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Compilation of Henry's law constants (version 5.0.0-rc.0) for water as solvent

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Abstract. Many atmospheric chemicals occur in the gas phase as well as in liquid cloud droplets and aerosol particles. Therefore, it is necessary to understand their distribution between the phases. According to Henry's law, the equilibrium ratio between the abundances in the gas phase and in the aqueous phase is constant for a dilute solution. Henry's law constants of trace gases of potential importance in environmental chemistry have been collected and converted into a uniform format. The compilation contains 46433 values of Henry's law constants for 10173 species, collected from 993 references. It will also be available on the internet at https://www.henrys-law.org. This article is a living review that supersedes the now obsolete publication by Sander (2015).

1 Introduction

Henry's law is named after the English chemist William Henry, who studied the topic in the early 19th century. In his publication about the quantity of gases absorbed by water (Henry, 1803), he described the results of his experiments:

> "[. . .] water takes up, of gas condensed by one, two, or more additional atmospheres, a quantity which, ordinarily compressed, would be equal to twice, thrice, &c. the volume absorbed under the common pressure of the atmosphere."

In other words, the amount of dissolved gas is proportional to its partial pressure in the gas phase. The proportionality factor is called Henry's law constant. In atmospheric chemistry, these constants are needed to describe the distribution of trace species between the air and liquid cloud droplets or aerosol particles. In other areas of environmental research, the constants are needed to calculate the vaporization of contaminants from rivers and during waste water treatment (e.g. Shen, 1982; Hawthorne et al., 1985; David et al., 2000).

Section 2 provides theoretical background about Henry's law and commonly used quantities and units. In Sect. 3, the compilation of Henry's law constants is described in detail. Additional information can be found in the electronic supplement, which is described in Sect. 4.

This article is a living review describing version 5.0.0-rc.0[1]. Compared to the now obsolete version 4.0 (Sander, 2015), the compilation contains 29083 additional values of Henry's law constants for 5541 additional species, collected from 304 additional references. In cases where experimental data are available for a large temperature range, the data were refitted to a 3-parameter equation, replacing the 2-parameter fits that were used previously. The symbols of the Henry's law constants have been adjusted in order to follow the new recommendations of the International Union of Pure and Applied Chemistry (IUPAC) by Sander et al. (2022). In addition to the CAS registry numbers, chemical species are now also identified by their InChIKeys (Heller et al., 2015).

2 Theoretical background

2.1 Fundamental types of Henry's law constants

There are many variants of Henry's law constants which can all be classified into two fundamental types: One possibility is to put the aqueous phase into the numerator and the gas phase into the denominator, i.e., define the constant as

[1]The name of this version indicates that it is a "release candidate" used for the interactive discussion in ACPD. If necessary, corrections can still be made. It is planned to release the final version 5.0.0 together with the final paper in ACP.

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Table 1. Variants of Henry's law constants H.

symbol	definition[a]	SI unit	other commonly used (non-SI) units[b]	conversion[c] from H_s^{cp}
		Henry's law solubility constants H_s		
H_s^{cp}	c_a/p	$\mathrm{mol\,m^{-3}\,Pa^{-1}}$	$\mathrm{M/atm}$	
H_s^{xp}	x/p	$\mathrm{Pa^{-1}}$	$\mathrm{atm^{-1}}$	$H_s^{xp} = H_s^{cp} \times M_{H_2O}/\varrho_{H_2O}$
H_s^{bp}	b/p	$\mathrm{mol\,kg^{-1}\,Pa^{-1}}$	$\mathrm{mol\,kg^{-1}\,atm^{-1}}$	$H_s^{bp} = H_s^{cp}/\varrho_{H_2O}$
H_s^{cc}	c_a/c_g	1 (dimensionless)		$H_s^{cc} = H_s^{cp} \times RT$
		Henry's law volatility constants H_v		
H_v^{pc}	p/c_a	$\mathrm{Pa\,m^3\,mol^{-1}}$	$\mathrm{atm\,m^3\,mol^{-1}}$	$H_v^{pc} = 1/H_s^{cp}$
H_v^{px}	p/x	Pa	atm	$H_v^{px} = (\varrho_{H_2O}/M_{H_2O})/H_s^{cp}$
H_v^{pw}	p/w	Pa	atm	$H_v^{pw} = (\varrho_{H_2O}/M_B)/H_s^{cp}$
H_v^{cc}	c_g/c_a	1 (dimensionless)		$H_v^{cc} = 1/(H_s^{cp} \times RT)$

[a] The definitions apply only at equilibrium and in the limit of infinite dilution.
[b] Here, M = mol/L and atm = 101 325 Pa.
[c] Here, M_{H_2O} and ϱ_{H_2O} are the molar mass and density of water, respectively. M_B is the molar mass of the solute. The simplified conversion formulas are valid only for binary solutions and ideal gases. More conversion formulas can be found in Tab. 2 of Sander et al. (2022).

the quotient A/G. Here, A and G are quantities describing the equilibrium composition (at infinite dilution) of the aqueous phase and the gas phase, respectively. Alternatively, the Henry's law constant can be defined as the quotient G/A, which results in the inverse value. There is no advantage or disadvantage in using one or the other, the two types exist purely for historical reasons. Unfortunately, the name "Henry's law constant" is used for both types. Therefore, expressions like "a large Henry's law constant" are meaningless unless the type is specified. Especially the dimensionless constants are very error-prone because their type cannot be deduced from the unit. In order to have a consistent terminology, the name "Henry's law solubility constant" (or "Henry solubility" for conciseness) should be used when refering to A/G. When refering to G/A, the name "Henry's law volatility constant" (or "Henry volatility") should be used.

2.2 Variants of Henry's law constants

For both of the fundamental types described in the previous section, there are several variants. This results from the multiplicity of quantities that can be chosen to describe the composition of the two phases. Typical choices for the aqueous phase are molar concentration (c_a), molality (b), and amount fraction (x). For the gas phase, molar concentration (c_g) and partial pressure (p) are often used. Note, however, that it is not possible to use the gas-phase amount fraction (y). At a given gas-phase amount fraction, the aqueous-phase concentration c_a depends on the total pressure and thus the ratio y/c_a is not a constant.

There are numerous combinations of these quantities. The eight variants recommended by IUPAC are summarized in Table 1. Numerical values of conversion factors between them are shown in Tables 2, 3, and 4.

2.3 Symbols

In the current literature, a plethora of different symbols is used for the Henry's law constants. Several symbols are used for the same variant, and sometimes the same symbol is used for different variants. However, for this work a consistent terminology is indispensable. Here, the IUPAC recommendations by Sander et al. (2022) are used: For Henry's law solubility constants, the symbol H_s is used, and for Henry's law volatility constants the symbol H_v is used.

To specify the exact variant of the Henry's law constant, two superscripts are used. They refer to the numerator and the denominator of the definition. For example, H_s^{cp} refers to the Henry solubility defined as c/p. If H_s refers to the reference temperature $T^\ominus = 298.15\,\mathrm{K}$, it will be denoted as $H_s^\ominus$. A summary of the symbols is shown in Table 5.

2.4 Temperature dependence of Henry's law constants

In spite of the name Henry's law "*constant*", it should be kept in mind that its value still depends on some parameters, e.g., the temperature T. The temperature dependence of equilibrium constants can be described with the van't Hoff equation, which also applies to Henry's law:

$$\frac{\mathrm{d}\ln H_s}{\mathrm{d}(1/T)} = \frac{-\Delta_{sol}H}{R}, \tag{1}$$

where $\Delta_{sol}H$ = enthalpy of dissolution and R = gas constant. Note that the letter H in the symbol $\Delta_{sol}H$ refers to enthalpy and is not related to the letter H for Henry's law constants. Integrating the above equation leads to

$$\ln H_s = \frac{-\Delta_{sol}H}{R}\frac{1}{T} + const \tag{2}$$

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Table 2. Conversion factors between several Henry's law solubility constants H_s (at $T^{\ominus}$ = 298.15 K and $\varrho^{\ominus}$ = 997 kg/m^3).

	$H_s^{cp} = \ldots \frac{\text{mol}}{\text{m}^3\,\text{Pa}}$	$H_s^{cp} = \ldots \frac{\text{M}}{\text{atm}}$	$H_s^{cc} = \ldots$	$H_s^{bp} = \ldots \frac{\text{mol}}{\text{kg}\,\text{Pa}}$	$H_s^{bp} = \ldots \frac{\text{mol}}{\text{kg}\,\text{atm}}$	$H_s^{xp} = \ldots \frac{1}{\text{atm}}$	$\alpha = \ldots$
$H_s^{cp} = 1\ \frac{\text{mol}}{\text{m}^3\,\text{Pa}}$	1.00000	101.325	2478.96	1.00301×10^{-3}	101.630	1.83089	2271.10
$H_s^{cp} = 1\ \frac{\text{M}}{\text{atm}}$	9.86923×10^{-3}	1.00000	24.4654	9.89893×10^{-6}	1.00301	0.0180695	22.4140
$H_s^{cc} = 1$	4.03395×10^{-4}	0.0408740	1.00000	4.04609×10^{-7}	0.0409970	7.38573×10^{-4}	0.916150
$H_s^{bp} = 1\ \frac{\text{mol}}{\text{kg}\,\text{Pa}}$	997.000	1.01021×10^{5}	2.47152×10^{6}	1.00000	1.01325×10^{5}	1825.40	2.26428×10^{6}
$H_s^{bp} = 1\ \frac{\text{mol}}{\text{kg}\,\text{atm}}$	9.83962×10^{-3}	0.997000	24.3920	9.86923×10^{-6}	1.00000	0.0180153	22.3467
$H_s^{xp} = 1\ \frac{1}{\text{atm}}$	0.546182	55.3419	1353.96	5.47826×10^{-4}	55.5084	1.00000	1240.43
$\alpha = 1$	4.40316×10^{-4}	0.0446150	1.09152	4.41641×10^{-7}	0.0447493	8.06171×10^{-4}	1.00000

Table 3. Conversion factors between several Henry's law volatility constants H_v (at $T^{\ominus}$ = 298.15 K and $\varrho^{\ominus}$ = 997 kg/m^3).

	$H_v^{px} = \ldots \text{atm}$	$H_v^{pc} = \ldots \frac{\text{m}^3\,\text{Pa}}{\text{mol}}$	$H_v^{pc} = \ldots \frac{\text{m}^3\,\text{atm}}{\text{mol}}$	$H_v^{cc} = \ldots$
$H_v^{px} = 1$ atm	1.00000	1.83089	1.80695×10^{-5}	7.38573×10^{-4}
$H_v^{pc} = 1\ \frac{\text{m}^3\,\text{Pa}}{\text{mol}}$	0.546182	1.00000	9.86923×10^{-6}	4.03395×10^{-4}
$H_v^{pc} = 1\ \frac{\text{m}^3\,\text{atm}}{\text{mol}}$	55341.9	1.01325×10^{5}	1.00000	40.8740
$H_v^{cc} = 1$	1353.96	2478.96	0.0244654	1.00000

Table 4. Products of Henry's law solubility constants H_s and Henry's law volatility constants H_v (at $T^{\ominus}$ = 298.15 K and $\varrho^{\ominus}$ = 997 kg/m^3). For example, if $H_v^{px} = 5$ atm, then $H_s^{bp} \approx 11$ mol/(kg atm) because $5 \times 11 \approx 55.5084$.

	$\frac{H_s^{cp}}{\text{mol}/(\text{m}^3\,\text{Pa})}$	$\frac{H_s^{cp}}{\text{M}/\text{atm}}$	$\frac{H_s^{cc}}{1}$	$\frac{H_s^{bp}}{\text{mol}/(\text{kg}\,\text{Pa})}$	$\frac{H_s^{bp}}{\text{mol}/(\text{kg}\,\text{atm})}$	$\frac{H_s^{xp}}{1/\text{atm}}$	$\frac{\alpha}{1}$
$\frac{H_v^{px}}{\text{atm}}$	0.546182	55.3419	1353.96	5.47826×10^{-4}	55.5084	1.00000	1240.43
$\frac{H_v^{pc}}{\text{m}^3\,\text{Pa}/\text{mol}}$	1.00000	101.325	2478.96	1.00301×10^{-3}	101.630	1.83089	2271.10
$\frac{H_v^{pc}}{\text{m}^3\,\text{atm}/\text{mol}}$	9.86923×10^{-6}	1.00000×10^{-3}	0.0244654	9.89893×10^{-9}	1.00301×10^{-3}	1.80695×10^{-5}	0.0224140
$\frac{H_v^{cc}}{1}$	4.03395×10^{-4}	0.0408740	1.00000	4.04609×10^{-7}	0.0409970	7.38573×10^{-4}	0.916150

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Table 5. List of Symbols.

symbol	quantity	SI unit*
ϱ	density	$\mathrm{kg\,m^{-3}}$
A	parameter for temperature dependence of H_s	1
b	molality	$\mathrm{mol\,kg^{-1}}$
B	parameter for temperature dependence of H_s	1
C	parameter for temperature dependence of H_s	1
c_a	aqueous-phase concentration	$\mathrm{mol\,m^{-3}}$
c_g	gas-phase concentration	$\mathrm{mol\,m^{-3}}$
D	parameter for temperature dependence of H_s	1
$\Delta_\mathrm{sol}H$	molar enthalpy of dissolution	$\mathrm{J\,mol^{-1}}$
H_s	Henry solubility (all variants)	miscellaneous
$H_\mathrm{s}^\ominus$	Henry solubility at the reference temperature $T^\ominus$	miscellaneous
H_s^{bp}	Henry solubility (defined as b/p)	$\mathrm{mol\,kg^{-1}\,Pa^{-1}}$
H_s^{cc}	Henry solubility (defined as c/c)	1
H_s^{cp}	Henry solubility (defined as c/p)	$\mathrm{mol\,m^{-3}\,Pa^{-1}}$
$H_\mathrm{s,eff}$	effective Henry solubility	miscellaneous
H'_s	$H \times K_\mathrm{A}$ (for strong acids)	miscellaneous
H_v	Henry volatility (all variants)	miscellaneous
$H_\mathrm{v}^\ominus$	Henry volatility at the reference temperature $T^\ominus$	miscellaneous
H_v^{cc}	Henry volatility (defined as c/c)	1
H_v^{pc}	Henry volatility (defined as p/c)	$\mathrm{Pa\,m^3\,mol^{-1}}$
H_v^{px}	Henry volatility (defined as p/x)	Pa
K_A	acid constant	$\mathrm{mol\,m^{-3}}$
M	molar mass	$\mathrm{kg\,mol^{-1}}$
p	partial pressure $= c_\mathrm{g}RT$	Pa
R	gas constant	$8.314\,\mathrm{J\,(mol\,K)^{-1}}$
T	temperature	K
$T^\ominus$	reference temperature	298.15 K
w	mass fraction in the aqueous phase	$\mathrm{kg\,kg^{-1}}$ (dimensionless)
x	amount fraction (molar mixing ratio) in the aqueous phase	$\mathrm{mol\,mol^{-1}}$ (dimensionless)
y	amount fraction (molar mixing ratio) in the gas phase	$\mathrm{mol\,mol^{-1}}$ (dimensionless)

*A unit of "1" denotes a quantity of dimension 1, commonly called "dimensionless quantity".

Calling the constant of integration A, and defining the parameter $B = -\Delta_\mathrm{sol}H/R$, we get:

$$\ln H_\mathrm{s} = A + \frac{B}{T} \tag{3}$$

or

$$H_\mathrm{s} = \exp(A) \times \exp\left(\frac{B}{T}\right) \tag{4}$$

To determine the parameters A and B experimentally, Henry's law constants are measured at several temperatures, and the method of least squares is used to fit the points to a function. Note that functions (3) and (4) produce slightly different fit parameters because the logarithmic function (3) puts less weight on errors of large Henry's law constants than the linear function (4) does. In this work, linear regression is performed using Eq. (3).

Thermodynamic data are often available at the temperature $T^\ominus = 298.15$ K. To present Henry's law constants at $T^\ominus$ and also show their temperature dependence, an alternative form of Eq. (4) can be used:

$$H_\mathrm{s} = H_\mathrm{s}^\ominus \times \exp\left(B\left(\frac{1}{T} - \frac{1}{T^\ominus}\right)\right). \tag{5}$$

where $H_\mathrm{s}^\ominus = \exp(A) \times \exp(B/T^\ominus)$. The enthalpy of dissolution $\Delta_\mathrm{sol}H$ is independent of temperature here:

$$\frac{-\Delta_\mathrm{sol}H}{R} = \frac{\mathrm{d}\ln H_\mathrm{s}}{\mathrm{d}(1/T)} = B \tag{6}$$

In this work, the values $H_\mathrm{s}^\ominus$ and $\mathrm{d}\ln H_\mathrm{s}/\mathrm{d}(1/T)$ are tabulated.

A simple equation based on the two parameters A and B is valid only for a limited temperature range, in which the enthalpy of dissolution $\Delta_\mathrm{sol}H$ can be considered constant. To accommodate a larger temperature range, a third parameter C is often added:

$$\ln H_\mathrm{s} = A + \frac{B}{T} + C \times \ln T. \tag{7}$$

Here, the fit parameters A and B are different from those calculated for function (3). The enthalpy of dissolution

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Table 6. Temperature-dependent terms and their analytical derivatives. Here, C, C_1 and C_2 are the empirical fit parameters defining $\ln(H_s)$. See Sect. 2.4 for details.

$\ln(H_s)$	$\frac{\mathrm{d}\ln H_s}{\mathrm{d}(1/T)}$
C	0
C/T	C
CT	$-CT^2$
CT^2	$-2CT^3$
C/T^2	$2C/T$
C/T^3	$3C/T^2$
$C\ln(T)$	$-CT$
$C_1\ln(C_2T)$	$-C_1T$ (independent of C_2)
$C\log_{10}(T)$	$-CT/\ln(10)$

$\Delta_{sol}H$ changes linearly with temperature in the 3-parameter fit:

$$\frac{-\Delta_{sol}H}{R} = \frac{\mathrm{d}\ln H_s}{\mathrm{d}(1/T)} = B - CT \tag{8}$$

To cover an even larger temperature range with an empirical formula, the dependence of $\ln H_s$ on T can be expressed as the sum of several terms. For example, Wilhelm et al. (1977) used the formula:

$$\ln H_s = A + B \times T^{-1} + C \times \ln T + D \times T. \tag{9}$$

The analytical derivative is simply the sum of the derivatives of the individual terms. Using the derivatives from Table 6, the temperature dependence of this expression can be calculated as:

$$\frac{\mathrm{d}\ln H_s}{\mathrm{d}(1/T)} = 0 + B - C \times T - D \times T^2. \tag{10}$$

When reporting Henry's law constants as such a function, it is important to present sufficient significant digits because H_s depends exponentially on the parameters.

Note that the temperature dependences for H_s^{cp} and H_s^{cc} are different since the conversion factor between them includes the temperature:

$$\begin{aligned} H_s^{cp} &= H_s^{cc}/(RT) \\ \Leftrightarrow \ln H_s^{cp} &= \ln H_s^{cc} + \ln(1/R) + \ln(1/T) \\ \Rightarrow \frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)} &= \frac{\mathrm{d}\ln H_s^{cc}}{\mathrm{d}(1/T)} + \frac{\mathrm{d}\ln(1/T)}{\mathrm{d}(1/T)} \\ &= \frac{\mathrm{d}\ln H_s^{cc}}{\mathrm{d}(1/T)} + T. \end{aligned} \tag{11}$$

2.5 Effective Henry's law solubility constants $H_{s,eff}$

The Henry's law constants mentioned so far describe the equilibrium between a chemical species in the gas phase and exactly the same species in the aqueous phase. This type is called the "intrinsic" Henry's law constant.

Once transferred into the aqueous phase, some species are involved in fast equilibria. In these cases, an "effective" Henry's law constant $H_{s,eff}$ can be defined, using a "total concentration" c_{tot}. Depending on the chemical class, there are different ways to define such a total concentration.

2.5.1 $H_{s,eff}$ for aldehydes

Aldehydes can be hydrated, forming geminal diols. For example, methanal (HCHO) is almost completely hydrated in aqueous solution:

$$\mathrm{HCHO + H_2O \rightleftharpoons H_2C(OH)_2} \tag{12}$$

The total concentration of dissolved methanal is:

$$c_{tot} = c(\mathrm{HCHO}) + c(\mathrm{H_2C(OH)_2}) \tag{13}$$

The intrinsic Henry's law solubility constant of HCHO is:

$$H_s = \frac{c(\mathrm{HCHO})}{p(\mathrm{HCHO})} \tag{14}$$

In contrast, the effective Henry's law constant $H_{s,eff}$ is defined as:

$$H_{s,eff} = \frac{c_{tot}}{p(\mathrm{HCHO})} = \frac{c(\mathrm{HCHO}) + c(\mathrm{H_2C(OH)_2})}{p(\mathrm{HCHO})} \tag{15}$$

2.5.2 $H_{s,eff}$ for acids and bases

Acids and bases undergo ionic dissociation upon dissolution, e.g.:

$$\mathrm{HCl \rightleftharpoons H^+ + Cl^-} \tag{16}$$

Defining the total concentration c_{tot} as

$$c_{tot} = c(\mathrm{HCl}) + c(\mathrm{Cl^-}), \tag{17}$$

the effective Henry's law constant is:

$$H_{s,eff} = \frac{c(\mathrm{HCl}) + c(\mathrm{Cl^-})}{p(\mathrm{HCl})} \tag{18}$$

Considering the acidity constant

$$K_a = \frac{c(\mathrm{H^+})\, c(\mathrm{Cl^-})}{c(\mathrm{HCl})}, \tag{19}$$

the relation between the intrinsic and the effective Henry's law constant for HCl can be written as:

$$H_{s,eff} = H_s \times \left(1 + \frac{K_a}{c(\mathrm{H^+})}\right) \tag{20}$$

Since the factor on the right-hand side contains $c(\mathrm{H^+})$, the conversion between the intrinsic and the effective Henry's law constant is pH-dependent. Proportionality between $p(\mathrm{HCl})$ and c_{tot} is restricted to conditions under which

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the uptake of gaseous HCl does not affect the acidity of the solution. Thus, effective Henry's law constants of acids and bases are not material constants but depend on the solution pH (Sander et al., 2022).

In order to obtain a pH-independent constant, the product of the intrinsic Henry's law constant H_s^{cp} and the acidity constant K_a is often used for HCl and other strong acids:

$$H'_s = H_s^{cp} \times K_a = \frac{c(H^+) \times c(Cl^-)}{p(HCl)} \quad (21)$$

Although H'_s is usually also called a Henry's law constant, it should be noted that it is a different quantity and it has different units than H_s^{cp}.

2.5.3 $H_{s,eff}$ for halogens

In the aqueous phase, halogens are in equilibrium with their hypohalous acids, e.g.:

$$Cl_2 + H_2O \rightleftharpoons HOCl + H^+ + Cl^-. \quad (22)$$

The equilibrium constant is:

$$K = \frac{c(HOCl)\, c(H^+)\, c(Cl^-)}{c(Cl_2)} \quad (23)$$

Since the sum of Cl_2 and HOCl is not affected by this equilibrium, a "total chlorine concentration" c_{tot} can be defined as:

$$c_{tot} = c(Cl_2) + c(HOCl), \quad (24)$$

Using c_{tot}, it is formally possible to define an effective Henry's law constant as:

$$H_{s,eff} = \frac{c_{tot}}{p(Cl_2)} = \frac{c(Cl_2) + c(HOCl)}{p(Cl_2)} \quad (25)$$

However, this definition is problematic because it doesn't work at infinite dilution. With decreasing Cl_2 concentration, the equilibrium in Eq. (22) will shift to the right (Le Chatelier's principle), i.e., $c(HOCl) \gg c(Cl_2)$, and the effective Henry's law solubility constant goes to infinity (e.g., Fig. 2 in Jones (1911) or Fig. A1 in Lin and Pehkonen (1998)). Therefore, the intrinsic Henry's law constant should be used for halogens, and the term "effective Henry's law constant" should be avoided here.

Instead of extrapolating to infinite dilution, the total chlorine solubility is sometimes reported at the fixed partial pressure of $p(Cl_2)$ = 101325 Pa. However, even in the vicinity of 101325 Pa, the total chlorine concentration c_{tot} is not proportional to $p(Cl_2)$.

In order to convert experimentally determined chlorine solubilities to the intrinsic constant $H_s(Cl_2)$, additional processes may have to be considered, e.g., aqueous-phase diffusion (Brian et al., 1962; Leaist, 1986) and the formation of chlorine hydrates (Adams and Edmonds, 1937; Young, 1983).

2.6 Dependence of Henry's law constants on the composition of the solution

Values of Henry's law constants for aqueous solutions depend on the composition of the solution, i.e., on its ionic strength and on dissolved organics. In general, the solubility of a gas decreases with increasing salinity ("salting out"). However, a "salting in" effect has also been observed, e.g., for the effective Henry's law constant of glyoxal (Kampf et al., 2013; Kurtén et al., 2015). The effect can be described with the Sechenov equation (Setschenow, 1889). Note that the scientific transliteration from Cyrillic is "Sechenov" but the original article was written in German and used the German transliteration "Setschenow". There are many alternative ways to define the Sechenov equation, depending on how the aqueous-phase composition is described (based on concentration, molality, or molar fraction) and which variant of the Henry's law constant is used. Describing the solution in terms of molality is preferred because molality is invariant to temperature and to the addition of dry salt to the solution (see Sander (1999) for details). Thus, the Sechenov equation can be written as:

$$\log_{10}\left(\frac{H_{s0}^{bp}}{H_s^{bp}}\right) = K_s \times b(salt) \quad (26)$$

where H_{s0}^{bp} = Henry's law constant in pure water, H_s^{bp} = Henry's law constant in the salt solution, K_s = molality-based Sechenov constant, and $b(salt)$ = molality of the salt.

Since the atmosphere contains very dilute cloud droplets as well as highly concentrated aerosols, adequate values of Henry's law constants should be used. Unfortunately, Sechenov parameters are unknown for many species.

3 Values of Henry's law constants

3.1 The data compilation

The compilation of Henry's law constants is presented in the appendix, and it will also be available online at https://www.henrys-law.org. It contains Henry's law constants for inorganic and organic species of potential importance in environmental chemistry. Most data were measured at ambient conditions (around 298 K and 1 atm). Data at high temperatures are excluded or (if possible) extrapolated to $T^{\ominus} = 298.15$ K. The data refer to aqueous solutions; octanol and other solvents are not included. The constants refer to pure water as solvent unless noted otherwise (e.g., sea water).

All Henry's law constants have been converted to a uniform format: H_s^{cp} with the unit $mol/(m^3\,Pa)$. In cases where the conversion involves the temperature-dependent density of water, the parameterization by Bettin and Spieweck (1990) was used to calculate ϱ_{H_2O} at the temperature T.

Inorganic substances are sorted according to the elements they contain. The order chosen is: O, H, N, F, Cl, Br, I,

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S, rare gases, others. Compounds with several of these elements are put into the last of the applicable sections. For example, nitryl chloride which contains O, N and Cl, is listed in the Cl section. Carbon-containing compounds (including CO and CO_2) are sorted somewhat arbitrarily by increasing chain length and complexity. Hetero atoms (O, N, F, Cl, Br, I, S, P, etc.) are sorted in the same order as for inorganic compounds. The table contains the following groups of species:

The first column of the table shows the systematic name, the chemical formula, trivial names (if any), the CAS registry number (in square brackets), and the InChIKey.

The column labeled "H_s^{cp}" contains Henry's law solubility constants at the reference temperature $T^\ominus = 298.15\,\mathrm{K}$. Values are rounded to two significant digits and given in the unit $\mathrm{mol/(m^3\,Pa)}$.

The column labeled "$\mathrm{d}\ln H_s/\mathrm{d}(1/T)$" contains the temperature dependence of the Henry solubility as defined in Eq. (5), rounded to two significant digits and given in the unit K. If the term $\Delta_{sol}H$ is temperature-dependent, the value of $\mathrm{d}\ln H_s/\mathrm{d}(1/T)$ is calculated at $T^\ominus = 298.15\,\mathrm{K}$.

For each table entry the column labeled "type" denotes how the Henry's law constant was obtained in the given reference. Literature reviews are usually most reliable, followed

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by original publications of experimental determinations of H_s. Other data has to be treated more carefully. The types listed here are roughly ordered by decreasing reliability:

"L" The cited paper is a *literature* review.

"M" Original publication of a *measured* value.

"V" *Vapor* pressure of the pure substance divided by aqueous solubility (sometimes called "VP/AS").

"R" The cited paper presents a *recalculation* of previously published material (e.g. extrapolation to a different temperature or concentration range).

"T" *Thermodynamical* calculation ($\Delta_{sol}G = -RT \ln H$, see Sander (1999) for details).

"X" The original paper was not available for this study. The data listed here was found in a secondary source.

"C" The paper is a *citation* of a reference which I could not obtain (personal communication, Ph.D. theses, grey literature).

"Q" The value was calculated with a "*quantitative* structure property relationship" (QSPR) or a similar theoretical method.

"E" The value is an *estimate*. Estimates are listed only if no reliable data are available.

"?" The cited paper doesn't clearly state how the value was obtained.

"W" The value is probably wrong, as explained in the note.

In some cases there might be good agreement between different authors. However, if the original work they refer to is not known one has to be careful when evaluating the reliability. It is possible that they were recalculating data from the same source. The similarity in that case would not be due to independent investigations.

The table entries in the pdf of this document are hyperlinked to endnotes with additional information. In order to avoid spreading of erroneous data, some of these notes identify errors in the original publications. Symbols and acronyms used here refer to those in the original publications.

The CAS numbers in the tables are hyperlinked to the NIST Chemistry WebBook.

3.2 Further sources of information

3.2.1 Review articles

Several reviews about Henry's law have been published, starting with Markham and Kobe (1941), up to more recent publications such as Wilhelm et al. (1977), Mackay and Shiu (1981), Staudinger and Roberts (1996), Staudinger and Roberts (2001), Fogg and Sangster (2003), and Burkholder et al. (2019). Practical guidance on the use of Henry's law has been published by Smith and Harvey (2007).

Experimental methods to obtain Henry's law constants as well as indirect (theoretical) methods have been described and compared by several authors. Only a brief summary of some articles is given here. For details, the reader is referred to the original publications:

- Battino and Clever (1966): Miscellaneous methods, partially of historical interest
- Betterton (1992): Head-space method, bubble column method, thermodynamic cycles, calculation from vapor pressure and solubility, linear correlations
- Turner et al. (1996): Static methods, mechanical recirculation methods, separate measurement of solubility and pure species vapor pressure, ebulliometry, perturbation chromatography
- Staudinger and Roberts (1996): Batch air stripping, concurrent flow technique, Equilibrium Partitioning in Closed Systems (EPICS), calculation via Quantitative Property Property Relationships (QPPR), Quantitative Structure Property Relationships (QSPR), UNIversal quasichemical Functional group Activity Coefficients (UNIFAC)
- Brennan et al. (1998): Comparison of predictive methods
- Sander (1999): QPPR, QSPR, thermodynamic calculations
- Fogg and Sangster (2003): Miscellaneous methods
- Dupeux et al. (2022): QSPR

3.2.2 Internet

On the internet, several pages provide Henry's law constants, e.g.:

- The PubChem database: https://pubchem.ncbi.nlm.nih.gov
- The NIST Chemistry WebBook: https://webbook.nist.gov/chemistry
- The ChemSpider database: https://www.chemspider.com
- The Generator for Explicit Chemistry and Kinetics of Organics in the Atmosphere (GECKO-A) provides Henry's law constants on the basis of experimental data and structure-activity relationships: http://geckoa.lisa.u-pec.fr/generateur_form.php

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- The Pesticide Properties Database (PPD): https://www.ars.usda.gov/Services/docs.htm?docid=14199
- HENRYWIN, a program to calculate Henry's law constants: https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface
- Vapor-liquid equilibrium data (mostly at elevated temperatures) from the "Dortmund Data Bank": http://www.ddbst.com/en/EED/VLE/VLEindex.php
- EPI Suite estimates from the Arctic Monitoring and Assessment Programme (AMAP) database: https://chemicals.amap.no/about

3.2.3 Vapor–liquid equilibrium data

Henry's law constants can be obtained from vapor–liquid equilibrium (VLE) data. For example, consider a binary mixture that consists of a solute dissolved in water. The total pressure P over the solution is the sum of the partial pressures of the components. The partial pressure of the solute can be defined via Henry's law, and the partial pressure of the water can be defined via Raoult's law:

$$\begin{aligned} P &= p_{\mathrm{solute}} + p_{\mathrm{water}} \\ &= x H_{\mathrm{v}}^{px} + (1-x) p_{\mathrm{sat}} \\ &= x(H_{\mathrm{v}}^{px} - p_{\mathrm{sat}}) + p_{\mathrm{sat}} \end{aligned} \tag{27}$$

where p_{sat} is the saturation vapor pressure of water. If VLE data with the total pressure at several small solute fractions x are available, the derivative $\mathrm{d}P/\mathrm{d}x$ (i.e., the slope of a plot P vs x) can be used to obtain the Henry's law constant:

$$\frac{\mathrm{d}P}{\mathrm{d}x} = H_{\mathrm{v}}^{px} - p_{\mathrm{sat}} \Rightarrow H_{\mathrm{v}}^{px} = \frac{\mathrm{d}P}{\mathrm{d}x} + p_{\mathrm{sat}} \tag{28}$$

4 The electronic supplement

The Supplement contains several files with additional information about the compiled Henry's law constants. It includes a `README` file with a detailed description. Here, only a short summary is given:

- The files `henry_*.f90` contain the Fortran 90 code that was used to convert the values from the original publications to a uniform format: H_{s}^{cp} with the unit $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$. The code and the comments in the code can be used to double-check that the conversion was done correctly.
- If the original publications contain measurements at different temperatures, the code often contains all individual data points, not just the regression line that was used to calculate the temperature dependence. In addition, the supplement contains data files with the temperature-dependent values of H_{s}^{cp} in `output/Tdep_data/*.dat` and plots of the data points as well as the regression lines according to Eqs. (5) and (7) in `output/gnuplot/Tdep.pdf`.
- If the Henry's law constants are needed in electronic form, it is cumbersome to extract them from the pdf of this article. Therefore, the supplement contains the files `output/*.f90` with declarations of the Henry's law constants (H_{s}^{cp}, H_{s}^{xp}, H_{s}^{bp}, H_{s}^{cc}, H_{v}^{pc}, H_{v}^{px}, and H_{v}^{cc}) in Fortran 90 syntax.
- For some references, the `util/` directory contains python scripts that preprocess input and perform other calculations related to the original data.

5 Summary and outlook

An updated and extended version of a compilation of Henry's law constants has been presented. The collection, which will also be available at https://www.henrys-law.org, will be continously maintained, updated and extended in the future. If necessary, errata will also be posted on the web page. In addition to providing a source of information, I hope that this work will help to identify gaps in our current knowledge and stimulate research projects. In particular, it seems that even for some well-known chemicals like HCl, Br_2, and BrCl, there is a large uncertainty in the value of the Henry's law constants. I always welcome information about new measurements of Henry's law constants to be included in the table.

Supplement. The supplement related to this article is available online at: https://doi.org/10.5194/acp-0-1-2023-supplement.

Competing interests. The author declares no competing interests.

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open access publication have been covered by the Max Planck Society.

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Appendix A: Appendix with data tables

A1 Inorganic species

A1.1 Oxygen (O)

Table A1.1: Oxygen (O)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
oxygen	1.3×10^{-5}	1500	Burkholder et al. (2019)	L	1
O_2	1.3×10^{-5}	1500	Burkholder et al. (2015)	L	1
[7782-44-7]			Clever et al. (2014)	L	2
MYMOFIZGZYHOMD-UHFFFAOYSA-N	1.2×10^{-5}	1700	Warneck and Williams (2012)	L	
	1.3×10^{-5}	1500	Sander et al. (2011)	L	1
	1.3×10^{-5}	1500	Sander et al. (2006)	L	1
	1.3×10^{-5}	1400	Fernández-Prini et al. (2003)	L	3
	1.3×10^{-5}	1500	Battino et al. (1983)	L	
	1.3×10^{-5}	1500	Battino (1981)	L	1
	1.3×10^{-5}	1500	Wilhelm et al. (1977)	L	
	1.2×10^{-5}	1400	Himmelblau (1960)	L	1
	1.2×10^{-5}	1600	Millero et al. (2002a)	M	4, 5
	1.2×10^{-5}	1600	Millero et al. (2002b)	M	6, 7
	1.3×10^{-5}	1500	Rettich et al. (2000)	M	8
	1.3×10^{-5}	1400	Sherwood et al. (1991)	M	9
	1.3×10^{-5}	1500	Rettich et al. (1981)	M	10
	1.3×10^{-5}	1500	Cosgrove and Walkley (1981)	M	11
	1.2×10^{-5}		da Silva et al. (1980)	M	12
	1.3×10^{-5}	1400	Cramer (1980)	M	
	1.3×10^{-5}	1400	Benson et al. (1979)	M	
	1.4×10^{-4}		Razumovskii and Zaikov (1971)	M	13
	1.1×10^{-5}		Power and Stegall (1970)	M	14
	1.3×10^{-5}	1500	Murray and Riley (1969)	M	15
	1.2×10^{-5}	1200	Shoor et al. (1969)	M	16
	1.2×10^{-5}	1600	Carpenter (1966)	M	17
	1.3×10^{-5}	1500	Morrison and Billett (1952)	M	18
	1.2×10^{-5}		Orcutt and Seevers (1937a)	M	
	1.3×10^{-5}	1500	Fox (1909)	M	
	1.2×10^{-5}	1700	Geffcken (1904)	M	
	1.3×10^{-5}	1400	Winkler (1891b)	M	19
	1.3×10^{-5}	1400	Bohr and Bock (1891)	M	
	1.2×10^{-5}	1800	Timofejew (1890)	M	
	1.2×10^{-5}	1200	Bunsen (1855a)	M	
	1.2×10^{-5}	1600	Wauchope and Haque (1972)	V	
	1.2×10^{-5}	1600	Wauchope and Haque (1972)	V	
	1.3×10^{-5}	1500	Wauchope and Haque (1972)	V	
	1.3×10^{-5}		Pierotti (1965)	T	
	1.4×10^{-5}		Nunn (1958)	C	12
	7.9×10^{-6}		Hayer et al. (2022)	Q	20
	1.3×10^{-5}	1500	Yaws et al. (1999)	?	21
	1.1×10^{-5}		Abraham and Weathersby (1994)	?	21

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Table A1.1: Oxygen (O) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-5}	1500	Dean and Lange (1999)	?	22, 23
	1.3×10^{-5}		Seinfeld (1986)	?	21
	1.3×10^{-4}		Smith and Bomberger (1980)	?	24
ozone O_3 [10028-15-6] CBENFWSGALASAD-UHFFFAOYSA-N	1.0×10^{-4}	2800	Burkholder et al. (2019)	L	
	1.0×10^{-4}	2800	Burkholder et al. (2015)	L	
			Clever et al. (2014)	L	25
	1.0×10^{-4}	2800	Sander et al. (2011)	L	
	1.0×10^{-4}	2800	Sander et al. (2006)	L	
	7.6×10^{-5}	3700	Biń (2005)	L	
	1.1×10^{-4}	2400	Warneck (2003)	L	
			Battino (1981)	L	26
	1.3×10^{-4}	2000	Wilhelm et al. (1977)	L	
	1.1×10^{-4}		Levanov et al. (2008)	M	12
	1.1×10^{-4}	2300	Gershenzon et al. (2001)	M	
	9.9×10^{-5}	2600	Rischbieter et al. (2000)	M	
	9.2×10^{-5}	2600	Andreozzi et al. (1996)	M	
	1.2×10^{-4}	1400	Sotelo et al. (1989)	M	
	1.1×10^{-4}	2300	Kosak-Channing and Helz (1983)	M	
	1.7×10^{-4}		Gurol and Singer (1982)	M	12
			Roth and Sullivan (1981)	M	27
	1.2×10^{-4}	1900	Stumm (1958)	M	
	9.9×10^{-5}	2600	Kilpatrick et al. (1956)	M	
	1.3×10^{-4}	2000	Briner and Perrottet (1939)	M	
	2.0×10^{-4}		Fischer and Tropsch (1917)	M	
	8.0×10^{-5}	2900	Luther (1905)	M	
	1.2×10^{-4}	4100	Mailfert (1894)	M	
	1.2×10^{-4}		Schöne (1873)	M	28
	1.1×10^{-4}	2600	Chameides (1984)	T	
	1.2×10^{-4}		Perry and Chilton (1973)	X	29
	1.2×10^{-4}		Hayer et al. (2022)	Q	20
			Lide and Frederikse (1995)	?	30
	9.3×10^{-5}	2500	Seinfeld (1986)	?	21
	9.3×10^{-5}	2500	Hoffmann and Jacob (1984)	?	21

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A1.2 Hydrogen (H)

Table A1.2: Hydrogen (H)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hydrogen atom	2.6×10^{-6}		Burkholder et al. (2019)	L	
H	2.6×10^{-6}		Burkholder et al. (2015)	L	
[12385-13-6]	2.6×10^{-6}		Sander et al. (2011)	L	
YZCKVEUIGOORGS-UHFFFAOYSA-N	2.6×10^{-6}		Sander et al. (2006)	L	
	3.1×10^{-6}		Armstrong et al. (2015)	T	
	3.4×10^{-6}		Parker (1992)	E	31
			Roduner and Bartels (1992)	?	32
hydrogen	7.8×10^{-6}	530	Fernández-Prini et al. (2003)	L	3
H_2	7.7×10^{-6}	490	Young (1981a)	L	1
[1333-74-0]	7.7×10^{-6}	490	Wilhelm et al. (1977)	L	
UFHFLCQGNIYNRP-UHFFFAOYSA-N	7.8×10^{-6}	600	Himmelblau (1960)	L	1
	7.8×10^{-6}	620	Schmidt (1979)	M	33, 34
	7.7×10^{-6}	480	Gordon et al. (1977)	M	35
	7.7×10^{-6}	520	Crozier and Yamamoto (1974)	M	36
	7.2×10^{-6}		Longo et al. (1970)	M	14
	7.2×10^{-6}		Power and Stegall (1970)	M	14
			Shoor et al. (1969)	M	37
	7.5×10^{-6}		Ruetschi and Amlie (1966)	M	38
	7.8×10^{-6}	510	Morrison and Billett (1952)	M	39
	7.8×10^{-6}	540	Geffcken (1904)	M	
	7.7×10^{-6}	1500	Braun (1900)	M	40
	7.7×10^{-6}	500	Winkler (1891a)	M	41
	7.5×10^{-6}	550	Bohr and Bock (1891)	M	
	7.8×10^{-6}	610	Timofejew (1890)	M	
	8.5×10^{-6}	20	Bunsen (1855a)	M	42, 43
	7.8×10^{-6}	500	Wauchope and Haque (1972)	V	
	7.7×10^{-6}		Hine and Weimar (1965)	R	
	8.3×10^{-6}		Pierotti (1965)	T	
	6.4×10^{-6}		Hayer et al. (2022)	Q	20
	7.7×10^{-6}	490	Yaws et al. (1999)	?	21
	7.7×10^{-6}		Abraham and Weathersby (1994)	?	21
	7.7×10^{-6}	500	Dean and Lange (1999)	?	44, 23
deuterium			Young (1981a)	L	45
D_2	7.9×10^{-6}	720	Muccitelli and Wen (1978)	M	46
[7782-39-0]	7.9×10^{-6}	720	Muccitelli and Wen (1978)	M	
UFHFLCQGNIYNRP-VVKOMZTBSA-N	8.2×10^{-6}		Hayer et al. (2022)	Q	20
hydroxyl radical	3.8×10^{-1}		Burkholder et al. (2019)	L	
OH	3.8×10^{-1}		Burkholder et al. (2015)	L	
[3352-57-6]	3.8×10^{-1}		Sander et al. (2011)	L	
TUJKJAMUKRIRHC-UHFFFAOYSA-N	3.8×10^{-1}		Sander et al. (2006)	L	
	2.9×10^{-1}	4300	Hanson et al. (1992)	T	
	3.2×10^{-1}		Mozurkewich (1986)	T	
	2.9×10^{-1}	3100	Berdnikov and Bazhin (1970)	T	47

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Table A1.2: Hydrogen (H) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	2.5×10^{-1}		Lelieveld and Crutzen (1991)	C	
	2.0		Lelieveld and Crutzen (1991)	C	
	8.9×10^{1}		Lelieveld and Crutzen (1991)	C	
	2.5×10^{-1}	5300	Jacob (1986)	C	48
hydroperoxy radical	6.8		Burkholder et al. (2019)	L	
HO_2	6.8		Burkholder et al. (2015)	L	
[3170-83-0]	6.8		Sander et al. (2011)	L	
MHAJPDPJQMAIIY-UHFFFAOYSA-M	6.8		Sander et al. (2006)	L	
	5.7×10^{1}		Régimbal and Mozurkewich (1997)	R	
	3.8×10^{1}	5900	Hanson et al. (1992)	T	
	8.9×10^{1}		Weinstein-Lloyd and Schwartz (1991)	T	
	8.9×10^{1}		Chameides (1984)	T	
	1.2×10^{1}		Schwartz (1984)	T	49
	4.6×10^{1}	4800	Berdnikov and Bazhin (1970)	T	47
		6600	Jacob (1986)	E	50
hydrogen peroxide	8.6×10^{2}	7300	Burkholder et al. (2019)	L	
H_2O_2	8.6×10^{2}	7300	Burkholder et al. (2015)	L	
[7722-84-1]	9.5×10^{2}	7200	Brockbank (2013)	L	1
MHAJPDPJQMAIIY-UHFFFAOYSA-N	9.1×10^{2}	6600	Warneck and Williams (2012)	L	
	8.3×10^{2}	7600	Sander et al. (2011)	L	
	7.6×10^{2}	7300	Sander et al. (2006)	L	
	9.8×10^{2}	6100	Fogg and Sangster (2003)	L	51
	1.2×10^{3}	5900	Rivera-Rios (2018)	M	
	1.1×10^{3}	7000	Huang and Chen (2010)	M	
	8.2×10^{2}	7400	O'Sullivan et al. (1996)	M	
	9.9×10^{2}	6300	Lind and Kok (1994)	M	52
			Staffelbach and Kok (1993)	M	53
	8.5×10^{2}	6500	Zhou and Lee (1992)	M	
	6.7×10^{2}	7900	Hwang and Dasgupta (1985)	M	
	1.4×10^{3}		Yoshizumi et al. (1984)	M	12
	9.6×10^{2}	6600	Chameides (1984)	T	
	7.0×10^{2}	7000	Martin and Damschen (1981)	T	
	6.4×10^{1}		Hilal et al. (2008)	Q	
	7.0×10^{2}	7300	Seinfeld (1986)	?	21
	7.0×10^{2}	7300	Hoffmann and Jacob (1984)	?	21
			Pandis and Seinfeld (1989)	W	54

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A1.3 Nitrogen (N)

Table A1.3: Nitrogen (N)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
nitrogen	6.4×10^{-6}	1300	Burkholder et al. (2019)	L	1
N_2	6.4×10^{-6}	1300	Burkholder et al. (2015)	L	1
[7727-37-9]	6.4×10^{-6}	1600	Warneck and Williams (2012)	L	
IJGRMHOSHXDMSA-UHFFFAOYSA-N	6.4×10^{-6}	1300	Sander et al. (2011)	L	1
	6.4×10^{-6}	1300	Sander et al. (2006)	L	1
	6.5×10^{-6}	1200	Fernández-Prini et al. (2003)	L	3
	6.5×10^{-6}	1200	Battino et al. (1984)	L	
	6.5×10^{-6}	1200	Battino (1982)	L	1
	6.4×10^{-6}	1300	Wilhelm et al. (1977)	L	
	5.4×10^{-6}		Steward et al. (1973)	L	14
	6.5×10^{-6}	1400	Allott et al. (1973)	L	
	6.3×10^{-6}	1300	Himmelblau (1960)	L	1
	6.4×10^{-6}	1300	Rettich et al. (1984)	M	55
	6.6×10^{-6}	1300	Cosgrove and Walkley (1981)	M	11
	5.5×10^{-6}		Power and Stegall (1970)	M	14
	6.4×10^{-6}	1300	Murray et al. (1969)	M	56
	6.5×10^{-6}	1400	Morrison and Billett (1952)	M	57
	6.6×10^{-6}		Orcutt and Seevers (1937a)	M	
	6.5×10^{-6}	1100	Van Slyke et al. (1934)	M	
	5.6×10^{-6}		Grollman (1929)	M	58
	6.4×10^{-6}	1200	Fox (1909)	M	
	6.3×10^{-6}	2200	Braun (1900)	M	59
	6.3×10^{-6}	1300	Winkler (1891b)	M	60
	6.7×10^{-6}	1400	Bohr and Bock (1891)	M	
	5.8×10^{-6}	1200	Bunsen (1855a)	M	43
	6.4×10^{-6}	1300	Wauchope and Haque (1972)	V	
	6.5×10^{-6}	1300	Wauchope and Haque (1972)	V	
	6.5×10^{-6}		Pierotti (1965)	T	
	7.2×10^{-6}		Nunn (1958)	C	12
	5.6×10^{-6}		Hayer et al. (2022)	Q	20
	6.4×10^{-6}	1600	Battino et al. (2018)	?	
	6.3×10^{-6}	1200	Yaws et al. (1999)	?	21
	5.7×10^{-6}		Abraham and Weathersby (1994)	?	21
	6.3×10^{-6}	1300	Dean and Lange (1999)	?	61, 23
ammonia	5.9×10^{-1}	4200	Burkholder et al. (2019)	L	
NH_3	5.9×10^{-1}	4200	Burkholder et al. (2015)	L	
[7664-41-7]	5.9×10^{-1}	4200	Sander et al. (2011)	L	
QGZKDVFQNNGYKY-UHFFFAOYSA-N	5.9×10^{-1}	4200	Sander et al. (2006)	L	
	5.8×10^{-1}	4400	Yoo et al. (1986)	L	1
	6.0×10^{-1}	4200	Edwards et al. (1978)	L	1
	1.0×10^{-1}	1500	Wilhelm et al. (1977)	L	
	2.8×10^{-1}	3200	Shi et al. (1999)	M	
	9.9	6600	Tsuji et al. (1990)	M	62
	6.0×10^{-1}	4200	Clegg and Brimblecombe (1989)	M	

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Table A1.3: Nitrogen (N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.5×10^{-1}	4100	Dasgupta and Dong (1986)	M	
	7.7×10^{-1}		Holzwarth et al. (1984)	M	
	7.4×10^{-1}	3700	Hales and Drewes (1979)	M	
	5.6×10^{-1}	4200	Dasgupta and Dong (1986)	T	
	5.7×10^{-1}	4100	Chameides (1984)	T	
	5.9×10^{-1}	4100	Edwards et al. (1975)	T	1
	6.1×10^{-1}		Van Krevelen et al. (1949)	X	63
	2.9×10^{-1}		Hayer et al. (2022)	Q	20
	2.7×10^{-1}	2400	Dean and Lange (1999)	?	64, 23
	5.7×10^{-1}		Abraham et al. (1990)	?	
	6.1×10^{-1}	4100	Seinfeld (1986)	?	21
	5.8×10^{-1}	4100	Hoffmann and Jacob (1984)	?	21
	5.2×10^{-1}		Bone et al. (1983)	?	65
hydrazoic acid HN_3 [7782-79-8] JUINSXZKUKVTMD-UHFFFAOYSA-N	1.2×10^{-1}	3800	Sander et al. (2011)	L	66
	9.8×10^{-2}	3100	Wilhelm et al. (1977)	L	
	1.2×10^{-1}	3700	Betterton and Robinson (1997)	M	
	9.9×10^{-2}		Templeton and King (1971)	M	38
	7.6×10^{-1}		Modarresi et al. (2007)	Q	67
			Burkholder et al. (2019)	W	68
			Burkholder et al. (2015)	W	69
hydrazine H_4N_2 [302-01-2] OAKJQQAXSVQMHS-UHFFFAOYSA-N	1.6×10^{1}		HSDB (2015)	V	
dinitrogen monoxide N_2O (nitrous oxide; laughing gas) [10024-97-2] GQPLMRYTRLFLPF-UHFFFAOYSA-N	2.4×10^{-4}	2600	Burkholder et al. (2019)	L	1
	2.1×10^{-4}	2600	Burkholder et al. (2019)	L	70
	2.4×10^{-4}	2600	Burkholder et al. (2015)	L	1
	2.1×10^{-4}	2600	Burkholder et al. (2015)	L	70
	2.4×10^{-4}	2700	Warneck and Williams (2012)	L	
	2.4×10^{-4}	2600	Sander et al. (2011)	L	1
	2.4×10^{-4}	2600	Sander et al. (2006)	L	1
	2.4×10^{-4}	2500	Young (1981b)	L	1
	2.4×10^{-4}	2600	Wilhelm et al. (1977)	L	
	1.8×10^{-4}		Steward et al. (1973)	L	14
	2.5×10^{-4}	2500	Allott et al. (1973)	L	
	2.4×10^{-4}	2500	Weiss and Price (1980)	M	71
	2.5×10^{-4}	2300	Gabel and Schultz (1973)	M	
	2.4×10^{-4}		Joosten and Danckwerts (1972)	M	
	1.9×10^{-4}		Bachofen and Farhi (1971)	M	14
	2.4×10^{-4}	2400	Saidman et al. (1966)	M	
	1.4×10^{-4}		Sy and Hasbrouck (1964)	M	14
	2.2×10^{-4}		Nunn (1958)	M	72
	2.4×10^{-4}		Orcutt and Seevers (1937a)	M	
	2.4×10^{-4}	2500	Kunerth (1922)	M	
	2.4×10^{-4}	2400	Siebeck (1909)	M	
	2.4×10^{-4}	2700	Geffcken (1904)	M	

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Table A1.3: Nitrogen (N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.3×10^{-4}	2900	Roth (1897)	M	73
	2.5×10^{-4}	2600	Carius (1855)	M	
	2.6×10^{-4}	2500	Gordon (1895)	X	74
	1.7×10^{-4}		Harris (1951)	X	14, 75
	3.0×10^{-4}		Macintosh et al. (1958)	X	12, 75
	1.7×10^{-4}		Orcutt and Seevers (1937b)	X	58, 75
	2.8×10^{-4}		Nunn (1958)	C	12
	2.2×10^{-4}		Hayer et al. (2022)	Q	20
		3600	Kühne et al. (2005)	Q	
		2700	Kühne et al. (2005)	?	
	2.4×10^{-4}	2500	Yaws et al. (1999)	?	21
	1.8×10^{-4}		Abraham and Weathersby (1994)	?	21
	2.4×10^{-4}	2800	Dean and Lange (1999)	?	23
	2.5×10^{-4}		Seinfeld (1986)	?	21
	2.5×10^{-4}		Liss and Slater (1974)	?	
nitrogen monoxide NO (nitric oxide) [10102-43-9] MWUXSHHQAYIFBG-UHFFFAOYSA-N	1.9×10^{-5}	1600	Warneck and Williams (2012)	L	
	1.9×10^{-5}	1600	Sander et al. (2011)	L	76, 1
	1.9×10^{-5}	1600	Sander et al. (2006)	L	77, 1
	1.9×10^{-5}	1500	Schwartz and White (1981)	L	
	1.9×10^{-5}	1400	Young (1981b)	L	78, 1
	1.3×10^{-5}		Zafiriou and McFarland (1980)	M	79
	2.3×10^{-5}		Komiyama and Inoue (1980)	M	80
	1.9×10^{-5}	1500	Komiyama and Inoue (1978)	M	
	1.9×10^{-5}	1400	Winkler (1901)	M	81
	3.4×10^{-5}		Pierotti (1965)	T	
	1.9×10^{-5}	1300	Loomis (1928)	C	82
	1.5×10^{-5}		Hayer et al. (2022)	Q	20
		1500	Kühne et al. (2005)	Q	
		1600	Kühne et al. (2005)	?	
	1.9×10^{-5}	1400	Yaws et al. (1999)	?	21
	1.9×10^{-5}	1500	Dean and Lange (1999)	?	83, 23
	1.9×10^{-5}		Seinfeld (1986)	?	21
	1.9×10^{-5}		Andrew and Hanson (1961)	?	
			Burkholder et al. (2019)	W	84
			Burkholder et al. (2015)	W	85
			Wilhelm et al. (1977)	W	86
nitrogen dioxide NO_2 [10102-44-0] JCXJVPUVTGWSNB-UHFFFAOYSA-N	1.2×10^{-4}	2400	Burkholder et al. (2019)	L	
	1.2×10^{-4}	2400	Burkholder et al. (2015)	L	
	9.9×10^{-5}		Warneck and Williams (2012)	L	
	1.2×10^{-4}	2400	Sander et al. (2011)	L	
	1.4×10^{-4}		Sander et al. (2006)	L	
	1.2×10^{-4}		Schwartz and White (1981)	L	
	1.4×10^{-4}		Cheung et al. (2000)	M	
	6.9×10^{-5}		Lee and Schwartz (1981)	M	87
	2.3×10^{-4}		Komiyama and Inoue (1980)	M	80
	1.2×10^{-4}	2500	Chameides (1984)	T	

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Table A1.3: Nitrogen (N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.4×10^{-4}	1800	Berdnikov and Bazhin (1970)	T	47
	9.9×10^{-5}		Pandis and Seinfeld (1989)	?	88
	9.9×10^{-5}		Seinfeld (1986)	?	21
	4.0×10^{-4}		Andrew and Hanson (1961)	?	
nitrogen trioxide NO_3 (nitrate radical) [12033-49-7] YPJKMVATUPSWOH-UHFFFAOYSA-N	3.8×10^{-4}		Burkholder et al. (2019)	L	
	3.8×10^{-4}		Burkholder et al. (2015)	L	
	3.8×10^{-4}		Sander et al. (2011)	L	
	3.8×10^{-4}		Sander et al. (2006)	L	
	1.8×10^{-2}		Thomas et al. (1998)	M	
	5.9×10^{-3}		Rudich et al. (1996)	M	89
	1.2×10^{-1}	1900	Chameides (1986)	T	
	3.4×10^{-4}	2000	Berdnikov and Bazhin (1970)	T	47
			Jacob (1986)	E	90
			Seinfeld and Pandis (1998)	?	91
dinitrogen trioxide N_2O_3 [10544-73-7] LZDSILRDTDCIQT-UHFFFAOYSA-N	5.9×10^{-3}		Schwartz and White (1981)	L	
	2.5×10^{-1}		Komiyama and Inoue (1978)	M	
dinitrogen tetroxide N_2O_4 [10544-72-6] WFPZPJSADLPSON-UHFFFAOYSA-N	1.4×10^{-2}		Schwartz and White (1981)	L	
	2.0×10^{-2}		Komiyama and Inoue (1980)	M	80
	1.6×10^{-2}	3500	Komiyama and Inoue (1978)	M	
	3.1×10^{-2}		Andrew and Hanson (1961)	M	
	1.3×10^{-2}	1100	Kramers et al. (1961)	M	
dinitrogen pentoxide N_2O_5 (nitric anhydride) [10102-03-1] ZWWCURLKEXEFQT-UHFFFAOYSA-N	3.0×10^{-2}		Cruzeiro et al. (2022)	T	92
	3.9×10^{-3}		Galib and Limmer (2021)	T	93
	4.9×10^{-3}		Hirshberg et al. (2018)	T	94
	8.7×10^{-4}	3600	Fried et al. (1994)	T	95
	3.9×10^{-2}	4300	Robinson et al. (1997)	Q	96
	4.9×10^{-2}		Mentel et al. (1999)	E	97
	∞		Sander and Crutzen (1996)	E	98
	∞		Jacob (1986)	E	98
hydroxylamine H_3NO [7803-49-8] AVXURJPOCDRRFD-UHFFFAOYSA-N	1.4×10^{3}		HSDB (2015)	Q	99
nitrous acid HNO_2 [7782-77-6] IOVCWXUNBOPUCH-UHFFFAOYSA-N	4.8×10^{-1}	4800	Schwartz and White (1981)	L	
	4.7×10^{-1}	4900	Becker et al. (1998)	M	
	4.7×10^{-1}	4900	Becker et al. (1996)	M	
	4.8×10^{-1}	4900	Park and Lee (1988)	M	
	3.7×10^{-1}	9000	Komiyama and Inoue (1978)	M	
	4.7×10^{-1}	4700	Martin (1984)	T	
	4.8×10^{-1}	4800	Chameides (1984)	T	
	4.8×10^{-1}		Seinfeld (1986)	?	21

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Table A1.3: Nitrogen (N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
nitric acid	8.8×10^{2}		Durham et al. (1981)	V	
HNO_3	2.1×10^{3}	8700	Lelieveld and Crutzen (1991)	R	100
[7697-37-2]			Clegg and Brimblecombe (1990)	T	101, 1
GRYLNZFGIOXLOG-UHFFFAOYSA-N			Brimblecombe and Clegg (1989)	T	102
	2.6×10^{4}	8700	Chameides (1984)	T	
	2.1×10^{3}		Schwartz and White (1981)	T	
	2.1×10^{3}		Pandis and Seinfeld (1989)	?	103
	2.1×10^{3}		Seinfeld (1986)	?	21
	3.4×10^{3}	8800	Hoffmann and Jacob (1984)	?	21
			Brimblecombe and Clegg (1988)	W	104
pernitric acid	3.9×10^{-1}	8400	Leu and Zhang (1999)	L	
HNO_4	3.9×10^{1}		Amels et al. (1996)	M	
[26404-66-0]	1.2×10^{2}	6900	Régimbal and Mozurkewich (1997)	T	
UUZZMWZGAZGXSF-UHFFFAOYSA-N	1.4×10^{2}		Warneck (1999)	C	
	2.0×10^{2}	0	Jacob et al. (1989)	C	
			Möller and Mauersberger (1992)	E	105

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A1.4 Fluorine (F)

Table A1.4: Fluorine (F)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
fluorine atom F [14762-94-8] YCKRFDGAMUMZLT-UHFFFAOYSA-N	2.0×10^{-4}	400	Berdnikov and Bazhin (1970)	T	47
hydrogen fluoride HF [7664-39-3] KRHYYFGTRYWZRS-UHFFFAOYSA-N	1.3×10^{2}		Fredenhagen and Wellmann (1932a)	M	
			Brimblecombe and Clegg (1989)	T	106
	6.8×10^{-4}		Hayer et al. (2022)	Q	20
			Brimblecombe and Clegg (1988)	W	104
difluorine monoxide F_2O [7783-41-7] UJMWVICAENGCRF-UHFFFAOYSA-N	2.9×10^{-5}		Schäfer and Lax (1962)	C	
nitrogen trifluoride NF_3 [7783-54-2] GVGCUCJTUSOZKP-UHFFFAOYSA-N	7.9×10^{-6}	1900	Burkholder et al. (2019)	L	1
	7.9×10^{-6}	1900	Burkholder et al. (2015)	L	1
	7.9×10^{-6}	1900	Sander et al. (2011)	L	1
	7.9×10^{-6}	1900	Wilhelm et al. (1977)	L	
	7.7×10^{-6}	1700	Dean et al. (1973)	M	107
	7.8×10^{-6}	1900	Ashton et al. (1968)	M	108
dinitrogen tetrafluoride N_2F_4 (tetrafluorohydrazine) [10036-47-2] GFADZIUESKAXAK-UHFFFAOYSA-N	8.4×10^{-6}	2500	Burkholder et al. (2019)	L	1
	8.4×10^{-6}	2500	Burkholder et al. (2015)	L	1
	8.4×10^{-6}	2500	Sander et al. (2011)	L	1
	8.4×10^{-6}	2500	Wilhelm et al. (1977)	L	
	8.4×10^{-6}	2400	Dean et al. (1973)	M	109

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A1.5 Chlorine (Cl)

Table A1.5: Chlorine (Cl)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chlorine (molecular) Cl_2 [7782-50-5] KZBUYRJDOAKODT-UHFFFAOYSA-N			Burkholder et al. (2019)	L	110
			Burkholder et al. (2015)	L	110
			Sander et al. (2011)	L	110
			Sander et al. (2006)	L	110
			Young (1983)	L	111
	6.1×10^{-4}	3200	Aieta and Roberts (1986)	M	
	6.2×10^{-4}	3500	Whitney and Vivian (1941a)	M	112
			Jones (1911)	M	110
			Winkler (1907)	M	110
	6.0×10^{-4}	3000	Yakovkin (1900)	M	113
			Bakhuis Roozeboom (1884)	M	110
			Goodwin (1883)	M	110
			Schoenfeld (1855)	M	110
	7.4×10^{-4}	2600	Lin and Pehkonen (1998)	R	
	5.9×10^{-4}		Leaist (1986)	R	114
		3200	Brian et al. (1962)	R	
			Adams and Edmonds (1937)	R	115
			Arkadiev (1918)	R	116
	6.1×10^{-4}	2800	Wagman et al. (1982)	T	
	8.7×10^{-4}		Hayer et al. (2022)	Q	20
			Bartlett and Margerum (1999)	?	110, 21, 117
			Yaws et al. (1999)	?	110
			Dean and Lange (1999)	?	110
			Wilhelm et al. (1977)	?	118, 110
chlorine atom Cl [22537-15-1] ZAMOUSCENKQFHK-UHFFFAOYSA-N	2.3×10^{-2}		Burkholder et al. (2019)	L	
	2.3×10^{-2}		Burkholder et al. (2015)	L	
	2.3×10^{-2}		Sander et al. (2011)	L	
	2.3×10^{-2}		Sander et al. (2006)	L	
	2.0×10^{-3}		Mozurkewich (1986)	T	119
	1.5×10^{-4}	1500	Berdnikov and Bazhin (1970)	T	47
hydrogen chloride HCl [7647-01-0] VEXZGXHMUGYJMC-UHFFFAOYSA-N			Clegg and Brimblecombe (1986)	L	120
	1.5×10^{1}		Chen et al. (1979)	R	
			Carslaw et al. (1995)	T	121, 1
			Brimblecombe and Clegg (1989)	T	122
	1.1×10^{-2}	2300	Marsh and McElroy (1985)	T	
			Wagman et al. (1982)	T	123
	2.0×10^{-1}		Graedel and Goldberg (1983)	C	
	2.4×10^{-1}		Hayer et al. (2022)	Q	20
			Seinfeld and Pandis (1998)	?	91
	1.9×10^{-1}	620	Dean and Lange (1999)	?	124, 23
	2.5×10^{1}		Seinfeld (1986)	?	21
	7.2	2000	Pandis and Seinfeld (1989)	W	125
			Brimblecombe and Clegg (1988)	W	104

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Table A1.5: Chlorine (Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hypochlorous acid	6.5	5900	Burkholder et al. (2019)	L	
HOCl	6.5	5900	Burkholder et al. (2015)	L	
[7790-92-3]	6.5	5900	Sander et al. (2011)	L	
QWPPOHNGKGFGJK-UHFFFAOYSA-N	6.5	5900	Sander et al. (2006)	L	
	6.5	5900	Huthwelker et al. (1995)	L	
	9.1		Blatchley et al. (1992)	M	12
	4.7	1600	Hanson and Ravishankara (1991)	M	126
	9.0		McCoy et al. (1990)	M	12
	6.0	4900	Holzwarth et al. (1984)	M	127
	1.2×10^{1}	5200	Imagawa (1950)	M	11
	6.4	8900	Ourisson and Kastner (1939)	M	
	2.6	5100	Wagman et al. (1982)	T	
	5.4		Hilal et al. (2008)	Q	
perchloric acid	9.9×10^{3}		Jaeglé et al. (1996)	E	128
$HClO_4$					
[7601-90-3]					
VLTRZXGMWDSKGL-UHFFFAOYSA-N					
monochlorine monoxide	7.0×10^{-3}		Burkholder et al. (2019)	L	
ClO	7.0×10^{-3}		Burkholder et al. (2015)	L	
[14989-30-1]	7.0×10^{-3}		Sander et al. (2011)	L	
MLWGAEVSWJXOQJ-UHFFFAOYSA-N	7.0×10^{-3}		Sander et al. (2006)	L	
dichlorine monoxide			Secoy and Cady (1941)	M	129
Cl_2O			Ourisson and Kastner (1939)	M	130
[7791-21-1]	3.4×10^{-2}	5900	this work	R	131, 132, 133
RCJVRSBWZCNNQT-UHFFFAOYSA-N	7.6×10^{-2}	5600	this work	R	132, 134
	7.0×10^{-2}		Roth (1942)	R	135
			Burkholder et al. (2019)	?	136
			Burkholder et al. (2015)	?	136
			Sander et al. (2011)	?	136
			Sander et al. (2006)	?	136
			Young (1983)	?	137
	1.7×10^{-1}	1800	Wilhelm et al. (1977)	?	138
chlorine dioxide	1.0×10^{-2}	3500	Burkholder et al. (2019)	L	
ClO_2	1.0×10^{-2}	3500	Burkholder et al. (2015)	L	
[10049-04-4]	1.0×10^{-2}	3500	Sander et al. (2011)	L	
OSVXSBDYLRYLIG-UHFFFAOYSA-N	1.0×10^{-2}	3500	Sander et al. (2006)	L	
	1.0×10^{-2}	3300	Young (1983)	L	1
	1.0×10^{-2}	3300	Wilhelm et al. (1977)	L	
	1.0×10^{-2}	3200	Kepinski and Trzeszczynski (1964)	M	
	1.1×10^{-2}	3100	Ishi (1958)	M	
	1.0×10^{-2}		Taube and Dodgen (1949)	M	
	6.6×10^{-3}	1200	Bigorgne (1947)	M	
	9.7×10^{-3}	3600	Holst (1944)	M	
			Haller and Northgraves (1955)	C	139

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Table A1.5: Chlorine (Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^{-2}	3100	Mavu (2011)	?	
	9.7×10^{-3}		Morrow et al. (2006)	?	
	1.0×10^{-2}	3300	Yaws et al. (1999)	?	21
perchloryl fluoride ClO_3F [7616-94-6] XHFXMNZYIKFCPN-UHFFFAOYSA-N	4.4×10^{-5}		Hayer et al. (2022)	Q	20
nitrosyl chloride NOCl [2696-92-6] VPCDQGACGWYTMC-UHFFFAOYSA-N	$>4.9\times10^{-4}$ $>4.9\times10^{-4}$ $>4.9\times10^{-4}$		Burkholder et al. (2019) Burkholder et al. (2015) Scheer et al. (1997)	L L M	
nitryl chloride $ClNO_2$ [13444-90-1] HSSFHZJIMRUXDM-UHFFFAOYSA-M	4.5×10^{-4} 2.4×10^{-4} 3.9×10^{-4}		Frenzel et al. (1998) Behnke et al. (1997) Roberts et al. (2008)	E E ?	 140
chlorine nitrate $ClNO_3$ [14545-72-3] XYLGPCWDPLOBGP-UHFFFAOYSA-N	7.0×10^{-2} ∞	4500	Robinson et al. (1997) Sander and Crutzen (1996)	Q E	141 98
chloramine NH_2Cl (chloramide) [10599-90-3] QDHHCQZDFGDHMP-UHFFFAOYSA-N	8.6×10^{-1} 8.6×10^{-1} 8.6×10^{-1} 8.6×10^{-1} 9.2×10^{-1} 4.6×10^{-5}	6000 6000 6000 6000 4800	Burkholder et al. (2019) Burkholder et al. (2015) Sander et al. (2011) Sander et al. (2006) Holzwarth et al. (1984) Hayer et al. (2022)	L L L L M Q	 20
dichloramine $NHCl_2$ (chlorimide) [3400-09-7] JSYGRUBHOCKMGQ-UHFFFAOYSA-N	2.9×10^{-1} 2.9×10^{-1} 2.9×10^{-1} 2.9×10^{-1} 2.8×10^{-1}	4200 4200 4200 4200 4200	Burkholder et al. (2019) Burkholder et al. (2015) Sander et al. (2011) Sander et al. (2006) Holzwarth et al. (1984)	L L L L M	
nitrogen trichloride NCl_3 [10025-85-1] QEHKBHWEUPXBCW-UHFFFAOYSA-N	9.9×10^{-4} 9.9×10^{-4} 9.9×10^{-4} 9.9×10^{-4} 9.9×10^{-4}	4100 4100 4100 4100 4100	Burkholder et al. (2019) Burkholder et al. (2015) Sander et al. (2011) Sander et al. (2006) Holzwarth et al. (1984)	L L L L M	

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A1.6 Bromine (Br)

Table A1.6: Bromine (Br)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bromine (molecular) Br_2 [7726-95-6] GDTBXPJZTBHREO-UHFFFAOYSA-N	7.2×10^{-3}	4400	Burkholder et al. (2019)	L	
	7.2×10^{-3}	4400	Burkholder et al. (2015)	L	
	7.2×10^{-3}	4400	Sander et al. (2011)	L	
	7.2×10^{-3}	4400	Sander et al. (2006)	L	
	1.8×10^{-2}	3600	Dubik et al. (1987)	M	142
	6.8×10^{-3}		Hill et al. (1968)	M	
	9.6×10^{-3}		Jenkins and King (1965)	M	12
	7.0×10^{-3}	4100	Kelley and Tartar (1956)	M	
	1.4×10^{-2}		Jones (1911)	M	80
	7.8×10^{-3}	3800	Winkler (1906)	M	
	7.9×10^{-3}	3600	Winkler (1899)	M	
	8.3×10^{-3}	4100	Fogg and Sangster (2003)	V	
	7.9×10^{-3}	3900	Jenkins and King (1965)	R	
	7.2×10^{-3}	4000	Wagman et al. (1982)	T	
	9.2×10^{-3}		Giona et al. (1969)	X	143, 12
	7.6×10^{-3}		Bartlett and Margerum (1999)	?	21, 117
	7.5×10^{-3}	3900	Dean and Lange (1999)	?	144, 23
bromine atom Br [10097-32-2] WKBOTKDWSSQWDR-UHFFFAOYSA-N	1.2×10^{-2}		Mozurkewich (1986)	T	119
	3.4×10^{-4}	1800	Berdnikov and Bazhin (1970)	T	47
hydrogen bromide HBr [10035-10-6] CPELXLSAUQHCOX-UHFFFAOYSA-N			Carslaw et al. (1995)	T	145, 1
			Brimblecombe and Clegg (1989)	T	146
			Wagman et al. (1982)	T	147
	6.8×10^{-2}		Hayer et al. (2022)	Q	20
			Chameides and Stelson (1992)	?	148
	2.4×10^{-1}	250	Dean and Lange (1999)	?	149, 23
			Brimblecombe and Clegg (1988)	W	104
hypobromous acid HOBr [13517-11-8] CUILPNURFADTPE-UHFFFAOYSA-N	$>1.3\times10^{1}$		Burkholder et al. (2019)	L	
	$>1.3\times10^{1}$		Burkholder et al. (2015)	L	
	$>1.9\times10^{1}$		Blatchley et al. (1992)	M	12
	1.9×10^{1}		McCoy et al. (1990)	M	12
	1.8×10^{-2}	4000	Mozurkewich (1995)	T	150
	6.0×10^{1}		Frenzel et al. (1998)	E	
	9.1×10^{-1}		Vogt et al. (1996)	E	
			Sander et al. (2011)	W	151
			Sander et al. (2006)	W	151
			Fickert (1998)	W	152
nitryl bromide $BrNO_2$ [13536-70-4] SEYAFCXQVVHRPY-UHFFFAOYSA-M	3.0×10^{-3}		Frenzel et al. (1998)	E	

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Table A1.6: Bromine (Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bromine nitrate $BrNO_3$ [40423-14-1] RRTWEEAEXPZMPY-UHFFFAOYSA-N	∞		Sander and Crutzen (1996)	E	98
bromine chloride BrCl [13863-41-7] CODNYICXDISAEA-UHFFFAOYSA-N	9.7×10^{-3}	5600	Burkholder et al. (2019)	L	
	9.7×10^{-3}	5600	Burkholder et al. (2015)	L	
	9.7×10^{-3}	5600	Sander et al. (2011)	L	
	9.7×10^{-3}	5600	Sander et al. (2006)	L	
	$<6.2\times10^{-2}$		Katrib et al. (2001)	M	153
	1.5×10^{-2}		Disselkamp et al. (1999)	M	154
	9.3×10^{-3}	5600	Bartlett and Margerum (1999)	M	
	4.2×10^{-2}	4000	Dubik et al. (1987)	M	142
	1.1×10^{-2}		this work	T	155
	6.9×10^{-4}	4000	Ordóñez et al. (2012)	E	
	5.8×10^{-3}		Frenzel et al. (1998)	E	

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A1.7 Iodine (I)

Table A1.7: Iodine (I)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
iodine (molecular) I_2 [7553-56-2] PNDPGZBMCMUPRI-UHFFFAOYSA-N	2.8×10^{-2} 2.8×10^{-2} 3.0×10^{-2} 3.1×10^{-2} 3.2×10^{-2} 1.1×10^{-2}	4300 3900 4400 4600 4800	Eguchi et al. (1973) Fogg and Sangster (2003) Palmer et al. (1985) Berdnikov and Bazhin (1970) Wagman et al. (1982) Thompson and Zafiriou (1983)	M V R R T C	 1 156
iodine atom I [14362-44-8] ZCYVEMRRCGMTRW-UHFFFAOYSA-N	7.9×10^{-4} 6.2×10^{-5}	 2300	Mozurkewich (1986) Berdnikov and Bazhin (1970)	T T	157 47
hydrogen iodide HI [10034-85-2] XMBWDFGMSWQBCA-UHFFFAOYSA-N	 2.5×10^{-1} ∞	 9800	Brimblecombe and Clegg (1989) Wagman et al. (1982) Ordóñez et al. (2012) Vogt et al. (1999) Brimblecombe and Clegg (1988)	T T E E W	158 159 98 104
iodine monoxide IO [14696-98-1] AFSVSXMRDKPOEW-UHFFFAOYSA-N	4.4		Saiz-Lopez et al. (2014)	?	160
iodine dioxide OIO [13494-92-3] WXDJHDMIIZKXSK-UHFFFAOYSA-N	9.9×10^{1}		Saiz-Lopez et al. (2014)	?	160
diiodine dioxide I_2O_2 [215239-62-6] IELAHHPSAVYAOC-UHFFFAOYSA-N	∞ ∞ 9.9×10^{1}		Badia et al. (2019) Vogt et al. (1999) Saiz-Lopez et al. (2014)	E E ?	161, 162 161, 98 161, 160
diiodine trioxide I_2O_3 [11085-17-9] NMNCVPKLBXOKQA-UHFFFAOYSA-N	∞ 9.9×10^{1}		Badia et al. (2019) Saiz-Lopez et al. (2014)	E ?	161, 162 161, 160
diiodine tetroxide I_2O_4 [1024652-24-1] XHTWXUOEQMOFEJ-UHFFFAOYSA-N	∞ 9.9×10^{1}		Badia et al. (2019) Saiz-Lopez et al. (2014)	E ?	161, 162 161, 160
hypoiodous acid HOI [14332-21-9] GEOVEUCEIQCBKH-UHFFFAOYSA-N	>4.1		Palmer et al. (1985) Thompson and Zafiriou (1983)	C E	 163

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Table A1.7: Iodine (I) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
iodine nitrite INO_2 [15465-40-4] PSZTWRLUACEPOW-UHFFFAOYSA-N	3.0×10^{-3} ∞		Badia et al. (2019) Vogt et al. (1999)	E E	164 98
iodine nitrate INO_3 [14696-81-2] CCJHDZZUWZIVJF-UHFFFAOYSA-N	∞		Vogt et al. (1999)	E	98
iodine chloride ICl [7790-99-0] QZRGKCOWNLSUDK-UHFFFAOYSA-N	1.1		Wagman et al. (1982)	T	
iodine bromide IBr [7789-33-5] CBEQRNSPHCCXSH-UHFFFAOYSA-N	2.4×10^{-1}		Wagman et al. (1982)	T	

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A1.8 Sulfur (S)

Table A1.8: Sulfur (S)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
sulfur S [7704-34-9] NINIDFKCEFEMDL-UHFFFAOYSA-N	2.0×10^{1}		Maniere et al. (2011)	?	12, 165
hydrogen sulfide H_2S [7783-06-4] RWSOTUBLDIXVET-UHFFFAOYSA-N	1.0×10^{-3}	2100	Burkholder et al. (2019)	L	1
	1.0×10^{-3}	2100	Burkholder et al. (2015)	L	1
	1.0×10^{-3}	2100	Sander et al. (2011)	L	1
	1.0×10^{-3}	2100	Sander et al. (2006)	L	1
	1.0×10^{-3}	2000	Fernández-Prini et al. (2003)	L	3
	1.0×10^{-3}	2200	Carroll and Mather (1989)	L	
	1.0×10^{-3}	2000	Fogg and Young (1988)	L	1, 166
	1.0×10^{-3}	2000	Yoo et al. (1986)	L	1
	1.0×10^{-3}	2100	Edwards et al. (1978)	L	1
	1.0×10^{-3}	2100	Wilhelm et al. (1977)	L	
	9.1×10^{-4}	1700	Rinker and Sandall (2000)	M	
	9.2×10^{-4}	1600	Munder et al. (2000)	M	
	8.6×10^{-4}	2100	De Bruyn et al. (1995b)	M	
	1.1×10^{-3}	2300	Suleimenov and Krupp (1994)	M	1
	1.2×10^{-3}	1700	Tsuji et al. (1990)	M	62
	9.4×10^{-4}	2300	Barrett et al. (1988)	M	
	1.0×10^{-3}	2100	Clarke and Glew (1971)	M	167
	1.0×10^{-3}	2300	Winkler (1907)	M	
	1.0×10^{-3}	2100	Winkler (1906)	M	
	1.1×10^{-3}	2000	Schoenfeld (1855)	M	168
	9.6×10^{-4}	2000	Iliuta and Larachi (2007)	R	1
	1.0×10^{-3}		Hine and Weimar (1965)	R	
	1.0×10^{-3}	2300	Edwards et al. (1975)	T	1
	7.0×10^{-4}		Hayer et al. (2022)	Q	20
	1.0×10^{-3}	2000	Yaws et al. (1999)	?	21
	1.0×10^{-3}	2100	Dean and Lange (1999)	?	169, 23
			Chapoy et al. (2005)	W	170, 1
deuterium sulfide D_2S [13536-94-2] RWSOTUBLDIXVET-ZSJDYOACSA-N	9.9×10^{-4}	2100	Clarke and Glew (1971)	M	171, 172
sulfur dioxide SO_2 [7446-09-5] RAHZWNYVWXNFOC-UHFFFAOYSA-N	1.3×10^{-2}	2900	Burkholder et al. (2019)	L	1
	1.3×10^{-2}	2900	Burkholder et al. (2015)	L	1
	1.3×10^{-2}	2900	Sander et al. (2011)	L	1
	1.3×10^{-2}	2900	Sander et al. (2006)	L	1
	1.2×10^{-2}	3100	Yoo et al. (1986)	L	1
	1.3×10^{-2}	2900	Young (1983)	L	1
	1.2×10^{-2}	3200	Maahs (1982)	L	
	1.2×10^{-2}	3000	Edwards et al. (1978)	L	1

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Table A1.8: Sulfur (S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.4×10^{-2}	2800	Wilhelm et al. (1977)	L	
	4.0×10^{-1}		St-Pierre et al. (2014)	M	173
	1.2×10^{-2}	3100	Johnstone and Leppla (1934)	M	
	1.4×10^{-2}	3400	Schoenfeld (1855)	M	174
	1.1×10^{-2}	1200	Terraglio and Manganelli (1967)	V	
	1.2×10^{-2}	3100	Chameides (1984)	T	
	1.2×10^{-2}	3100	Edwards et al. (1975)	T	1
	1.2×10^{-2}		Rodríguez-Sevilla et al. (2001)	X	175
	1.2×10^{-2}	3100	Pandis and Seinfeld (1989)	C	
	1.2×10^{-2}	3300	Beilke and Gravenhorst (1978)	C	
	2.9×10^{-2}		Hayer et al. (2022)	Q	20
	1.3×10^{-2}	2900	Yaws et al. (1999)	?	21
	1.5×10^{-2}	3100	Dean and Lange (1999)	?	176, 23
	1.2×10^{-2}	3100	Seinfeld (1986)	?	21
	1.2×10^{-2}	3100	Hoffmann and Jacob (1984)	?	21
sulfur trioxide SO_3 [7446-11-9] AKEJUJNQAAGONA-UHFFFAOYSA-N	5.1×10^{-8}		Hayer et al. (2022)	Q	20
	∞		Sander and Crutzen (1996)	E	98
sulfuric acid H_2SO_4 [7664-93-9] QAOWNCQODCNURD-UHFFFAOYSA-N			Marti et al. (1997)	M	177
			Ayers et al. (1980)	M	178
			Gmitro and Vermeulen (1964)	M	179
			Clegg et al. (1998)	V	180
	1.3×10^{13}	20000	Hoffmann and Calvert (1985)	T	
	2.9×10^{7}	10000	Ayers (1983)	T	
sulfur hexafluoride SF_6 [2551-62-4] SFZCNBIFKDRMGX-UHFFFAOYSA-N	2.4×10^{-6}	3100	Warneck and Williams (2012)	L	
	2.5×10^{-6}	2100	Fernández-Prini et al. (2003)	L	3
	2.4×10^{-6}	2400	Wilhelm et al. (1977)	L	
	2.3×10^{-6}	2700	Bullister et al. (2002)	M	181
	1.4×10^{-6}		Guitart et al. (1989)	M	14
	2.4×10^{-6}		Park et al. (1982)	M	
	2.5×10^{-6}	260	Cosgrove and Walkley (1981)	M	42, 11
	1.7×10^{-6}		Longo et al. (1970)	M	14
	1.7×10^{-6}		Power and Stegall (1970)	M	14
			Shoor et al. (1969)	M	182
	2.4×10^{-6}	2400	Ashton et al. (1968)	M	183
	2.2×10^{-6}	3500	Friedman (1954)	M	
	2.2×10^{-6}		Giardino et al. (1988)	V	
	2.6×10^{-6}		Hayer et al. (2022)	Q	20
	2.2×10^{-5}		Keshavarz et al. (2022)	Q	
	2.6×10^{-5}		Duchowicz et al. (2020)	Q	184
		3200	Kühne et al. (2005)	Q	
	2.2×10^{-6}		Duchowicz et al. (2020)	?	185, 21
		2800	Kühne et al. (2005)	?	
	2.4×10^{-6}	2400	Yaws et al. (1999)	?	21
	1.9×10^{-6}		Abraham and Weathersby (1994)	?	21

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Table A1.8: Sulfur (S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
sulfuryl fluoride	8.9×10^{-5}	3100	Cady and Misra (1974)	M	
SO_2F_2	7.3×10^{-5}		Duchowicz et al. (2020)	V	186
[2699-79-8]	3.2		Duchowicz et al. (2020)	Q	
OBTWBSRJZRCYQV-UHFFFAOYSA-N	6.3×10^{-6}		Maniere et al. (2011)	?	12, 165

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A1.9 Rare gases (He, Ne, Ar, Kr, Xe, Rn)

Table A1.9: Rare gases (He, Ne, Ar, Kr, Xe, Rn)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
helium	3.9×10^{-6}	15	Fernández-Prini et al. (2003)	L	3
He	3.8×10^{-6}	83	Abraham and Matteoli (1988)	L	
[7440-59-7]	3.8×10^{-6}	83	Clever (1979a)	L	1
SWQJXJOGLNCZEY-UHFFFAOYSA-N	3.8×10^{-6}	92	Wilhelm et al. (1977)	L	
	3.7×10^{-6}	320	Himmelblau (1960)	L	1
	3.9×10^{-6}	69	Krause and Benson (1989)	M	
			Shoor et al. (1969)	M	187
	3.7×10^{-6}	120	Morrison and Johnstone (1954)	M	188
	3.8×10^{-6}		Friedman (1954)	M	
	3.8×10^{-6}	210	Lannung (1930)	M	189
	3.7×10^{-6}	380	Cady et al. (1922)	M	
	6.3×10^{-6}	-700	von Antropoff (1910)	M	42
	3.7×10^{-6}	220	Wauchope and Haque (1972)	V	
	5.3×10^{-6}		Pierotti (1965)	T	
	4.5×10^{-6}		Hayer et al. (2022)	Q	20
	3.3×10^{-6}	4	Linnemann et al. (2020)	Q	42
	3.3×10^{-6}	71	Linnemann et al. (2020)	Q	42, 190
	3.9×10^{-6}		Warr et al. (2015)	Q	12
	3.8×10^{-6}	83	Yaws et al. (1999)	?	21
	3.9×10^{-6}		Abraham and Weathersby (1994)	?	21
	3.7×10^{-6}	200	Dean and Lange (1999)	?	191, 23
	3.8×10^{-6}		Abraham et al. (1990)	?	
neon	4.5×10^{-6}	430	Fernández-Prini et al. (2003)	L	3
Ne	4.4×10^{-6}	470	Abraham and Matteoli (1988)	L	
[7440-01-9]	4.5×10^{-6}	470	Clever (1979a)	L	1
GKAOGPIIYCISHV-UHFFFAOYSA-N	4.4×10^{-6}	450	Wilhelm et al. (1977)	L	
	4.5×10^{-6}	440	Krause and Benson (1989)	M	
	4.4×10^{-6}	510	Crovetto et al. (1982)	M	
	4.3×10^{-6}		Power and Stegall (1970)	M	14
	4.5×10^{-6}	460	Morrison and Johnstone (1954)	M	192
	4.6×10^{-6}	37	Lannung (1930)	M	193
	6.6×10^{-6}	-990	von Antropoff (1910)	M	
	4.5×10^{-6}	510	Wauchope and Haque (1972)	V	
	8.8×10^{-6}		Pierotti (1965)	T	
	4.5×10^{-6}		Hayer et al. (2022)	Q	20
	3.4×10^{-6}	250	Linnemann et al. (2020)	Q	33
	4.7×10^{-6}	470	Linnemann et al. (2020)	Q	33, 190
	3.6×10^{-6}		Warr et al. (2015)	Q	12
	4.5×10^{-6}	470	Yaws et al. (1999)	?	21
	4.4×10^{-6}		Abraham and Weathersby (1994)	?	21
	4.5×10^{-6}	550	Dean and Lange (1999)	?	194, 23
	4.4×10^{-6}		Abraham et al. (1990)	?	

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Table A1.9: Rare gases (He, Ne, Ar, Kr, Xe, Rn) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
argon	1.4×10^{-5}	1700	Warneck and Williams (2012)	L	
Ar	1.4×10^{-5}	1400	Fernández-Prini et al. (2003)	L	3
[7440-37-1]	1.4×10^{-5}	1500	Abraham and Matteoli (1988)	L	
XKRFYHLGVUSROY-UHFFFAOYSA-N	1.4×10^{-5}	1500	Clever (1980)	L	1
	1.4×10^{-5}	1500	Wilhelm et al. (1977)	L	
	1.4×10^{-5}	1400	Rettich et al. (1992)	M	195
	1.4×10^{-5}	1400	Krause and Benson (1989)	M	
	1.4×10^{-5}		Park et al. (1982)	M	
	1.4×10^{-5}	1500	Crovetto et al. (1982)	M	
	1.4×10^{-5}	1200	Cosgrove and Walkley (1981)	M	11
	1.4×10^{-5}	1300	Potter II and Clynne (1978)	M	
	1.4×10^{-5}	1500	Murray and Riley (1970)	M	196
	1.4×10^{-5}	1600	Shoor et al. (1969)	M	197
	1.4×10^{-5}	1500	Ashton et al. (1968)	M	198
	1.3×10^{-5}	1500	Morrison and Johnstone (1954)	M	199
	1.4×10^{-5}	1800	Friedman (1954)	M	
	1.4×10^{-5}	1400	Lannung (1930)	M	200
	1.6×10^{-5}	1300	von Antropoff (1910)	M	
	1.5×10^{-5}	1400	Winkler (1906)	M	
	1.4×10^{-5}	1400	Wauchope and Haque (1972)	V	
	1.4×10^{-5}	1400	Wauchope and Haque (1972)	V	
	1.8×10^{-5}		Pierotti (1965)	T	
	9.5×10^{-6}		Hayer et al. (2022)	Q	20
	7.8×10^{-6}	1200	Linnemann et al. (2020)	Q	190
	1.1×10^{-5}	1100	Linnemann et al. (2020)	Q	201
	1.2×10^{-5}		Warr et al. (2015)	Q	12
	1.4×10^{-5}	1500	Yaws et al. (1999)	?	21
	1.2×10^{-5}		Abraham and Weathersby (1994)	?	21
	1.4×10^{-5}	1500	Dean and Lange (1999)	?	202, 23
	1.4×10^{-5}		Abraham et al. (1990)	?	
krypton	2.5×10^{-5}	1700	Fernández-Prini et al. (2003)	L	3
Kr	2.5×10^{-5}	1900	Abraham and Matteoli (1988)	L	
[7439-90-9]	2.5×10^{-5}	1900	Clever (1979b)	L	1
DNNSSWSSYDEUBZ-UHFFFAOYSA-N	2.5×10^{-5}	1900	Wilhelm et al. (1977)	L	
	2.0×10^{-5}		Steward et al. (1973)	L	14
	2.5×10^{-5}	2000	Allott et al. (1973)	L	
	2.5×10^{-5}	1800	Krause and Benson (1989)	M	
	2.5×10^{-5}	1900	Crovetto et al. (1982)	M	
	2.6×10^{-5}	1800	Cosgrove and Walkley (1981)	M	11
	2.4×10^{-5}	1700	Morrison and Johnstone (1954)	M	203
	3.4×10^{-5}	1400	von Antropoff (1910)	M	204
	2.8×10^{-5}	1900	von Antropoff (1910)	M	204
	2.4×10^{-5}	1800	Wauchope and Haque (1972)	V	
	4.4×10^{-5}		Pierotti (1965)	T	
	2.6×10^{-5}		Hayer et al. (2022)	Q	20
	1.5×10^{-5}	1600	Linnemann et al. (2020)	Q	190
	1.6×10^{-5}	1400	Linnemann et al. (2020)	Q	201

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Table A1.9: Rare gases (He, Ne, Ar, Kr, Xe, Rn) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.5×10^{-5}		Warr et al. (2015)	Q	12
	2.5×10^{-5}	1900	Yaws et al. (1999)	?	21
	2.0×10^{-5}		Abraham and Weathersby (1994)	?	21
	2.5×10^{-5}	1800	Dean and Lange (1999)	?	205, 23
	2.5×10^{-5}		Abraham et al. (1990)	?	
xenon Xe [7440-63-3] FHNFHKCVQCLJFQ-UHFFFAOYSA-N	4.4×10^{-5}	2200	Fernández-Prini et al. (2003)	L	3
	4.3×10^{-5}	2300	Abraham and Matteoli (1988)	L	
	4.3×10^{-5}	2300	Clever (1979b)	L	1
	4.2×10^{-5}	2200	Wilhelm et al. (1977)	L	
	3.3×10^{-5}		Steward et al. (1973)	L	14
	4.5×10^{-5}	2400	Allott et al. (1973)	L	
	4.0×10^{-5}	2400	Himmelblau (1960)	L	1, 206
	4.3×10^{-5}	2300	Krause and Benson (1989)	M	
	4.2×10^{-5}	2400	Crovetto et al. (1982)	M	
	4.2×10^{-5}	2200	Morrison and Johnstone (1954)	M	207
	4.4×10^{-5}	2500	von Antropoff (1910)	M	
	4.2×10^{-5}	2200	Wauchope and Haque (1972)	V	
	5.5×10^{-5}		Pierotti (1965)	T	
	2.5×10^{-5}		Hayer et al. (2022)	Q	20
	7.0×10^{-5}	2300	Linnemann et al. (2020)	Q	190
	2.9×10^{-5}	1800	Linnemann et al. (2020)	Q	201
	8.2×10^{-5}		Warr et al. (2015)	Q	12
	4.3×10^{-5}	2300	Yaws et al. (1999)	?	21
	3.4×10^{-5}		Abraham and Weathersby (1994)	?	21
	4.9×10^{-5}	2200	Dean and Lange (1999)	?	208, 23
	4.3×10^{-5}		Abraham et al. (1990)	?	
xenon-133 ^{133}Xe [14932-42-4] FHNFHKCVQCLJFQ-NJFSPNSNSA-N	3.2×10^{-5}		Ercan (1979)	M	14
radon Rn [10043-92-2] SYUHGPGVQRZVTB-UHFFFAOYSA-N	9.1×10^{-5}	2900	Abraham and Matteoli (1988)	L	
	9.1×10^{-5}	2600	Clever (1979b)	L	1
	9.2×10^{-5}	2600	Wilhelm et al. (1977)	L	
	9.4×10^{-5}	2600	Lewis et al. (1987)	M	209
	1.0×10^{-4}	2700	Ramstedt (1911)	M	
	1.2×10^{-4}		Pierotti (1965)	T	
	1.0×10^{-4}		Hayer et al. (2022)	Q	20
	7.4×10^{-5}	2400	Linnemann et al. (2020)	Q	210
	9.1×10^{-5}	2600	Yaws et al. (1999)	?	21
	8.3×10^{-5}	2800	Dean and Lange (1999)	?	211, 23
	9.1×10^{-5}		Abraham et al. (1990)	?	

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A1.10 Other elements (B, Se, P, As, Hg)

Table A1.10: Other elements (B, Se, P, As, Hg)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
boric acid H_3BO_3 [10043-35-3] KGBXLFKZBHKPEV-UHFFFAOYSA-N	3.8×10^{6}		HSDB (2015)	V	
selenium hydride H_2Se [7783-07-5] BUGBHKTXTAQXES-UHFFFAOYSA-N	8.1×10^{-4} 8.3×10^{-4} 8.3×10^{-4}	1700 1900 1900	Fogg and Young (1988) Wilhelm et al. (1977) Sisi et al. (1971)	L L M	1 212
phosphorus trihydride PH_3 (phosphine) [7803-51-2] XYFCBTPGUUZFHI-UHFFFAOYSA-N	8.1×10^{-5} 5.9×10^{-5} 8.1×10^{-5}	2000 3000 2000	Wilhelm et al. (1977) Fu et al. (2013) Yaws et al. (1999)	L M ?	 213 21
arsenic hydride AsH_3 (arsine) [7784-42-1] RQNWIZPPADIBDY-UHFFFAOYSA-N	8.8×10^{-5}	2100	Wilhelm et al. (1977)	L	
mercury Hg [7439-97-6] QSHDDOUJBYECFT-UHFFFAOYSA-N	1.3×10^{-3} 1.3×10^{-3} 1.2×10^{-3} 1.1×10^{-3} 1.3×10^{-3} 1.3×10^{-3} 8.7×10^{-4} 1.1×10^{-3} 1.2×10^{-3} 1.4×10^{-3} 1.4×10^{-3} 1.3×10^{-3} 1.3×10^{-3} 9.2×10^{-4}	2600 2600 5400 4800 2600 2500 5700 2300 2700 	Burkholder et al. (2019) Burkholder et al. (2015) Clever (1987) Clever et al. (1985) Andersson et al. (2008) Sanemasa (1975) Mackay and Leinonen (1975) Glew and Hames (1971) Shon et al. (2005) WHO (1990) Abraham et al. (2008) Schroeder and Munthe (1998) Schroeder and Munthe (1998) Petersen et al. (1998) Brimblecombe (1986)	L L L L M M V V C C Q ? ? ? ?	 1 1 1 12 214 12, 21 21 215 80
mercury(II) oxide HgO [21908-53-2] UKWHYYKOEPRTIC-UHFFFAOYSA-N	3.2×10^{4} 2.7×10^{10} 1.4×10^{4}		Shon et al. (2005) Schroeder and Munthe (1998) Petersen et al. (1998)	? ? ?	216 21 215
mercury dihydroxide $Hg(OH)_2$ [12135-13-6] VLKKXDVIWIBHHS-UHFFFAOYSA-L	1.3×10^{2} 1.3×10^{2}	4200 4200	WHO (1990) Lindqvist and Rodhe (1985)	C C	

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Table A1.10: Other elements (B, Se, P, As, Hg) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
mercury dichloride	1.0×10^3		Severit (1997)	M	217
$HgCl_2$	1.6×10^4		Abraham et al. (2008)	V	
[7487-94-7]	4.2×10^4		Abraham et al. (2008)	V	
LWJROJCJINYWOX-UHFFFAOYSA-L	1.3×10^4	7400	Kanefke (2008)	R	
	2.4×10^5		Shon et al. (2005)	C	
	1.4×10^4	5300	WHO (1990)	C	
	1.4×10^4	5300	Lindqvist and Rodhe (1985)	C	
	4.2×10^4	7400	Abraham et al. (2008)	Q	218
	2.7×10^4		Schroeder and Munthe (1998)	?	12, 21
	1.4×10^4	9500	Braun and Dransfeld (1989)	?	11
	6.3×10^2		Iverfeldt and Persson (1985)	?	219
mercury dibromide	1.2×10^3		Abraham et al. (2008)	V	
$HgBr_2$	9.6×10^2	7400	Kanefke (2008)	C	
[7789-47-1]	4.4×10^3	7100	Abraham et al. (2008)	Q	218
NGYIMTKLQULBOO-UHFFFAOYSA-L	2.7×10^4		Hedgecock et al. (2005)	?	220
	5.2×10^1		Iverfeldt and Persson (1985)	?	219
mercury diiodide	5.7×10^1		Abraham et al. (2008)	V	
HgI_2	2.0×10^2	6700	Abraham et al. (2008)	Q	218
[7774-29-0]	1.9		Iverfeldt and Persson (1985)	?	219
YFDLHELOZYVNJE-UHFFFAOYSA-L					

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A2 Hydrocarbons (C, H)

A2.1 Alkanes

Table A2.1: Alkanes

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methane	1.4×10^{-5}	1600	Burkholder et al. (2019)	L	1
CH_4	1.2×10^{-5}	1100	Burkholder et al. (2019)	L	70
[74-82-8]	1.4×10^{-5}	1600	Burkholder et al. (2015)	L	1
VNWKTOKETHGBQD-UHFFFAOYSA-N	1.2×10^{-5}	1100	Burkholder et al. (2015)	L	70
	1.4×10^{-5}	1900	Warneck and Williams (2012)	L	
	1.4×10^{-5}	1600	Sander et al. (2011)	L	1
	1.4×10^{-5}	1600	Sander et al. (2006)	L	1
	1.4×10^{-5}	1500	Fernández-Prini et al. (2003)	L	3
	1.4×10^{-5}	1600	Plyasunov and Shock (2000)	L	
	1.4×10^{-5}	1600	Abraham and Matteoli (1988)	L	
			Clever and Young (1987)	L	221
	1.5×10^{-5}		Mackay and Shiu (1981)	L	
	1.4×10^{-5}	1700	Wilhelm et al. (1977)	L	
	1.3×10^{-5}	1500	Himmelblau (1960)	L	1
	1.6×10^{-5}		Liu et al. (2021)	M	
	1.4×10^{-5}	1800	Lutsyk et al. (2005)	M	
	1.2×10^{-5}	2400	Lekvam and Bishnoi (1997)	M	
	1.3×10^{-5}	1400	Reichl (1995)	M	222
	1.4×10^{-5}	1600	Scharlin and Battino (1995)	M	223
	1.2×10^{-5}		Guitart et al. (1989)	M	14
	1.4×10^{-5}	1800	Ben-Naim and Battino (1985)	M	
	1.4×10^{-5}	1600	Crovetto et al. (1982)	M	
	1.4×10^{-5}	1600	Rettich et al. (1981)	M	
	1.4×10^{-5}	1600	Cosgrove and Walkley (1981)	M	11
	1.3×10^{-5}	1700	Shoor et al. (1969)	M	224
	1.5×10^{-5}		McAuliffe (1966)	M	225
	1.4×10^{-5}	1600	Wetlaufer et al. (1964)	M	
	1.5×10^{-5}		McAuliffe (1963)	M	226
	1.3×10^{-5}	1600	Morrison and Billett (1952)	M	227
	1.3×10^{-5}	1700	Winkler (1901)	M	228
	1.5×10^{-5}		Duchowicz et al. (2020)	V	186
	1.5×10^{-5}		HSDB (2015)	V	
	1.5×10^{-5}		Meylan and Howard (1991)	V	
	1.5×10^{-5}		Hine and Mookerjee (1975)	V	
	1.3×10^{-5}	1600	Wauchope and Haque (1972)	V	
	9.2×10^{-5}		Butler and Ramchandani (1935)	V	
	1.4×10^{-5}		Hine and Weimar (1965)	R	
	1.4×10^{-5}		Pierotti (1965)	T	
	9.6×10^{-6}		Liss and Slater (1974)	C	
	1.3×10^{-5}		Deno and Berkheimer (1960)	C	
	1.1×10^{-5}		Hayer et al. (2022)	Q	20
	3.4×10^{-3}		Duchowicz et al. (2020)	Q	
	7.0×10^{-7}		Gharagheizi et al. (2012)	Q	

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.5×10^{-5}		Hilal et al. (2008)	Q	
		2300	Kühne et al. (2005)	Q	
	3.0×10^{-5}		Yao et al. (2002)	Q	229
	3.0×10^{-5}		English and Carroll (2001)	Q	230, 231
	8.6×10^{-6}		Katritzky et al. (1998)	Q	
	1.6×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	2.1×10^{-5}		Suzuki et al. (1992)	Q	232
	2.4×10^{-5}		Meylan and Howard (1991)	Q	
		1700	Kühne et al. (2005)	?	
	1.6×10^{-5}		Yaws (1999)	?	21
	1.4×10^{-5}	1600	Yaws et al. (1999)	?	21
	1.2×10^{-5}		Abraham and Weathersby (1994)	?	21
	1.3×10^{-5}	1700	Dean and Lange (1999)	?	233, 23
	1.5×10^{-5}		Yaws and Yang (1992)	?	21
	1.4×10^{-5}		Abraham et al. (1990)	?	
ethane C_2H_6 [74-84-0] OTMSDBZUPAUEDD-UHFFFAOYSA-N	1.9×10^{-5}	2400	Burkholder et al. (2019)	L	1
	1.9×10^{-5}	2400	Burkholder et al. (2015)	L	1
	1.9×10^{-5}	2400	Sander et al. (2011)	L	1
	1.9×10^{-5}	2400	Sander et al. (2006)	L	1
	1.9×10^{-5}	2400	Fernández-Prini et al. (2003)	L	3
	1.9×10^{-5}	2300	Plyasunov and Shock (2000)	L	
	1.9×10^{-5}	2300	Abraham and Matteoli (1988)	L	
	1.9×10^{-5}	2300	Hayduk (1982)	L	1
	2.0×10^{-5}		Mackay and Shiu (1981)	L	
	1.8×10^{-5}	2400	Wilhelm et al. (1977)	L	
	2.0×10^{-5}	2300	Reichl (1995)	M	234
	1.3×10^{-5}		Guitart et al. (1989)	M	14
	1.8×10^{-5}	2700	Ben-Naim and Battino (1985)	M	
	1.9×10^{-5}	2300	Rettich et al. (1981)	M	
	1.8×10^{-5}	2700	Cosgrove and Walkley (1981)	M	11
	2.0×10^{-5}		McAuliffe (1966)	M	225
	2.0×10^{-5}	2400	Wetlaufer et al. (1964)	M	
	2.0×10^{-5}		McAuliffe (1963)	M	226
	1.7×10^{-5}	2100	Morrison and Billett (1952)	M	235
	1.8×10^{-5}	2400	Winkler (1901)	M	236
	2.0×10^{-5}		Duchowicz et al. (2020)	V	186
	2.0×10^{-5}		HSDB (2015)	V	
	2.0×10^{-5}		Hine and Mookerjee (1975)	V	
	1.7×10^{-5}	2000	Wauchope and Haque (1972)	V	
	1.0×10^{-4}		Butler and Ramchandani (1935)	V	
	4.0×10^{-5}		Pierotti (1965)	T	
	2.0×10^{-5}		Yaws (2003)	X	237
	1.8×10^{-5}		Deno and Berkheimer (1960)	C	
	1.8×10^{-5}		Hayer et al. (2022)	Q	20
	1.3×10^{-3}		Duchowicz et al. (2020)	Q	
	1.1×10^{-4}		Wang et al. (2017)	Q	80, 238
	1.1×10^{-5}		Wang et al. (2017)	Q	80, 239

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.0×10^{-5}		Wang et al. (2017)	Q	80, 240
	2.0×10^{-5}		Li et al. (2014)	Q	241
	3.3×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	4.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
	2.0×10^{-5}		Hilal et al. (2008)	Q	
	7.8×10^{-6}		Modarresi et al. (2007)	Q	67
		2600	Kühne et al. (2005)	Q	
	4.6×10^{-6}		Modarresi et al. (2005)	Q	247
	2.1×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	2.1×10^{-5}		Yao et al. (2002)	Q	229
	1.8×10^{-5}		English and Carroll (2001)	Q	230, 231
	1.5×10^{-5}		Katritzky et al. (1998)	Q	
	2.4×10^{-5}		Suzuki et al. (1992)	Q	232
	2.2×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	1.1×10^{-5}		Irmann (1965)	Q	
		2500	Kühne et al. (2005)	?	
	2.0×10^{-5}		Yaws (1999)	?	21
	1.9×10^{-5}	2300	Yaws et al. (1999)	?	21
	1.5×10^{-5}		Abraham and Weathersby (1994)	?	21
	1.8×10^{-5}	2400	Dean and Lange (1999)	?	250, 23
	2.0×10^{-5}		Yaws and Yang (1992)	?	21
	1.9×10^{-5}		Abraham et al. (1990)	?	
propane	1.5×10^{-5}	2700	Burkholder et al. (2019)	L	1
C_3H_8	1.5×10^{-5}	2700	Burkholder et al. (2015)	L	1
[74-98-6]	1.5×10^{-5}	2700	Sander et al. (2011)	L	1
ATUOYWHBWRKTHZ-UHFFFAOYSA-N	1.5×10^{-5}	2700	Sander et al. (2006)	L	1
	1.5×10^{-5}	2800	Plyasunov and Shock (2000)	L	
	1.5×10^{-5}	2800	Abraham and Matteoli (1988)	L	
	1.5×10^{-5}	2700	Hayduk (1986)	L	1
	1.4×10^{-5}		Mackay and Shiu (1981)	L	
	1.5×10^{-5}	2700	Wilhelm et al. (1977)	L	
	1.6×10^{-5}	2700	Chapoy et al. (2004)	M	1
	1.5×10^{-5}	2700	Reichl (1995)	M	251
	9.7×10^{-6}		Guitart et al. (1989)	M	14
	1.4×10^{-5}	3000	Ben-Naim and Battino (1985)	M	
	1.4×10^{-5}		McAuliffe (1966)	M	225
	1.6×10^{-5}	2700	Wetlaufer et al. (1964)	M	
	1.4×10^{-5}		McAuliffe (1963)	M	226
	1.5×10^{-5}	2600	Morrison and Billett (1952)	M	252
	1.4×10^{-5}		Duchowicz et al. (2020)	V	186
	1.4×10^{-5}		HSDB (2015)	V	
	1.4×10^{-5}		Hine and Mookerjee (1975)	V	
	1.5×10^{-5}	2600	Wauchope and Haque (1972)	V	
	1.5×10^{-5}	2700	Wauchope and Haque (1972)	V	

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.3×10^{-5}		Irmann (1965)	V	
	1.4×10^{-5}		Yaws (2003)	X	237
	1.4×10^{-5}		Deno and Berkheimer (1960)	C	
	1.7×10^{-5}		Hayer et al. (2022)	Q	20
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	8.7×10^{-5}		Wang et al. (2017)	Q	80, 238
	9.3×10^{-6}		Wang et al. (2017)	Q	80, 239
	1.9×10^{-5}		Wang et al. (2017)	Q	80, 240
	4.1×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	2.4×10^{-5}		Gharagheizi et al. (2010)	Q	246
	1.4×10^{-5}		Hilal et al. (2008)	Q	
	7.2×10^{-6}		Modarresi et al. (2007)	Q	67
		2900	Kühne et al. (2005)	Q	
	3.7×10^{-6}		Modarresi et al. (2005)	Q	247
	1.4×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	2.0×10^{-5}		Yao et al. (2002)	Q	229
	1.4×10^{-5}		English and Carroll (2001)	Q	230, 231
	1.5×10^{-5}		Katritzky et al. (1998)	Q	
	1.7×10^{-5}		Suzuki et al. (1992)	Q	232
	1.6×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	1.3×10^{-5}		Irmann (1965)	Q	
		2800	Kühne et al. (2005)	?	
	1.4×10^{-5}		Yaws (1999)	?	21
	1.5×10^{-5}	4500	Yaws et al. (1999)	?	21
	1.4×10^{-5}		Yaws and Yang (1992)	?	21
	1.5×10^{-5}		Abraham et al. (1990)	?	
butane C_4H_{10} [106-97-8] IJDNQMDRQITEOD-UHFFFAOYSA-N	1.2×10^{-5}	3100	Burkholder et al. (2019)	L	253, 1
	1.2×10^{-5}	3100	Burkholder et al. (2015)	L	254, 1
	1.2×10^{-5}	3100	Sander et al. (2011)	L	255, 1
	1.2×10^{-5}	3100	Sander et al. (2006)	L	256, 1
	1.2×10^{-5}	3100	Plyasunov and Shock (2000)	L	
	1.3×10^{-5}	3100	Abraham and Matteoli (1988)	L	
	1.2×10^{-5}	3000	Hayduk (1986)	L	1
	1.0×10^{-5}		Mackay and Shiu (1981)	L	
	1.2×10^{-5}	3100	Wilhelm et al. (1977)	L	
	1.3×10^{-5}	2300	Carroll et al. (1997)	M	1
	8.0×10^{-6}		Guitart et al. (1989)	M	14
	1.2×10^{-5}	3200	Ben-Naim and Battino (1985)	M	
	1.1×10^{-5}		McAuliffe (1966)	M	225
	1.3×10^{-5}	3200	Wetlaufer et al. (1964)	M	
	1.1×10^{-5}		McAuliffe (1963)	M	226
	1.1×10^{-5}	2900	Morrison and Billett (1952)	M	257
	1.0×10^{-5}		Duchowicz et al. (2020)	V	186
	1.0×10^{-5}		HSDB (2015)	V	

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.0×10^{-5}		Mackay et al. (2006a)	V	
	1.0×10^{-5}		Mackay et al. (1993)	V	
	9.6×10^{-6}		Hwang et al. (1992)	V	
	1.1×10^{-5}		Hine and Mookerjee (1975)	V	
	1.1×10^{-5}	2900	Wauchope and Haque (1972)	V	
	1.2×10^{-5}	3100	Wauchope and Haque (1972)	V	
	1.2×10^{-5}		Irmann (1965)	V	
	4.8×10^{-5}		Butler and Ramchandani (1935)	V	
	1.1×10^{-5}		Yaws (2003)	X	258
	1.1×10^{-5}		Yaws (2003)	X	237
	1.1×10^{-5}		Deno and Berkheimer (1960)	C	
	1.6×10^{-5}		Dupeux et al. (2022)	Q	259
	1.6×10^{-5}		Hayer et al. (2022)	Q	20
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	7.8×10^{-5}		Wang et al. (2017)	Q	80, 238
	1.1×10^{-5}		Wang et al. (2017)	Q	80, 239
	1.8×10^{-5}		Wang et al. (2017)	Q	80, 240
	1.1×10^{-5}		Li et al. (2014)	Q	241
	4.6×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	246
	1.2×10^{-5}		Hilal et al. (2008)	Q	
		3300	Kühne et al. (2005)	Q	
	3.5×10^{-6}		Modarresi et al. (2005)	Q	247
	1.1×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	1.6×10^{-5}		Yao et al. (2002)	Q	229
	1.0×10^{-5}		English and Carroll (2001)	Q	230, 260
	1.5×10^{-5}		Katritzky et al. (1998)	Q	
	1.3×10^{-5}		Suzuki et al. (1992)	Q	232
	1.2×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	1.2×10^{-5}		Irmann (1965)	Q	
		3300	Kühne et al. (2005)	?	
	1.1×10^{-5}		Yaws (1999)	?	21
	1.2×10^{-5}	3000	Yaws et al. (1999)	?	21
	1.1×10^{-5}		Yaws and Yang (1992)	?	21
	1.2×10^{-5}		Abraham et al. (1990)	?	
2-methylpropane	9.1×10^{-6}	2700	Burkholder et al. (2019)	L	261, 1
$HC(CH_3)_3$	9.1×10^{-6}	2700	Burkholder et al. (2015)	L	262, 1
(isobutane)	9.1×10^{-6}	2700	Sander et al. (2011)	L	263, 1
[75-28-5]	9.1×10^{-6}	2700	Sander et al. (2006)	L	264, 1
NNPPMTNAJDCUHE-UHFFFAOYSA-N			Fogg and Sangster (2003)	L	265
	9.2×10^{-6}	2900	Plyasunov and Shock (2000)	L	
	9.1×10^{-6}	2700	Hayduk (1986)	L	266, 1
	8.3×10^{-6}		Mackay and Shiu (1981)	L	
	8.0×10^{-6}	2700	Wilhelm et al. (1977)	L	

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^{-4}	5100	Mohebbi et al. (2012)	M	
	8.5×10^{-6}		McAuliffe (1966)	M	225
	9.9×10^{-6}	2700	Wetlaufer et al. (1964)	M	
	8.5×10^{-6}		McAuliffe (1963)	M	226
	8.3×10^{-6}		Duchowicz et al. (2020)	V	186
	8.3×10^{-6}		HSDB (2015)	V	
	8.3×10^{-6}		Mackay et al. (2006a)	V	
	8.3×10^{-6}		Mackay et al. (1993)	V	
	8.4×10^{-6}		Hine and Mookerjee (1975)	V	
	9.7×10^{-6}		Irmann (1965)	V	
	8.5×10^{-6}		Yaws (2003)	X	237
	1.3×10^{-5}		Hayer et al. (2022)	Q	20
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	8.3×10^{-5}		Wang et al. (2017)	Q	80, 238
	5.3×10^{-6}		Wang et al. (2017)	Q	80, 239
	2.0×10^{-5}		Wang et al. (2017)	Q	80, 240
	3.1×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
	5.6×10^{-6}		Hilal et al. (2008)	Q	
	5.8×10^{-6}		Modarresi et al. (2007)	Q	67
		3300	Kühne et al. (2005)	Q	
	3.7×10^{-6}		Modarresi et al. (2005)	Q	247
	8.4×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	8.4×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	9.8×10^{-6}		Yao et al. (2002)	Q	229, 267
	1.0×10^{-5}		English and Carroll (2001)	Q	230, 231
	1.5×10^{-5}		Katritzky et al. (1998)	Q	
	1.1×10^{-5}		Suzuki et al. (1992)	Q	232
	1.0×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	1.1×10^{-5}		Irmann (1965)	Q	
		2900	Kühne et al. (2005)	?	
	8.6×10^{-6}		Yaws (1999)	?	21
	9.1×10^{-6}	2700	Yaws et al. (1999)	?	21
	8.5×10^{-6}		Yaws and Yang (1992)	?	21
	8.0×10^{-6}		Abraham et al. (1990)	?	
	7.9×10^{-6}		Abraham (1979)	?	
pentane C_5H_{12} [109-66-0] OFBQJSOFQDEBGM-UHFFFAOYSA-N	7.2×10^{-6}	3900	Brockbank (2013)	L	1, 268
	8.7×10^{-6}	3500	Plyasunov and Shock (2000)	L	
	8.0×10^{-6}	3400	Abraham and Matteoli (1988)	L	
	8.0×10^{-6}		Mackay and Shiu (1981)	L	
	8.7×10^{-6}	3400	Jou and Mather (2000)	M	269, 270
	8.2×10^{-6}	3600	Jönsson et al. (1982)	M	
	7.8×10^{-6}		Rytting et al. (1978)	M	
	7.8×10^{-6}		Mackay et al. (2006a)	V	

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.8×10^{-6}		Mackay et al. (1993)	V	
	8.3×10^{-6}		Eastcott et al. (1988)	V	
	7.8×10^{-6}		Amoore and Buttery (1978)	V	
	7.9×10^{-6}		Hine and Mookerjee (1975)	V	
	8.3×10^{-6}		McAuliffe (1966)	V	225
	8.3×10^{-6}		McAuliffe (1963)	V	226
		3000	Gill et al. (1976)	T	
	7.8×10^{-6}		Yaws (2003)	X	258
	7.8×10^{-6}		Yaws (2003)	X	237
	1.3×10^{-5}		Dupeux et al. (2022)	Q	259
	4.9×10^{-5}		Keshavarz et al. (2022)	Q	
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	184
	6.5×10^{-5}		Wang et al. (2017)	Q	80, 238
	9.3×10^{-6}		Wang et al. (2017)	Q	80, 239
	1.7×10^{-5}		Wang et al. (2017)	Q	80, 240
	4.7×10^{-6}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	8.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
	9.9×10^{-6}		Hilal et al. (2008)	Q	
	6.6×10^{-6}		Modarresi et al. (2007)	Q	67
		3600	Kühne et al. (2005)	Q	
	3.1×10^{-6}		Modarresi et al. (2005)	Q	247
	8.4×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	1.5×10^{-5}		Yao et al. (2002)	Q	229
	8.0×10^{-6}		English and Carroll (2001)	Q	230, 231
	1.5×10^{-5}		Katritzky et al. (1998)	Q	
	1.0×10^{-5}		Suzuki et al. (1992)	Q	232
	9.9×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
	7.9×10^{-6}		Duchowicz et al. (2020)	?	185, 21
		4200	Kühne et al. (2005)	?	
	7.8×10^{-6}		Yaws (1999)	?	21
	5.1×10^{-6}		Abraham and Weathersby (1994)	?	21
	7.8×10^{-6}		Yaws and Yang (1992)	?	21
	8.0×10^{-6}		Abraham et al. (1990)	?	
2-methylbutane C_5H_{12} (isopentane) [78-78-4] QWTDNUCVQCZILF-UHFFFAOYSA-N	7.7×10^{-6}	3000	Plyasunov and Shock (2000)	L	
	7.2×10^{-6}		Mackay and Shiu (1981)	L	
	7.0×10^{-6}		Duchowicz et al. (2020)	V	186
	7.0×10^{-6}		HSDB (2015)	V	
	7.2×10^{-6}		Mackay et al. (2006a)	V	
	2.1×10^{-6}		Mackay et al. (1993)	V	
	7.2×10^{-6}		Eastcott et al. (1988)	V	
	7.2×10^{-6}		Cabani et al. (1981)	V	
	7.6×10^{-6}		McAuliffe (1966)	V	225
	7.6×10^{-6}		McAuliffe (1963)	V	226
	7.2×10^{-6}		Yaws (2003)	X	237

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	7.3×10^{-5}		Wang et al. (2017)	Q	80, 238
	6.0×10^{-6}		Wang et al. (2017)	Q	80, 239
	2.0×10^{-5}		Wang et al. (2017)	Q	80, 240
	3.8×10^{-6}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	271, 243
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	8.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
	6.4×10^{-6}		Hilal et al. (2008)	Q	
	7.2×10^{-6}		Modarresi et al. (2007)	Q	67
	3.8×10^{-6}		Modarresi et al. (2005)	Q	247
	5.8×10^{-6}		Yaffe et al. (2003)	Q	248, 272
	8.4×10^{-6}		Yao et al. (2002)	Q	229
	7.9×10^{-6}		English and Carroll (2001)	Q	230, 231
	1.5×10^{-5}		Katritzky et al. (1998)	Q	
	8.4×10^{-6}		Nirmalakhandan et al. (1997)	Q	
	7.2×10^{-6}		Yaws (1999)	?	21
	7.2×10^{-6}		Yaws and Yang (1992)	?	21
dimethylpropane	6.0×10^{-6}	3000	Plyasunov and Shock (2000)	L	
$C(CH_3)_4$	2.7×10^{-6}		Mackay and Shiu (1981)	L	
(neopentane)	5.9×10^{-6}	3300	Wilhelm et al. (1977)	L	
[463-82-1]	5.5×10^{-6}	2800	Shoor et al. (1969)	M	273
CRSOQBOWXPBRES-UHFFFAOYSA-N	4.7×10^{-6}		McAuliffe (1966)	M	
	6.3×10^{-6}	3200	Wetlaufer et al. (1964)	M	
	2.7×10^{-6}		Duchowicz et al. (2020)	V	186
	2.7×10^{-6}		HSDB (2015)	V	
	4.5×10^{-6}		Mackay et al. (2006a)	V	
	4.5×10^{-6}		Mackay et al. (1993)	V	
	4.5×10^{-6}		Hine and Mookerjee (1975)	V	
	4.7×10^{-6}		Yaws (2003)	X	237
	7.5×10^{-5}		Duchowicz et al. (2020)	Q	
	4.5×10^{-5}		Wang et al. (2017)	Q	80, 238
	2.1×10^{-6}		Wang et al. (2017)	Q	80, 239
	2.5×10^{-5}		Wang et al. (2017)	Q	80, 240
	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	8.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
	2.5×10^{-6}		Hilal et al. (2008)	Q	
	5.3×10^{-6}		Modarresi et al. (2007)	Q	67
		3600	Kühne et al. (2005)	Q	
	3.6×10^{-6}		Modarresi et al. (2005)	Q	247
	4.6×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	3.8×10^{-6}		Yao et al. (2002)	Q	229, 267
	8.0×10^{-6}		English and Carroll (2001)	Q	230, 274

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.4×10^{-5}		Katritzky et al. (1998)	Q	
	7.3×10^{-6}		Suzuki et al. (1992)	Q	232
	6.2×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
		3100	Kühne et al. (2005)	?	
	4.7×10^{-6}		Yaws (1999)	?	21
	4.7×10^{-6}		Yaws and Yang (1992)	?	21
	5.8×10^{-6}		Abraham et al. (1990)	?	
	5.9×10^{-6}		Abraham (1979)	?	
hexane C_6H_{14} [110-54-3] VLKZOEOYAKHREP-UHFFFAOYSA-N	5.7×10^{-6}	4400	Brockbank (2013)	L	1, 275
	6.9×10^{-6}	3800	Plyasunov and Shock (2000)	L	
	6.1×10^{-6}	3800	Abraham and Matteoli (1988)	L	
	5.9×10^{-6}		Mackay and Shiu (1981)	L	
	6.1×10^{-6}		Ryu and Park (1999)	M	
	7.4×10^{-6}		Park et al. (1997)	M	276
	2.4×10^{-4}	8700	Kolb et al. (1992)	M	277
	6.7×10^{-6}		Guitart et al. (1989)	M	14
	9.9×10^{-6}	7500	Ashworth et al. (1988)	M	278
	6.7×10^{-6}	4200	Tsonopoulos and Wilson (1983)	M	1
	5.9×10^{-6}	4000	Jönsson et al. (1982)	M	
	5.4×10^{-6}		Rytting et al. (1978)	M	
	5.5×10^{-6}		Duchowicz et al. (2020)	V	186
	5.5×10^{-6}		HSDB (2015)	V	
	5.5×10^{-6}		Mackay et al. (2006a)	V	
	5.5×10^{-6}		Mackay et al. (1993)	V	
	5.5×10^{-6}		Hwang et al. (1992)	V	
	7.1×10^{-6}		Eastcott et al. (1988)	V	
	6.1×10^{-6}		Cabani et al. (1981)	V	
	5.4×10^{-6}		Hine and Mookerjee (1975)	V	
	5.9×10^{-6}		McAuliffe (1966)	V	225
	5.9×10^{-6}		McAuliffe (1963)	V	226
	6.7×10^{-6}	3800	Plyasunov et al. (2001)	T	
		3800	Gill et al. (1976)	T	
	7.6×10^{-6}		Yaws (2003)	X	258
	7.6×10^{-6}		Yaws (2003)	X	237
	1.0×10^{-5}		Dupeux et al. (2022)	Q	259
	5.7×10^{-6}		Hayer et al. (2022)	Q	20
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	5.0×10^{-5}		Wang et al. (2017)	Q	80, 238
	6.9×10^{-6}		Wang et al. (2017)	Q	80, 239
	1.6×10^{-5}		Wang et al. (2017)	Q	80, 240
	2.3×10^{-5}		Li et al. (2014)	Q	241
	4.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	5.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
	7.7×10^{-6}		Hilal et al. (2008)	Q	

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.2×10^{-6}		Modarresi et al. (2007)	Q	67
		4000	Kühne et al. (2005)	Q	
	2.9×10^{-6}		Modarresi et al. (2005)	Q	247
	5.8×10^{-6}		Yaffe et al. (2003)	Q	248, 272
	6.0×10^{-6}		Yao et al. (2002)	Q	229
	6.2×10^{-6}		English and Carroll (2001)	Q	230, 231
	1.4×10^{-5}		Katritzky et al. (1998)	Q	
	1.4×10^{-5}		Russell et al. (1992)	Q	279
	7.9×10^{-6}		Suzuki et al. (1992)	Q	232
	7.9×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
		4100	Kühne et al. (2005)	?	
	7.6×10^{-6}		Yaws (1999)	?	21
	3.4×10^{-6}		Abraham and Weathersby (1994)	?	21
	7.6×10^{-6}		Yaws and Yang (1992)	?	21
	6.1×10^{-6}		Abraham et al. (1990)	?	
2-methylpentane	6.4×10^{-6}	4500	Brockbank (2013)	L	1
C_6H_{14}	5.7×10^{-6}	3900	Plyasunov and Shock (2000)	L	
(isohexane)	5.9×10^{-6}		Mackay and Shiu (1981)	L	
[107-83-5]	1.3×10^{-5}	960	Ashworth et al. (1988)	M	42, 278
AFABGHUZZDYHJO-UHFFFAOYSA-N	5.8×10^{-6}		Duchowicz et al. (2020)	V	186
	5.8×10^{-6}		HSDB (2015)	V	
	5.7×10^{-6}		Mackay et al. (2006a)	V	
	5.7×10^{-6}		Mackay et al. (1993)	V	
	5.7×10^{-6}		Eastcott et al. (1988)	V	
	5.7×10^{-6}		Hine and Mookerjee (1975)	V	
	6.0×10^{-6}		McAuliffe (1966)	V	225
	6.0×10^{-6}		McAuliffe (1963)	V	226
			Staudinger and Roberts (1996)	R	280
	5.7×10^{-6}		Yaws (2003)	X	237
	6.2×10^{-6}		Hilal et al. (2008)	C	
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	6.0×10^{-5}		Wang et al. (2017)	Q	80, 238
	4.5×10^{-6}		Wang et al. (2017)	Q	80, 239
	1.9×10^{-5}		Wang et al. (2017)	Q	80, 240
	3.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	5.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
	4.8×10^{-6}		Hilal et al. (2008)	Q	
	5.9×10^{-6}		Modarresi et al. (2007)	Q	67
		4000	Kühne et al. (2005)	Q	
	3.9×10^{-6}		Modarresi et al. (2005)	Q	247
	5.8×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	8.0×10^{-6}		Yao et al. (2002)	Q	229
	6.1×10^{-6}		English and Carroll (2001)	Q	230, 231
	1.4×10^{-5}		Katritzky et al. (1998)	Q	

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	7.0×10^{-6}		Suzuki et al. (1992)	Q	232
	6.7×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
		4000	Kühne et al. (2005)	?	
	5.7×10^{-6}		Yaws (1999)	?	21
	3.6×10^{-6}		Abraham and Weathersby (1994)	?	21
	5.7×10^{-6}		Yaws and Yang (1992)	?	21
3-methylpentane C_6H_{14} [96-14-0] PFEOZHBOMNWTJB-UHFFFAOYSA-N	5.9×10^{-6}		Brockbank (2013)	L	
	5.9×10^{-6}		Plyasunov and Shock (2000)	L	
	5.8×10^{-6}		Mackay and Shiu (1981)	L	
	5.9×10^{-6}		Duchowicz et al. (2020)	V	186
	5.8×10^{-6}		HSDB (2015)	V	
	5.9×10^{-6}		Mackay et al. (2006a)	V	
	5.9×10^{-6}		Mackay et al. (1993)	V	
	5.9×10^{-6}		Eastcott et al. (1988)	V	
	5.8×10^{-6}		Hine and Mookerjee (1975)	V	
	6.0×10^{-6}		McAuliffe (1966)	V	
	8.2×10^{-6}		Yaws (2003)	X	237
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	6.0×10^{-5}		Wang et al. (2017)	Q	80, 238
	5.8×10^{-6}		Wang et al. (2017)	Q	80, 239
	1.9×10^{-5}		Wang et al. (2017)	Q	80, 240
	4.1×10^{-6}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	271, 243
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	5.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
	6.2×10^{-6}		Hilal et al. (2008)	Q	
	7.0×10^{-6}		Modarresi et al. (2007)	Q	67
		4000	Kühne et al. (2005)	Q	
	3.1×10^{-6}		Modarresi et al. (2005)	Q	247
	5.8×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	6.7×10^{-6}		Yao et al. (2002)	Q	229
	6.1×10^{-6}		English and Carroll (2001)	Q	230, 260
	1.4×10^{-5}		Katritzky et al. (1998)	Q	
	7.2×10^{-6}		Suzuki et al. (1992)	Q	232
	7.0×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
		4700	Kühne et al. (2005)	?	
	8.2×10^{-6}		Yaws (1999)	?	21
	3.7×10^{-6}		Abraham and Weathersby (1994)	?	21
	8.8×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2-dimethylbutane	5.7×10^{-6}		Brockbank (2013)	L	
C_6H_{14}	5.6×10^{-6}	3500	Plyasunov and Shock (2000)	L	
[75-83-2]	5.8×10^{-6}		Mackay and Shiu (1981)	L	
HNRMPXKDFBEGFZ-UHFFFAOYSA-N	6.5×10^{-6}		Duchowicz et al. (2020)	V	186
	5.8×10^{-6}		HSDB (2015)	V	
	5.0×10^{-6}		Mackay et al. (2006a)	V	
	5.0×10^{-6}		Mackay et al. (1993)	V	
	5.8×10^{-6}		Eastcott et al. (1988)	V	
	5.1×10^{-6}		Hine and Mookerjee (1975)	V	
	5.5×10^{-6}		McAuliffe (1966)	V	225
	5.5×10^{-6}		McAuliffe (1963)	V	226
	6.5×10^{-6}		Yaws (2003)	X	237
	7.5×10^{-5}		Duchowicz et al. (2020)	Q	
	4.0×10^{-5}		Wang et al. (2017)	Q	80, 238
	2.8×10^{-6}		Wang et al. (2017)	Q	80, 239
	2.5×10^{-5}		Wang et al. (2017)	Q	80, 240
	2.7×10^{-6}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	271, 243
	3.1×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-6}		Gharagheizi et al. (2010)	Q	246
	3.4×10^{-6}		Hilal et al. (2008)	Q	
	7.2×10^{-6}		Modarresi et al. (2007)	Q	67
	3.9×10^{-6}		Modarresi et al. (2005)	Q	247
	5.3×10^{-6}		Yaffe et al. (2003)	Q	248, 272
	3.4×10^{-6}		Yao et al. (2002)	Q	229
	6.2×10^{-6}		English and Carroll (2001)	Q	230, 231
	1.3×10^{-5}		Katritzky et al. (1998)	Q	
	6.0×10^{-6}		Suzuki et al. (1992)	Q	232
	5.3×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
	6.5×10^{-6}		Yaws (1999)	?	21
	3.4×10^{-6}		Abraham and Weathersby (1994)	?	21
	6.5×10^{-6}		Yaws and Yang (1992)	?	21
2,3-dimethylbutane	8.0×10^{-6}	4400	Brockbank (2013)	L	1
C_6H_{14}	7.6×10^{-6}		Plyasunov and Shock (2000)	L	
[79-29-8]	7.7×10^{-6}		Mackay and Shiu (1981)	L	
ZFFMLCVRJBZUDZ-UHFFFAOYSA-N	8.4×10^{-6}		Duchowicz et al. (2020)	V	186
	8.2×10^{-6}		HSDB (2015)	V	
	6.9×10^{-6}		Mackay et al. (2006a)	V	
	6.9×10^{-6}		Mackay et al. (1993)	V	
	7.1×10^{-6}		Eastcott et al. (1988)	V	
	7.6×10^{-6}		Yaws (2003)	X	237
	6.7×10^{-5}		Duchowicz et al. (2020)	Q	
	6.8×10^{-5}		Wang et al. (2017)	Q	80, 238
	4.9×10^{-6}		Wang et al. (2017)	Q	80, 239
	2.2×10^{-5}		Wang et al. (2017)	Q	80, 240
	3.5×10^{-6}		Gharagheizi et al. (2012)	Q	

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	5.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
	5.3×10^{-6}		Hilal et al. (2008)	Q	
	7.6×10^{-6}		Modarresi et al. (2007)	Q	67
		4000	Kühne et al. (2005)	Q	
	5.2×10^{-6}		Modarresi et al. (2005)	Q	247
	7.7×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	4.2×10^{-6}		Yao et al. (2002)	Q	229
	6.1×10^{-6}		English and Carroll (2001)	Q	230, 274
	1.3×10^{-5}		Katritzky et al. (1998)	Q	
	5.8×10^{-6}		Nirmalakhandan et al. (1997)	Q	
		4200	Kühne et al. (2005)	?	
	7.6×10^{-6}		Yaws (1999)	?	21
	7.6×10^{-6}		Yaws and Yang (1992)	?	21
heptane	4.4×10^{-6}	4500	Brockbank (2013)	L	1
C_7H_{16}	4.9×10^{-6}	4200	Plyasunov and Shock (2000)	L	
[142-82-5]	4.4×10^{-6}	4100	Abraham and Matteoli (1988)	L	
IMNFDUFMRHMDMM-UHFFFAOYSA-N	4.3×10^{-6}		Mackay and Shiu (1981)	L	
	4.5×10^{-6}		Ryu and Park (1999)	M	
	5.5×10^{-6}		Park et al. (1997)	M	276
	1.2×10^{-5}	3700	Hansen et al. (1993)	M	281
	6.0×10^{-6}		Guitart et al. (1989)	M	14
	4.2×10^{-6}	4700	Jönsson et al. (1982)	M	
	4.8×10^{-6}		Rytting et al. (1978)	M	
	4.9×10^{-6}		Duchowicz et al. (2020)	V	186
	5.5×10^{-6}		HSDB (2015)	V	
	4.8×10^{-6}		Mackay et al. (2006a)	V	
	4.8×10^{-6}		Mackay et al. (1993)	V	
	5.0×10^{-6}		Eastcott et al. (1988)	V	
	4.8×10^{-6}		Hine and Mookerjee (1975)	V	
	5.2×10^{-6}		McAuliffe (1966)	V	225
	5.2×10^{-6}		McAuliffe (1963)	V	226
	3.7×10^{-6}		Yaws (2003)	X	258
	3.7×10^{-6}		Yaws (2003)	X	237
	8.2×10^{-6}		Dupeux et al. (2022)	Q	259
	1.1×10^{-5}		Hayer et al. (2022)	Q	20
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	4.7×10^{-5}		Wang et al. (2017)	Q	80, 238
	4.9×10^{-6}		Wang et al. (2017)	Q	80, 239
	8.0×10^{-6}		Wang et al. (2017)	Q	80, 240
	4.1×10^{-6}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-6}		Raventos-Duran et al. (2010)	Q	271, 243
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	3.4×10^{-6}		Gharagheizi et al. (2010)	Q	246

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.4×10^{-6}		Hilal et al. (2008)	Q	
	5.3×10^{-6}		Modarresi et al. (2007)	Q	67
		4300	Kühne et al. (2005)	Q	
	2.4×10^{-6}		Modarresi et al. (2005)	Q	247
	4.1×10^{-6}		Yaffe et al. (2003)	Q	248, 272
	5.1×10^{-6}		Yao et al. (2002)	Q	229
	1.3×10^{-5}		Katritzky et al. (1998)	Q	
	6.5×10^{-6}		Russell et al. (1992)	Q	279
	6.0×10^{-6}		Suzuki et al. (1992)	Q	232
	6.2×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
		4900	Kühne et al. (2005)	?	
	3.7×10^{-6}		Yaws (1999)	?	21
	2.8×10^{-6}		Abraham and Weathersby (1994)	?	21
	3.6×10^{-6}		Yaws and Yang (1992)	?	21
	4.4×10^{-6}		Abraham et al. (1990)	?	
2-methylhexane C_7H_{16} (isoheptane) [591-76-4] GXDHCNNESPLIKD-UHFFFAOYSA-N	2.9×10^{-6}		Brockbank (2013)	L	
	2.9×10^{-6}		Plyasunov and Shock (2000)	L	
	2.9×10^{-6}		Mackay and Shiu (1981)	L	
	1.9×10^{-5}	-3600	Hansen et al. (1993)	M	281, 282
	2.9×10^{-6}		Duchowicz et al. (2020)	V	186
	2.9×10^{-6}		Mackay et al. (2006a)	V	
	2.9×10^{-6}		Mackay et al. (1993)	V	
	2.9×10^{-6}		Eastcott et al. (1988)	V	
	2.9×10^{-6}		Yaws (2003)	X	237
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	4.7×10^{-5}		Wang et al. (2017)	Q	80, 238
	3.2×10^{-6}		Wang et al. (2017)	Q	80, 239
	1.7×10^{-5}		Wang et al. (2017)	Q	80, 240
	3.2×10^{-6}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-6}		Raventos-Duran et al. (2010)	Q	271, 243
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	3.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
	3.7×10^{-6}		Hilal et al. (2008)	Q	
	5.2×10^{-6}		Modarresi et al. (2007)	Q	67
	2.8×10^{-6}		Modarresi et al. (2005)	Q	247
	2.9×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	3.4×10^{-6}		Yao et al. (2002)	Q	229
	1.3×10^{-5}		Katritzky et al. (1998)	Q	
	5.2×10^{-6}		Nirmalakhandan et al. (1997)	Q	
	2.9×10^{-6}		Yaws (1999)	?	21
	2.9×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methylhexane	3.2×10^{-6}		Brockbank (2013)	L	
C_7H_{16}	4.5×10^{-6}		Plyasunov and Shock (2000)	L	
[589-34-4]	4.2×10^{-6}		Mackay and Shiu (1981)	L	
VLJXXKKOSFGPHI-UHFFFAOYSA-N	6.0×10^{-6}		Duchowicz et al. (2020)	V	186
	4.0×10^{-6}		Mackay et al. (2006a)	V	
	4.0×10^{-6}		Mackay et al. (1993)	V	
	3.2×10^{-6}		Eastcott et al. (1988)	V	
	3.2×10^{-6}		Yaws (2003)	X	237
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	4.7×10^{-5}		Wang et al. (2017)	Q	80, 238
	3.8×10^{-6}		Wang et al. (2017)	Q	80, 239
	1.8×10^{-5}		Wang et al. (2017)	Q	80, 240
	3.6×10^{-6}		Gharagheizi et al. (2012)	Q	
	3.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
	4.5×10^{-6}		Hilal et al. (2008)	Q	
	6.1×10^{-6}		Modarresi et al. (2007)	Q	67
	2.7×10^{-6}		Modarresi et al. (2005)	Q	247
	4.1×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	3.4×10^{-6}		Yao et al. (2002)	Q	229
	4.6×10^{-6}		English and Carroll (2001)	Q	230, 231
	1.3×10^{-5}		Katritzky et al. (1998)	Q	
	5.3×10^{-6}		Nirmalakhandan et al. (1997)	Q	
	3.2×10^{-6}		Yaws (1999)	?	21
	2.5×10^{-6}		Abraham and Weathersby (1994)	?	21
	3.2×10^{-6}		Yaws and Yang (1992)	?	21
2,2-dimethylpentane	3.1×10^{-6}		Plyasunov and Shock (2000)	L	
C_7H_{16}	3.1×10^{-6}		Mackay and Shiu (1981)	L	
[590-35-2]	3.1×10^{-6}		Duchowicz et al. (2020)	V	186
CXOWYJMDMMMMJO-UHFFFAOYSA-N	3.1×10^{-6}		Mackay et al. (2006a)	V	
	3.1×10^{-6}		Mackay et al. (1993)	V	
	3.1×10^{-6}		Eastcott et al. (1988)	V	
	3.1×10^{-6}		Yaws (2003)	X	237
	7.5×10^{-5}		Duchowicz et al. (2020)	Q	
	2.4×10^{-6}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-6}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
	2.5×10^{-6}		Hilal et al. (2008)	Q	
	5.2×10^{-6}		Modarresi et al. (2007)	Q	67
	3.1×10^{-6}		Modarresi et al. (2005)	Q	247
	3.1×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	3.7×10^{-6}		Yao et al. (2002)	Q	229
	3.6×10^{-6}		English and Carroll (2001)	Q	230, 231
	1.2×10^{-5}		Katritzky et al. (1998)	Q	
	4.1×10^{-6}		Nirmalakhandan et al. (1997)	Q	
	3.1×10^{-6}		Yaws (1999)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.1×10^{-6}		Yaws and Yang (1992)	?	21
2,3-dimethylpentane	5.7×10^{-6}		Plyasunov and Shock (2000)	L	
C_7H_{16}	5.7×10^{-6}		Mackay and Shiu (1981)	L	
[565-59-3]	5.7×10^{-6}		Duchowicz et al. (2020)	V	186
WGECXQBGLLYSFP-UHFFFAOYSA-N	5.7×10^{-6}		Mackay et al. (1993)	V	
	5.7×10^{-6}		Eastcott et al. (1988)	V	
	5.7×10^{-6}		Yaws (2003)	X	237
	6.7×10^{-5}		Duchowicz et al. (2020)	Q	
	3.6×10^{-6}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-6}		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	3.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
	4.8×10^{-6}		Hilal et al. (2008)	Q	
	7.1×10^{-6}		Modarresi et al. (2007)	Q	67
	5.8×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	4.7×10^{-6}		English and Carroll (2001)	Q	230, 231
	1.2×10^{-5}		Katritzky et al. (1998)	Q	
	4.7×10^{-6}		Nirmalakhandan et al. (1997)	Q	
	5.7×10^{-6}		Yaws (1999)	?	21
	5.7×10^{-6}		Yaws and Yang (1992)	?	21
2,4-dimethylpentane	2.9×10^{-6}		Brockbank (2013)	L	
C_7H_{16}	3.3×10^{-6}		Plyasunov and Shock (2000)	L	
[108-08-7]	3.3×10^{-6}		Mackay and Shiu (1981)	L	
BZHMBWZPUJHVEE-UHFFFAOYSA-N	5.2×10^{-6}		Duchowicz et al. (2020)	V	186
	3.1×10^{-6}		Mackay et al. (2006a)	V	
	3.1×10^{-6}		Mackay et al. (1993)	V	
	3.4×10^{-6}		Eastcott et al. (1988)	V	
	3.1×10^{-6}		Hine and Mookerjee (1975)	V	
	3.1×10^{-6}		McAuliffe (1966)	V	
	3.3×10^{-6}		Yaws (2003)	X	237
	6.7×10^{-5}		Duchowicz et al. (2020)	Q	
	2.4×10^{-6}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-6}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	3.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
	2.2×10^{-6}		Hilal et al. (2008)	Q	
	5.2×10^{-6}		Modarresi et al. (2007)	Q	67
	3.0×10^{-6}		Modarresi et al. (2005)	Q	247
	5.3×10^{-6}		Yaffe et al. (2003)	Q	248, 272
	4.0×10^{-6}		Yao et al. (2002)	Q	229
	4.7×10^{-6}		English and Carroll (2001)	Q	230, 274
	1.2×10^{-5}		Katritzky et al. (1998)	Q	
	4.7×10^{-6}		Suzuki et al. (1992)	Q	232
	4.5×10^{-6}		Nirmalakhandan and Speece (1988)	Q	

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.4×10^{-6}		Yaws (1999)	?	21
	3.3×10^{-6}		Yaws and Yang (1992)	?	21
3,3-dimethylpentane	5.6×10^{-6}	3000	Brockbank (2013)	L	1, 283
C_7H_{16}	5.3×10^{-6}		Plyasunov and Shock (2000)	L	
[562-49-2]	5.4×10^{-6}		Mackay and Shiu (1981)	L	
AEXMKKGTQYQZCS-UHFFFAOYSA-N	5.4×10^{-6}		Duchowicz et al. (2020)	V	186
	5.4×10^{-6}		Mackay et al. (2006a)	V	
	5.4×10^{-6}		Mackay et al. (1993)	V	
	5.4×10^{-6}		Eastcott et al. (1988)	V	
	5.4×10^{-6}		Yaws (2003)	X	237
	7.5×10^{-5}		Duchowicz et al. (2020)	Q	
	3.3×10^{-6}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
	4.0×10^{-6}		Hilal et al. (2008)	Q	
	7.5×10^{-6}		Modarresi et al. (2007)	Q	67
		4300	Kühne et al. (2005)	Q	
	3.5×10^{-6}		Modarresi et al. (2005)	Q	247
	5.3×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	2.8×10^{-6}		Yao et al. (2002)	Q	229
	3.6×10^{-6}		English and Carroll (2001)	Q	230, 231
	1.2×10^{-5}		Katritzky et al. (1998)	Q	
	4.4×10^{-6}		Nirmalakhandan et al. (1997)	Q	
		3000	Kühne et al. (2005)	?	
	5.4×10^{-6}		Yaws (1999)	?	21
	5.3×10^{-6}		Yaws and Yang (1992)	?	21
3-ethylpentane	3.8×10^{-6}		Yaws (2003)	X	237
C_7H_{16}	3.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[617-78-7]	3.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
AORMDLNPRGXHHL-UHFFFAOYSA-N	5.3×10^{-6}		Hilal et al. (2008)	Q	
	2.5×10^{-6}		Modarresi et al. (2005)	Q	247
	4.8×10^{-6}		Yao et al. (2002)	Q	229, 267
	3.8×10^{-6}		Yaws (1999)	?	21
	3.9×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3-trimethylbutane	3.2×10^{-6}		Mackay et al. (2006a)	V	
C_7H_{16}	3.2×10^{-6}		Mackay et al. (1993)	V	
[464-06-2]	4.2×10^{-6}		Yaws (2003)	X	237
ZISSAWUMDACLOM-UHFFFAOYSA-N	2.8×10^{-6}		Gharagheizi et al. (2012)	Q	
	3.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
	3.3×10^{-6}		Hilal et al. (2008)	Q	
	7.2×10^{-6}		Modarresi et al. (2007)	Q	67
	3.1×10^{-6}		Modarresi et al. (2005)	Q	247
	3.1×10^{-6}		Yaffe et al. (2003)	Q	248, 272
	1.8×10^{-6}		Yao et al. (2002)	Q	229
	4.2×10^{-6}		Yaws (1999)	?	21
	4.1×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
octane	3.4×10^{-6}	5300	Brockbank (2013)	L	1
C_8H_{18}	4.0×10^{-6}	4600	Plyasunov and Shock (2000)	L	
[111-65-9]	3.1×10^{-6}	4300	Abraham and Matteoli (1988)	L	
TVMXDCGIABBOFY-UHFFFAOYSA-N	3.3×10^{-6}		Mackay and Shiu (1981)	L	
	3.4×10^{-6}		Ryu and Park (1999)	M	
	3.3×10^{-6}		Park et al. (1997)	M	276
	3.0×10^{-5}	8000	Hansen et al. (1993)	M	281
	3.1×10^{-6}	4100	Heidman et al. (1985)	M	1
	2.9×10^{-6}	5400	Jönsson et al. (1982)	M	
	3.1×10^{-6}		Rytting et al. (1978)	M	
	3.1×10^{-6}		Duchowicz et al. (2020)	V	186
	3.1×10^{-6}		HSDB (2015)	V	
	8.6×10^{-7}		Abraham and Acree (2007)	V	
	3.2×10^{-6}		Mackay et al. (2006a)	V	
	3.8×10^{-6}	4800	Sarraute et al. (2004)	V	
	3.2×10^{-6}		Mackay et al. (1993)	V	
	3.0×10^{-6}		Hwang et al. (1992)	V	
	3.1×10^{-6}		Meylan and Howard (1991)	V	
	3.2×10^{-6}		Eastcott et al. (1988)	V	
	3.1×10^{-6}		Hine and Mookerjee (1975)	V	
	3.1×10^{-6}		Mackay and Leinonen (1975)	V	
	3.9×10^{-6}		McAuliffe (1966)	V	225
	3.9×10^{-6}		McAuliffe (1963)	V	226
	2.0×10^{-6}		Yaws (2003)	X	258
	2.0×10^{-6}		Yaws (2003)	X	237
	6.8×10^{-6}		Dupeux et al. (2022)	Q	259
	2.8×10^{-5}		Hayer et al. (2022)	Q	20
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	3.6×10^{-5}		Wang et al. (2017)	Q	80, 238
	3.4×10^{-6}		Wang et al. (2017)	Q	80, 239
	4.2×10^{-6}		Wang et al. (2017)	Q	80, 240
	3.1×10^{-6}		Li et al. (2014)	Q	241
	3.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	2.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
	3.9×10^{-6}		Hilal et al. (2008)	Q	
	4.6×10^{-6}		Modarresi et al. (2007)	Q	67
		4700	Kühne et al. (2005)	Q	
	2.9×10^{-6}		Yaffe et al. (2003)	Q	248, 272
	3.7×10^{-6}		English and Carroll (2001)	Q	230, 231
	1.2×10^{-5}		Katritzky et al. (1998)	Q	
	2.6×10^{-6}		Russell et al. (1992)	Q	279
	4.6×10^{-6}		Suzuki et al. (1992)	Q	232
	3.3×10^{-6}		Meylan and Howard (1991)	Q	
	5.0×10^{-6}		Nirmalakhandan and Speece (1988)	Q	

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Table A2.1: Alkanes (. . . continued)

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		5400	Kühne et al. (2005)	?	
	2.0×10^{-6}		Yaws (1999)	?	21
	2.0×10^{-6}		Abraham and Weathersby (1994)	?	21
	2.0×10^{-6}		Yaws and Yang (1992)	?	21
	3.1×10^{-6}		Abraham et al. (1990)	?	
2-methylheptane	2.9×10^{-6}		Mackay et al. (2006a)	V	
C_8H_{18}	2.9×10^{-6}		Mackay et al. (1993)	V	
[592-27-8]	2.4×10^{-6}		Yaws (2003)	X	237
JVSWJIKNEAIKJW-UHFFFAOYSA-N	2.8×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
	2.7×10^{-6}		Hilal et al. (2008)	Q	
	2.1×10^{-6}		Modarresi et al. (2005)	Q	247
	3.1×10^{-6}		Yao et al. (2002)	Q	229, 267
	2.4×10^{-6}		Yaws (1999)	?	21
	2.7×10^{-6}		Hoff et al. (1993)	?	21
	2.7×10^{-6}		Yaws and Yang (1992)	?	21
3-methylheptane	2.6×10^{-6}		Brockbank (2013)	L	
C_8H_{18}	2.7×10^{-6}		Plyasunov and Shock (2000)	L	
[589-81-1]	2.7×10^{-6}		Mackay and Shiu (1981)	L	
LAIUFBWHERIJIH-UHFFFAOYSA-N	2.7×10^{-6}		Duchowicz et al. (2020)	V	186
	2.7×10^{-6}		Eastcott et al. (1988)	V	
	2.6×10^{-6}		Yaws (2003)	X	237
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	3.0×10^{-6}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
	3.3×10^{-6}		Hilal et al. (2008)	Q	
	5.5×10^{-6}		Modarresi et al. (2007)	Q	67
	2.0×10^{-6}		Modarresi et al. (2005)	Q	247
	2.9×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	3.0×10^{-6}		Yao et al. (2002)	Q	229
	3.6×10^{-6}		English and Carroll (2001)	Q	230, 260
	4.2×10^{-6}		Nirmalakhandan et al. (1997)	Q	
	2.7×10^{-6}		Yaws (1999)	?	21
	2.7×10^{-6}		Yaws and Yang (1992)	?	21
4-methylheptane	2.7×10^{-6}		Brockbank (2013)	L	
C_8H_{18}	2.4×10^{-6}		Yaws (2003)	X	237
[589-53-7]	2.9×10^{-6}		Gharagheizi et al. (2012)	Q	
CHBAWFGIXDBEBT-UHFFFAOYSA-N	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
	3.0×10^{-6}		Hilal et al. (2008)	Q	
	2.2×10^{-6}		Modarresi et al. (2005)	Q	247
	2.7×10^{-6}		Yao et al. (2002)	Q	229
	2.4×10^{-6}		Yaws (1999)	?	21
	2.7×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2-dimethylhexane	2.4×10^{-6}	4600	Brockbank (2013)	L	1
C_8H_{18}	2.4×10^{-6}	4600	Dohányosová et al. (2004)	M	284
[590-73-8]	2.7×10^{-7}		Duchowicz et al. (2020)	V	186
FLTJDUOFAQWHDF-UHFFFAOYSA-N	2.7×10^{-6}		Yaws (2003)	X	237
	7.5×10^{-5}		Duchowicz et al. (2020)	Q	
	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
	1.9×10^{-6}		Hilal et al. (2008)	Q	
		4700	Kühne et al. (2005)	Q	
	4.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.8×10^{-6}		Yao et al. (2002)	Q	229
		5100	Kühne et al. (2005)	?	
	2.7×10^{-6}		Yaws (1999)	?	21
	2.9×10^{-6}		Yaws and Yang (1992)	?	21
2,3-dimethylhexane	2.4×10^{-6}		Yaws (2003)	X	237
C_8H_{18}	2.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[584-94-1]	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
JXPOLSKBTUYKJB-UHFFFAOYSA-N	3.4×10^{-6}		Hilal et al. (2008)	Q	
	2.4×10^{-6}		Yaws (1999)	?	21
	2.6×10^{-6}		Yaws and Yang (1992)	?	21
2,4-dimethylhexane	2.6×10^{-6}		Yaws (2003)	X	237
C_8H_{18}	2.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[589-43-5]	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
HDGQICNBXPAKLR-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	2.6×10^{-6}		Yaws (1999)	?	21
	2.8×10^{-6}		Yaws and Yang (1992)	?	21
2,5-dimethylhexane	3.1×10^{-6}	4000	Brockbank (2013)	L	1, 285
C_8H_{18}	2.4×10^{-6}	4000	Dohányosová et al. (2004)	M	286
[592-13-2]	2.6×10^{-6}		Yaws (2003)	X	237
UWNADWZGEHDQAB-UHFFFAOYSA-N	2.2×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
	1.7×10^{-6}		Hilal et al. (2008)	Q	
		4700	Kühne et al. (2005)	Q	
	2.4×10^{-6}		Modarresi et al. (2005)	Q	247
	2.3×10^{-6}		Yao et al. (2002)	Q	229
		4700	Kühne et al. (2005)	?	
	2.7×10^{-6}		Yaws (1999)	?	21
	2.9×10^{-6}		Yaws and Yang (1992)	?	21
3,3-dimethylhexane	2.4×10^{-6}		Yaws (2003)	X	237
C_8H_{18}	2.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[563-16-6]	2.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
KUMXLFIBWFCMOJ-UHFFFAOYSA-N	2.9×10^{-6}		Hilal et al. (2008)	Q	
	1.9×10^{-6}		Modarresi et al. (2005)	Q	247
	1.5×10^{-6}		Yao et al. (2002)	Q	229
	2.4×10^{-6}		Yaws (1999)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.6×10^{-6}		Yaws and Yang (1992)	?	21
3,4-dimethylhexane	2.2×10^{-6}		Yaws (2003)	X	237
C_8H_{18}	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
[583-48-2]	3.8×10^{-6}		Hilal et al. (2008)	Q	
RNTWWGNZUXGTAX-UHFFFAOYSA-N	2.3×10^{-6}		Yaws (1999)	?	21
	2.4×10^{-6}		Yaws and Yang (1992)	?	21
3-ethylhexane	2.3×10^{-6}		Yaws (2003)	X	237
C_8H_{18}	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
[619-99-8]	3.7×10^{-6}		Hilal et al. (2008)	Q	
SFRKSDZMZHIISH-UHFFFAOYSA-N	2.3×10^{-6}		Yaws (1999)	?	21
	2.6×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3-trimethylpentane	2.4×10^{-6}		Yaws (2003)	X	237
C_8H_{18}	2.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[564-02-3]	2.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
XTDQDBVBDLYELW-UHFFFAOYSA-N	2.7×10^{-6}		Hilal et al. (2008)	Q	
	7.3×10^{-6}		Modarresi et al. (2007)	Q	67
	2.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.7×10^{-6}		Yao et al. (2002)	Q	229
	2.4×10^{-6}		Yaws (1999)	?	21
	2.6×10^{-6}		Yaws and Yang (1992)	?	21
2,2,4-trimethylpentane	3.0×10^{-6}		Plyasunov and Shock (2000)	L	
C_8H_{18}	3.0×10^{-6}		Mackay and Shiu (1981)	L	
(isooctane)	4.6×10^{-6}		Guitart et al. (1989)	M	14
[540-84-1]	3.3×10^{-6}		Mackay et al. (2006a)	V	
NHTMVDHEPJAVLT-UHFFFAOYSA-N	3.3×10^{-6}		Mackay et al. (1993)	V	
	3.1×10^{-6}		Eastcott et al. (1988)	V	
	3.3×10^{-6}		Hine and Mookerjee (1975)	V	
	3.2×10^{-6}		Mackay and Leinonen (1975)	V	
	3.6×10^{-6}		McAuliffe (1966)	V	225
	3.6×10^{-6}		McAuliffe (1963)	V	226
	2.8×10^{-6}		Yaws (2003)	X	237
	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	3.3×10^{-6}		Zhang et al. (2010)	Q	287, 288
	1.7×10^{-6}		Zhang et al. (2010)	Q	287, 289
	2.2×10^{-5}		Zhang et al. (2010)	Q	287, 290
	1.6×10^{-5}		Zhang et al. (2010)	Q	287, 291
	2.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
	1.2×10^{-6}		Hilal et al. (2008)	Q	
	4.8×10^{-6}		Modarresi et al. (2007)	Q	67
		4700	Kühne et al. (2005)	Q	
	3.4×10^{-6}		Modarresi et al. (2005)	Q	247
	6.2×10^{-6}		Yaffe et al. (2003)	Q	248, 272

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.0×10^{-6}		Yao et al. (2002)	Q	229
	3.7×10^{-6}		English and Carroll (2001)	Q	230, 274
	3.1×10^{-6}		Suzuki et al. (1992)	Q	232
	2.9×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
		4000	Kühne et al. (2005)	?	
	2.9×10^{-6}		Yaws (1999)	?	21
	2.9×10^{-6}		Yaws and Yang (1992)	?	21
2,3,3-trimethylpentane	2.1×10^{-6}		Yaws (2003)	X	237
C_8H_{18}	3.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[560-21-4]	2.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
OKVWYBALHQFVFP-UHFFFAOYSA-N	3.6×10^{-6}		Hilal et al. (2008)	Q	
	2.0×10^{-6}		Modarresi et al. (2005)	Q	247
	1.6×10^{-6}		Yao et al. (2002)	Q	229
	2.2×10^{-6}		Yaws (1999)	?	21
	2.4×10^{-6}		Yaws and Yang (1992)	?	21
2,3,4-trimethylpentane	3.3×10^{-6}		Brockbank (2013)	L	
C_8H_{18}	4.3×10^{-6}		Plyasunov and Shock (2000)	L	
[565-75-3]	5.3×10^{-6}		Mackay and Shiu (1981)	L	
RLPGDEORIPLBNF-UHFFFAOYSA-N			Mackay et al. (2006a)	V	292
	4.9×10^{-6}		Mackay et al. (1993)	V	
	5.6×10^{-6}		Eastcott et al. (1988)	V	
	5.6×10^{-6}		Yaws (2003)	X	237
	2.9×10^{-6}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
	3.1×10^{-6}		Hilal et al. (2008)	Q	
	7.0×10^{-6}		Modarresi et al. (2007)	Q	67
		4700	Kühne et al. (2005)	Q	
	2.0×10^{-6}		Modarresi et al. (2005)	Q	247
	5.3×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	2.1×10^{-6}		Yao et al. (2002)	Q	229
	3.7×10^{-6}		English and Carroll (2001)	Q	230, 231
	1.1×10^{-5}		Katritzky et al. (1998)	Q	
	3.2×10^{-6}		Nirmalakhandan et al. (1997)	Q	
		4900	Kühne et al. (2005)	?	
	5.6×10^{-6}		Yaws (1999)	?	21
	5.6×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2-methylpentane	2.3×10^{-6}		Yaws (2003)	X	237
C_8H_{18}	3.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[609-26-7]	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
DUPUVYJQZSLSJB-UHFFFAOYSA-N	3.6×10^{-6}		Hilal et al. (2008)	Q	
	2.2×10^{-6}		Modarresi et al. (2005)	Q	247
	2.5×10^{-6}		Yao et al. (2002)	Q	229
	2.3×10^{-6}		Yaws (1999)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.6×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-3-methylpentane	2.1×10^{-6}		Yaws (2003)	X	237
C_8H_{18}	3.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[1067-08-9]	2.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
GIEZWIDCIFCQPS-UHFFFAOYSA-N	4.5×10^{-6}		Hilal et al. (2008)	Q	
	2.0×10^{-6}		Modarresi et al. (2005)	Q	247
	2.2×10^{-6}		Yao et al. (2002)	Q	229
	2.1×10^{-6}		Yaws (1999)	?	21
	2.3×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3,3-tetramethylbutane	3.3×10^{-6}		Yaws (2003)	X	237
C_8H_{18}	2.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[594-82-1]	2.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
OMMLUKLXGSRPHK-UHFFFAOYSA-N	3.4×10^{-6}		Hilal et al. (2008)	Q	
	2.6×10^{-6}		Yaws and Yang (1992)	?	21
nonane	2.3×10^{-6}	6600	Brockbank (2013)	L	1, 293
C_9H_{20}	2.1×10^{-6}		Plyasunov and Shock (2000)	L	
[111-84-2]	2.0×10^{-6}		Mackay and Shiu (1981)	L	
BKIMMITUMNQMOS-UHFFFAOYSA-N	2.2×10^{-6}		Ryu and Park (1999)	M	
	1.9×10^{-6}		Park et al. (1997)	M	276
	2.3×10^{-5}	190	Ashworth et al. (1988)	M	42, 278
	1.8×10^{-6}	7300	Jönsson et al. (1982)	M	
	2.9×10^{-6}		Duchowicz et al. (2020)	V	186
	2.9×10^{-6}		HSDB (2015)	V	
	3.0×10^{-6}		Mackay et al. (2006a)	V	
	3.0×10^{-6}		Mackay et al. (1993)	V	
	1.7×10^{-6}		Eastcott et al. (1988)	V	
	2.0×10^{-6}		Abraham (1984)	V	
	1.6×10^{-6}		Yaws (2003)	X	237
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	2.9×10^{-5}		Wang et al. (2017)	Q	80, 238
	2.5×10^{-6}		Wang et al. (2017)	Q	80, 239
	2.3×10^{-5}		Wang et al. (2017)	Q	80, 240
	3.0×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-6}		Raventos-Duran et al. (2010)	Q	271, 243
	3.9×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	1.8×10^{-6}		Gharagheizi et al. (2010)	Q	246
	3.0×10^{-6}		Hilal et al. (2008)	Q	
	4.3×10^{-6}		Modarresi et al. (2007)	Q	67
		5000	Kühne et al. (2005)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	247
	2.0×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	4.6×10^{-6}		Yao et al. (2002)	Q	229
	1.1×10^{-5}		Katritzky et al. (1998)	Q	
	3.8×10^{-6}		Nirmalakhandan et al. (1997)	Q	
		4100	Kühne et al. (2005)	?	

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
2-methyloctane	1.6×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[3221-61-2]	1.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
ZUBZATZOEPUUQF-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	2.1×10^{-6}		Modarresi et al. (2005)	Q	247
	3.3×10^{-6}		Yao et al. (2002)	Q	229
	1.6×10^{-6}		Yaws (1999)	?	21
	2.1×10^{-6}		Yaws and Yang (1992)	?	21
3-methyloctane	1.5×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[2216-33-3]	1.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
SEEOMASXHIJCDV-UHFFFAOYSA-N	2.4×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	247
	2.8×10^{-6}		Yao et al. (2002)	Q	229
	1.5×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21
4-methyloctane	9.7×10^{-7}		Plyasunov and Shock (2000)	L	
C_9H_{20}	1.0×10^{-6}		Mackay and Shiu (1981)	L	
[2216-34-4]	9.9×10^{-7}		Duchowicz et al. (2020)	V	186
DOGIHOCMZJUJNR-UHFFFAOYSA-N	9.9×10^{-7}		Eastcott et al. (1988)	V	
	9.8×10^{-7}		Yaws (2003)	X	237
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	2.4×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-6}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
	2.3×10^{-6}		Hilal et al. (2008)	Q	
	4.9×10^{-6}		Modarresi et al. (2007)	Q	67
	1.6×10^{-6}		Modarresi et al. (2005)	Q	247
	2.9×10^{-6}		Yao et al. (2002)	Q	229
	9.8×10^{-7}		Yaws (1999)	?	21
	9.9×10^{-7}		Yaws and Yang (1992)	?	21
2,3-dimethylheptane	1.4×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[3074-71-3]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
WBRFDUJXCLCKPX-UHFFFAOYSA-N	2.4×10^{-6}		Hilal et al. (2008)	Q	
	2.4×10^{-6}		Modarresi et al. (2005)	Q	247
	2.0×10^{-6}		Yao et al. (2002)	Q	229, 267
	1.5×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2-dimethylheptane	1.7×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[1071-26-7]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
PSABUFWDVWCFDP-UHFFFAOYSA-N	1.4×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	247
	2.0×10^{-6}		Yao et al. (2002)	Q	229
	1.7×10^{-6}		Yaws (1999)	?	21
	2.1×10^{-6}		Yaws and Yang (1992)	?	21
2,4-dimethylheptane	1.7×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[2213-23-2]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
AUKVIBNBLXQNIZ-UHFFFAOYSA-N	1.4×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	247
	1.8×10^{-6}		Yao et al. (2002)	Q	229
	1.7×10^{-6}		Yaws (1999)	?	21
	2.1×10^{-6}		Yaws and Yang (1992)	?	21
2,5-dimethylheptane	1.6×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[2216-30-0]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
HQZHQNKZOYIKQC-UHFFFAOYSA-N	1.5×10^{-6}		Hilal et al. (2008)	Q	
	2.0×10^{-6}		Yao et al. (2002)	Q	229
	1.6×10^{-6}		Yaws (1999)	?	21
	2.0×10^{-6}		Yaws and Yang (1992)	?	21
2,6-dimethylheptane	1.7×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[1072-05-5]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
KBPCCVWUMVGXGF-UHFFFAOYSA-N	1.2×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	247
	2.2×10^{-6}		Yao et al. (2002)	Q	229
	1.7×10^{-6}		Yaws (1999)	?	21
	2.1×10^{-6}		Yaws and Yang (1992)	?	21
3,3-dimethylheptane	2.3×10^{-6}		Hilal et al. (2008)	Q	
C_9H_{20}	1.9×10^{-6}		Yaws and Yang (1992)	?	21
[4032-86-4]					
BVAKDOXCVSMKHE-UHFFFAOYSA-N					
3,4-dimethylheptane	1.4×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[922-28-1]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
MAKRYGRRIKSDES-UHFFFAOYSA-N	2.6×10^{-6}		Hilal et al. (2008)	Q	
	1.7×10^{-6}		Modarresi et al. (2005)	Q	247
	1.6×10^{-6}		Yao et al. (2002)	Q	229
	1.4×10^{-6}		Yaws (1999)	?	21
	1.8×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,5-dimethylheptane	1.6×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[926-82-9]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
DZJTZGHZAWTWGA-UHFFFAOYSA-N	1.5×10^{-6}		Hilal et al. (2008)	Q	
	1.7×10^{-6}		Modarresi et al. (2005)	Q	247
	1.6×10^{-6}		Yao et al. (2002)	Q	229
	1.6×10^{-6}		Yaws (1999)	?	21
	2.0×10^{-6}		Yaws and Yang (1992)	?	21
4,4-dimethylheptane	1.5×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[1068-19-5]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
WSOKFYJGNBQDPW-UHFFFAOYSA-N	2.1×10^{-6}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	247
	1.5×10^{-6}		Yao et al. (2002)	Q	229
	1.5×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21
3-ethylheptane	1.4×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-80-4]	1.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
PSVQKOKKLWHNRP-UHFFFAOYSA-N	2.6×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	247
	2.4×10^{-6}		Yao et al. (2002)	Q	229
	1.4×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21
4-ethylheptane	1.5×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[2216-32-2]	1.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
XMROPFQWHHUFFS-UHFFFAOYSA-N	2.5×10^{-6}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	247
	2.8×10^{-6}		Yao et al. (2002)	Q	229
	1.5×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3-trimethylhexane	1.5×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-25-4]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
CBVFSZDQEHBJEQ-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	247
	9.0×10^{-7}		Yao et al. (2002)	Q	229
	1.5×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
2,2,4-trimethylhexane	1.7×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-26-5]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
AFTPEBDOGXRMNQ-UHFFFAOYSA-N	1.1×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	247
	1.0×10^{-6}		Yao et al. (2002)	Q	229
	1.7×10^{-6}		Yaws (1999)	?	21
	2.1×10^{-6}		Yaws and Yang (1992)	?	21
2,2,5-trimethylhexane	1.9×10^{-6}	6200	Brockbank (2013)	L	1
C_9H_{20}	2.8×10^{-6}		Plyasunov and Shock (2000)	L	
[3522-94-9]	2.9×10^{-6}		Mackay and Shiu (1981)	L	
HHOSMYBYIHNXNO-UHFFFAOYSA-N	4.1×10^{-6}		Mackay et al. (2006a)	V	
	4.1×10^{-6}		Mackay et al. (1993)	V	
	4.1×10^{-6}		Cabani et al. (1981)	V	
	3.9×10^{-6}		McAuliffe (1966)	V	
	1.8×10^{-6}		Yaws (2003)	X	237
	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
	9.0×10^{-7}		Hilal et al. (2008)	Q	
	1.7×10^{-6}		Modarresi et al. (2005)	Q	247
	2.9×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	1.5×10^{-6}		Yao et al. (2002)	Q	229
	2.2×10^{-6}		Nirmalakhandan et al. (1997)	Q	
	1.8×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21
2,3,3-trimethylhexane	1.4×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-28-7]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
DJYSEQMMCZAKGT-UHFFFAOYSA-N	2.4×10^{-6}		Hilal et al. (2008)	Q	
	2.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.0×10^{-6}		Yao et al. (2002)	Q	229
	1.4×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
2,3,4-trimethylhexane	1.4×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[921-47-1]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
RUTNOQHQISEBGT-UHFFFAOYSA-N	2.6×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	247
	1.1×10^{-6}		Yao et al. (2002)	Q	229
	1.4×10^{-6}		Yaws (1999)	?	21
	1.8×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,5-trimethylhexane	1.7×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[1069-53-0]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
ODGLTLJZCVNPBU-UHFFFAOYSA-N	1.4×10^{-6}		Hilal et al. (2008)	Q	
	2.1×10^{-6}		Modarresi et al. (2005)	Q	247
	1.1×10^{-6}		Yao et al. (2002)	Q	229, 267
	2.8×10^{-6}		English and Carroll (2001)	Q	230, 231
	1.7×10^{-6}		Yaws (1999)	?	21
	2.0×10^{-6}		Yaws and Yang (1992)	?	21
2,4,4-trimethylhexane	1.5×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-30-1]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
SVEMKBCPZYWEPH-UHFFFAOYSA-N	1.4×10^{-6}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	247
	1.1×10^{-6}		Yao et al. (2002)	Q	229
	1.5×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21
3,3,4-trimethylhexane	1.3×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-31-2]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
ARWOOWBJJKVYOV-UHFFFAOYSA-N	2.9×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	247
	1.1×10^{-6}		Yao et al. (2002)	Q	229
	1.3×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2-methylhexane	1.5×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[16789-46-1]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
MVLOWDRGPHBNNF-UHFFFAOYSA-N	2.3×10^{-6}		Hilal et al. (2008)	Q	
	2.2×10^{-6}		Modarresi et al. (2005)	Q	247
	1.2×10^{-6}		Yao et al. (2002)	Q	229
	1.5×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21
4-ethyl-2-methylhexane	1.6×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[3074-75-7]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
KYCZJIBOPKRSOV-UHFFFAOYSA-N	1.5×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	247
	1.5×10^{-6}		Yao et al. (2002)	Q	229, 267
	1.7×10^{-6}		Yaws (1999)	?	21
	2.0×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-3-methylhexane	1.3×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[3074-76-8]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
CYWROHZCELEGSE-UHFFFAOYSA-N	3.2×10^{-6}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	247
	1.2×10^{-6}		Yao et al. (2002)	Q	229
	1.3×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-4-methylhexane	1.4×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[3074-77-9]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
OKCRKWVABWILDR-UHFFFAOYSA-N	3.1×10^{-6}		Hilal et al. (2008)	Q	
	1.9×10^{-6}		Modarresi et al. (2005)	Q	247
	1.2×10^{-6}		Yao et al. (2002)	Q	229
	1.4×10^{-6}		Yaws (1999)	?	21
	1.8×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3,3-tetramethylpentane	1.2×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[7154-79-2]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
QUKOJKFJIHSBKV-UHFFFAOYSA-N	3.6×10^{-6}		Hilal et al. (2008)	Q	
	2.1×10^{-6}		Modarresi et al. (2005)	Q	247
	1.0×10^{-6}		Yao et al. (2002)	Q	229, 267
	1.2×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3,4-tetramethylpentane	1.4×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[1186-53-4]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
VZFMYOCAEQDWDY-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	247
	2.8×10^{-6}		Yao et al. (2002)	Q	229
	1.4×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
2,2,4,4-tetramethylpentane	1.7×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[1070-87-7]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
GUMULFRCHLJNDY-UHFFFAOYSA-N	9.0×10^{-7}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	247
	1.4×10^{-6}		Yao et al. (2002)	Q	229
	1.7×10^{-6}		Yaws (1999)	?	21
	1.9×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3,4-tetramethylpentane	1.2×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	3.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-38-9]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
JLCYYQOQSAMWTA-UHFFFAOYSA-N	2.7×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	247
	1.2×10^{-6}		Yao et al. (2002)	Q	229
	1.2×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,2-dimethylpentane	1.5×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-32-3]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
CLZCPQKGOAXOJT-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	247
	1.6×10^{-6}		Yao et al. (2002)	Q	229, 267
	1.5×10^{-6}		Yaws (1999)	?	21
	1.8×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,3-dimethylpentane	1.2×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	3.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-33-4]	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
MMASVVOQIKCFJZ-UHFFFAOYSA-N	3.5×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Modarresi et al. (2005)	Q	247
	1.6×10^{-6}		Yao et al. (2002)	Q	229
	1.2×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,4-dimethylpentane	1.4×10^{-6}		Yaws (2003)	X	237
C_9H_{20}	2.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[1068-87-7]	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
VLHAGZNBWKUMRW-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	2.0×10^{-6}		Modarresi et al. (2005)	Q	247
	1.8×10^{-6}		Yao et al. (2002)	Q	229
	1.4×10^{-6}		Yaws (1999)	?	21
	1.8×10^{-6}		Yaws and Yang (1992)	?	21
3,3-diethylpentane		4900	Abraham and Nasehzadeh (1981)	R	
C_9H_{20}	1.1×10^{-6}		Yaws (2003)	X	237
[1067-20-5]	3.4×10^{-6}		Gharagheizi et al. (2012)	Q	
BGXXXYLRPIRDHJ-UHFFFAOYSA-N	1.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
	4.1×10^{-6}		Hilal et al. (2008)	Q	
	2.0×10^{-6}		Modarresi et al. (2005)	Q	247
	1.7×10^{-6}		Yao et al. (2002)	Q	229
	1.1×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
	9.5×10^{-6}		Abraham et al. (1990)	?	
	9.4×10^{-6}		Abraham (1979)	?	

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
decane	1.3×10^{-6}		Brockbank (2013)	L	
$C_{10}H_{22}$	1.1×10^{-6}		Plyasunov and Shock (2000)	L	
[124-18-5]	1.4×10^{-6}		Mackay and Shiu (1981)	L	
DIOQZVSQGTUSAI-UHFFFAOYSA-N	1.9×10^{-6}		Duchowicz et al. (2020)	V	186
	1.9×10^{-6}		HSDB (2015)	V	
	2.1×10^{-6}		Mackay et al. (2006a)	V	
	2.1×10^{-6}		Mackay et al. (1993)	V	
	2.0×10^{-6}		Hwang et al. (1992)	V	
	2.3×10^{-6}		Eastcott et al. (1988)	V	
	1.9×10^{-6}		Abraham (1984)	V	
	1.9×10^{-6}		Yaws (2003)	X	258
	1.9×10^{-6}		Yaws (2003)	X	237
	4.4×10^{-6}		Dupeux et al. (2022)	Q	259
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	2.3×10^{-5}		Wang et al. (2017)	Q	80, 238
	1.7×10^{-6}		Wang et al. (2017)	Q	80, 239
	6.5×10^{-6}		Wang et al. (2017)	Q	80, 240
	3.7×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-6}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
	2.2×10^{-6}		Hilal et al. (2008)	Q	
	3.8×10^{-6}		Modarresi et al. (2007)	Q	67
	2.0×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	2.2×10^{-6}		English and Carroll (2001)	Q	230, 231
	1.0×10^{-5}		Katritzky et al. (1998)	Q	
	2.9×10^{-6}		Nirmalakhandan et al. (1997)	Q	
	1.9×10^{-6}		Yaws (1999)	?	21
	2.1×10^{-6}		Yaws and Yang (1992)	?	21
2-methylnonane	1.2×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[871-83-0]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
SGVYKUFIHHTIFL-UHFFFAOYSA-N	1.5×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	3.1×10^{-6}		Yao et al. (2002)	Q	229, 267
	1.2×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
3-methylnonane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[5911-04-6]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
PLZDDPSCZHRBOY-UHFFFAOYSA-N	1.7×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	2.8×10^{-6}		Yao et al. (2002)	Q	229
	1.1×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[17301-94-9]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
IALRSQMWHFKJJA-UHFFFAOYSA-N	1.6×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	2.7×10^{-6}		Yao et al. (2002)	Q	229
	1.0×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
5-methylnonane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-85-9]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
TYSIILFJZXHVPU-UHFFFAOYSA-N	1.7×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	4.2×10^{-6}		Yao et al. (2002)	Q	229
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
2,2-dimethyloctane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-87-1]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
GPBUTTSWJNPYJL-UHFFFAOYSA-N	1.3×10^{-6}		Hilal et al. (2008)	Q	
	1.1×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
2,3-dimethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[7146-60-3]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
YPMNDMUOGQJCLW-UHFFFAOYSA-N	1.7×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	1.6×10^{-6}		Yao et al. (2002)	Q	229
	1.0×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
2,4-dimethyloctane	1.2×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[4032-94-4]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
IXAVTTRPEXFVSX-UHFFFAOYSA-N	1.2×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.7×10^{-6}		Yao et al. (2002)	Q	229
	1.2×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

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2,5-dimethyloctane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-89-3]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
HOAAQUNESXYFDT-UHFFFAOYSA-N	1.3×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	2.0×10^{-6}		Yao et al. (2002)	Q	229, 267
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
2,6-dimethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[2051-30-1]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
ZALHPSXXQIPKTQ-UHFFFAOYSA-N	1.2×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.8×10^{-6}		Yao et al. (2002)	Q	229
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
2,7-dimethyloctane	1.2×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[1072-16-8]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
KEVMYFLMMDUPJE-UHFFFAOYSA-N	1.0×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	1.9×10^{-6}		Yao et al. (2002)	Q	229
	1.2×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
3,3-dimethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[4110-44-5]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
DBULLUBYDONGLT-UHFFFAOYSA-N	1.7×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.4×10^{-6}		Yao et al. (2002)	Q	229
	1.0×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
3,4-dimethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-92-8]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
QQCWGAMGBCGAQJ-UHFFFAOYSA-N	2.0×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	1.6×10^{-6}		Yao et al. (2002)	Q	229
	1.0×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,5-dimethyloctane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-93-9]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
VRHRGVJOUHJULC-UHFFFAOYSA-N	1.4×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	1.6×10^{-6}		Yao et al. (2002)	Q	229
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
3,6-dimethyloctane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-94-0]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
JEEQUUSFXYRPRK-UHFFFAOYSA-N	1.3×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	1.6×10^{-6}		Yao et al. (2002)	Q	229
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
4,4-dimethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-95-1]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
ZMEDGZAGMLTROM-UHFFFAOYSA-N	1.5×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.4×10^{-6}		Yao et al. (2002)	Q	229, 267
	1.1×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
4,5-dimethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-96-2]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
DOYJTLUPPPUSMD-UHFFFAOYSA-N	2.1×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.4×10^{-6}		Yao et al. (2002)	Q	229
	1.0×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyloctane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[5881-17-4]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
OEYGTUAKNZFCDJ-UHFFFAOYSA-N	2.2×10^{-6}		Hilal et al. (2008)	Q	
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
4-ethyloctane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[15869-86-0]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
NRJUFUBKIFIKFI-UHFFFAOYSA-N	2.4×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	2.8×10^{-6}		Yao et al. (2002)	Q	229
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,3-trimethylheptane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[52896-92-1]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
ACYHSTUWOQNWCX-UHFFFAOYSA-N	1.6×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	9.4×10^{-7}		Yao et al. (2002)	Q	229
	1.0×10^{-6}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
2,2,4-trimethylheptane	1.2×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[14720-74-2]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
IIYGOARYARWJBO-UHFFFAOYSA-N	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.0×10^{-6}		Yao et al. (2002)	Q	229
	1.2×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
2,2,5-trimethylheptane	1.2×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[20291-95-6]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
GZJFAWOTMWATOS-UHFFFAOYSA-N	1.5×10^{-6}		Modarresi et al. (2005)	Q	247
	1.1×10^{-6}		Yao et al. (2002)	Q	229, 267
	1.2×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
2,2,6-trimethylheptane	1.2×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[1190-83-6]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
FHJCGIUZJXWNET-UHFFFAOYSA-N	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	1.3×10^{-6}		Yao et al. (2002)	Q	229
	1.3×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
2,3,3-trimethylheptane	9.5×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[52896-93-2]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
QACXEXNKLFWKLK-UHFFFAOYSA-N	1.6×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	9.7×10^{-7}		Yao et al. (2002)	Q	229
	9.5×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
2,3,4-trimethylheptane	9.9×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[52896-95-4]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
UVVYAKOLFKEZEE-UHFFFAOYSA-N	1.6×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	9.0×10^{-7}		Yao et al. (2002)	Q	229
	9.9×10^{-7}		Yaws (1999)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
2,3,5-trimethylheptane	9.5×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[20278-85-7]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
YKPNYFKOKKKGNM-UHFFFAOYSA-N	1.1×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	1.1×10^{-6}		Yao et al. (2002)	Q	229
	9.5×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
2,3,6-trimethylheptane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[4032-93-3]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
IHPXJGBVRWFEJB-UHFFFAOYSA-N	1.1×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	1.2×10^{-6}		Yao et al. (2002)	Q	229
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
2,4,4-trimethylheptane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[4032-92-2]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
QALGVLROELGEEM-UHFFFAOYSA-N	1.1×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	8.6×10^{-7}		Yao et al. (2002)	Q	229
	1.1×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
2,4,5-trimethylheptane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[20278-84-6]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
YMBNRMDSLJNNPF-UHFFFAOYSA-N	1.1×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	9.0×10^{-7}		Yao et al. (2002)	Q	229, 267
	1.1×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
2,4,6-trimethylheptane	1.3×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[2613-61-8]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
YNLBBDHDNIXQNL-UHFFFAOYSA-N	7.5×10^{-7}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.0×10^{-6}		Yao et al. (2002)	Q	229
	1.3×10^{-6}		Yaws (1999)	?	21
	1.8×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,5,5-trimethylheptane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[1189-99-7]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
SOYLPZSOEXZMLE-UHFFFAOYSA-N	1.1×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.2×10^{-6}		Yao et al. (2002)	Q	229
	1.1×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
3,3,4-trimethylheptane	9.0×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[20278-87-9]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
WRBHKVWLEIYLDZ-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	7.6×10^{-7}		Yao et al. (2002)	Q	229
	9.0×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21
3,3,5-trimethylheptane	9.9×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[7154-80-5]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
VRVRZZWPKABUOE-UHFFFAOYSA-N	1.2×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	8.3×10^{-7}		Yao et al. (2002)	Q	229
	1.0×10^{-6}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
3,4,4-trimethylheptane	9.0×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[20278-88-0]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
BLNBSBLKPFFJKQ-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	7.7×10^{-7}		Yao et al. (2002)	Q	229
	9.0×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21
3,4,5-trimethylheptane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[20278-89-1]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
LJIIBBYARMPSMT-UHFFFAOYSA-N	2.3×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	8.9×10^{-7}		Yao et al. (2002)	Q	229
	9.4×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-2-methylheptane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[14676-29-0]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
NKMJCVVUYDKHAV-UHFFFAOYSA-N	2.0×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.4×10^{-6}		Yao et al. (2002)	Q	229
	1.0×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
4-ethyl-2-methylheptane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[52896-88-5]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
OJDKRASKNKPYDH-UHFFFAOYSA-N	1.4×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.5×10^{-6}		Yao et al. (2002)	Q	229
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
5-ethyl-2-methylheptane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[13475-78-0]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
DGEMPTLPTFNEHJ-UHFFFAOYSA-N	1.4×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	1.5×10^{-6}		Yao et al. (2002)	Q	229
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-3-methylheptane	9.1×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-01-1]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
HSOMNBKXPGCNBH-UHFFFAOYSA-N	2.2×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.3×10^{-6}		Yao et al. (2002)	Q	229, 267
	9.2×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
4-ethyl-3-methylheptane	9.8×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[52896-89-6]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
BTGGSWBKRYMHQK-UHFFFAOYSA-N	2.2×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	1.2×10^{-6}		Yao et al. (2002)	Q	229
	9.8×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-5-methylheptane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[52896-90-9]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
VXARVYMIZCGZGG-UHFFFAOYSA-N	1.3×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.6×10^{-6}		Yao et al. (2002)	Q	229
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-4-methylheptane	9.7×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[52896-91-0]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
JZBKRUIGSVOOIC-UHFFFAOYSA-N	2.2×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.1×10^{-6}		Yao et al. (2002)	Q	229
	9.8×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
4-ethyl-4-methylheptane	9.5×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-04-4]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
MPYQJQDSICRCJJ-UHFFFAOYSA-N	2.4×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.0×10^{-6}		Yao et al. (2002)	Q	229
	9.5×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
4-propylheptane	1.2×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[3178-29-8]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
ABYGSZMCWVXFCQ-UHFFFAOYSA-N	1.6×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	2.6×10^{-6}		Yao et al. (2002)	Q	229
	1.2×10^{-6}		Yaws (1999)	?	21
	1.7×10^{-6}		Yaws and Yang (1992)	?	21
4-(1-methylethyl)-heptane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
(4-isopropylheptane)	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
[52896-87-4]	2.1×10^{-6}		Hilal et al. (2008)	Q	
AZLAWGCUDHUQDB-UHFFFAOYSA-N	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	2.0×10^{-6}		Yao et al. (2002)	Q	229
	1.0×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,3,3-tetramethylhexane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[13475-81-5]	9.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
RMQHJMMCLSJULX-UHFFFAOYSA-N	1.8×10^{-6}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	247
	4.9×10^{-7}		Yao et al. (2002)	Q	229
	8.4×10^{-7}		Yaws (1999)	?	21
	1.2×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3,4-tetramethylhexane	8.7×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-08-2]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
MHPSPNGWFAGBNH-UHFFFAOYSA-N	1.2×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	5.9×10^{-7}		Yao et al. (2002)	Q	229
	8.7×10^{-7}		Yaws (1999)	?	21
	1.2×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3,5-tetramethylhexane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-09-3]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
GCFKTDRTZYDRBI-UHFFFAOYSA-N	8.4×10^{-7}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	6.6×10^{-7}		Yao et al. (2002)	Q	229, 267
	1.1×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
2,2,4,4-tetramethylhexane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[51750-65-3]	9.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
PXHNHTBJHHSVPT-UHFFFAOYSA-N	8.8×10^{-7}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	6.5×10^{-7}		Yao et al. (2002)	Q	229
	8.3×10^{-7}		Yaws (1999)	?	21
	1.1×10^{-6}		Yaws and Yang (1992)	?	21
2,2,4,5-tetramethylhexane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-42-5]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
KDRZICOOQNIJDN-UHFFFAOYSA-N	8.0×10^{-7}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	7.3×10^{-7}		Yao et al. (2002)	Q	229
	1.1×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,5,5-tetramethylhexane	1.4×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	8.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[1071-81-4]	9.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
HXQDUXXBVMMIKL-UHFFFAOYSA-N	4.6×10^{-7}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	247
	1.1×10^{-6}		Yao et al. (2002)	Q	229
	1.4×10^{-6}		Yaws (1999)	?	21
	1.8×10^{-6}		Yaws and Yang (1992)	?	21
2,3,3,4-tetramethylhexane	7.9×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-10-6]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
HIHSOGFAVTVMCY-UHFFFAOYSA-N	1.4×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	6.0×10^{-7}		Yao et al. (2002)	Q	229
	7.9×10^{-7}		Yaws (1999)	?	21
	1.2×10^{-6}		Yaws and Yang (1992)	?	21
2,3,3,5-tetramethylhexane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-11-7]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
GCGFXFIPOBRMQT-UHFFFAOYSA-N	9.2×10^{-7}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	5.9×10^{-7}		Yao et al. (2002)	Q	229
	1.0×10^{-6}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
2,3,4,4-tetramethylhexane	8.2×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-12-8]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
XDRDDPSGUQMOBO-UHFFFAOYSA-N	1.3×10^{-6}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	247
	6.3×10^{-7}		Yao et al. (2002)	Q	229
	8.3×10^{-7}		Yaws (1999)	?	21
	1.2×10^{-6}		Yaws and Yang (1992)	?	21
2,3,4,5-tetramethylhexane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-15-1]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
BHGNYYIOYPFWKC-UHFFFAOYSA-N	1.2×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	6.6×10^{-7}		Yao et al. (2002)	Q	229, 267
	1.0×10^{-6}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3,4,4-tetramethylhexane	6.6×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[5171-84-6]	9.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
MCEYLFHKATVXLN-UHFFFAOYSA-N	2.2×10^{-6}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Modarresi et al. (2005)	Q	247
	6.2×10^{-7}		Yao et al. (2002)	Q	229
	6.7×10^{-7}		Yaws (1999)	?	21
	1.0×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,2-dimethylhexane	9.8×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[20291-91-2]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
XYDYODCWVCBIOQ-UHFFFAOYSA-N	1.8×10^{-6}		Hilal et al. (2008)	Q	
	1.8×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	7.1×10^{-7}		Yao et al. (2002)	Q	229
	9.8×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
4-ethyl-2,2-dimethylhexane	1.2×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[52896-99-8]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
QHLDBFLIDFTHQI-UHFFFAOYSA-N	1.1×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	9.9×10^{-7}		Yao et al. (2002)	Q	229
	1.2×10^{-6}		Yaws (1999)	?	21
	1.6×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,3-dimethylhexane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-00-4]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
PJIFKODHGMUPFH-UHFFFAOYSA-N	2.0×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	6.6×10^{-7}		Yao et al. (2002)	Q	229
	8.6×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21
4-ethyl-2,3-dimethylhexane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-01-5]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
RHMRCCBCYFAZIK-UHFFFAOYSA-N	1.6×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	7.2×10^{-7}		Yao et al. (2002)	Q	229
	9.5×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-2,4-dimethylhexane	9.5×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[7220-26-0]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
OSKIMJMPFNLVOU-UHFFFAOYSA-N	1.6×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	7.1×10^{-7}		Yao et al. (2002)	Q	229, 267
	9.5×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
4-ethyl-2,4-dimethylhexane	9.1×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-03-7]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
SIKFMUYSQCEQOO-UHFFFAOYSA-N	1.3×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	7.2×10^{-7}		Yao et al. (2002)	Q	229
	9.1×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,5-dimethylhexane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-04-8]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
UJEUVDLASLOZIV-UHFFFAOYSA-N	1.1×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.1×10^{-6}		Yao et al. (2002)	Q	229
	1.1×10^{-6}		Yaws (1999)	?	21
	1.5×10^{-6}		Yaws and Yang (1992)	?	21
4-ethyl-3,3-dimethylhexane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-05-9]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
ZRTXVJYJVBTXHE-UHFFFAOYSA-N	1.9×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	7.3×10^{-7}		Yao et al. (2002)	Q	229
	8.6×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-3,4-dimethylhexane	8.6×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-06-0]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
ZGJCTUKRTSBTIQ-UHFFFAOYSA-N	2.2×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	7.7×10^{-7}		Yao et al. (2002)	Q	229
	8.6×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3-diethylhexane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-02-2]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
WWNGLKDLYKNGGT-UHFFFAOYSA-N	3.4×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	7.7×10^{-7}		Yao et al. (2002)	Q	229
	8.5×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21
3,4-diethylhexane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[19398-77-7]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
VBZCRMTUDYIWIH-UHFFFAOYSA-N	1.8×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	7.9×10^{-7}		Yao et al. (2002)	Q	229
	9.3×10^{-7}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
2-methyl-3-(1-methylethyl)-hexane	7.5×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.2×10^{-6}		Gharagheizi et al. (2012)	Q	
(3-isopropyl-2-methylhexane)	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
[62016-13-1]	1.5×10^{-6}		Hilal et al. (2008)	Q	
YBOXGRMAQIYMGV-UHFFFAOYSA-N	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	8.5×10^{-7}		Yao et al. (2002)	Q	229, 267
	7.5×10^{-7}		Yaws (1999)	?	21
	1.1×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3,3,4-pentamethylpentane	6.8×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-44-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
WKQBIIUOSATALN-UHFFFAOYSA-N	1.3×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	8.8×10^{-7}		Yao et al. (2002)	Q	229, 267
	6.8×10^{-7}		Yaws (1999)	?	21
	1.0×10^{-6}		Yaws and Yang (1992)	?	21
2,2,3,4,4-pentamethylpentane	7.2×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-45-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
OWFKEHICSVOVAC-UHFFFAOYSA-N	8.6×10^{-7}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	1.0×10^{-6}		Yao et al. (2002)	Q	229
	7.2×10^{-7}		Yaws (1999)	?	21
	1.0×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-2,2,3-trimethylpentane	6.6×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-17-3]	9.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
AJDIFHIHSYVDGP-UHFFFAOYSA-N	2.1×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	9.2×10^{-7}		Yao et al. (2002)	Q	229
	6.6×10^{-7}		Yaws (1999)	?	21
	1.0×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,2,4-trimethylpentane	9.2×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-18-4]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
VLIZIVHXZXQRDE-UHFFFAOYSA-N	1.2×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	1.1×10^{-6}		Yao et al. (2002)	Q	229
	9.2×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21
3-ethyl-2,3,4-trimethylpentane	7.0×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-19-5]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
OHZNMGSGEFVFTI-UHFFFAOYSA-N	1.5×10^{-6}		Hilal et al. (2008)	Q	
	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.0×10^{-6}		Yao et al. (2002)	Q	229
	7.0×10^{-7}		Yaws (1999)	?	21
	1.1×10^{-6}		Yaws and Yang (1992)	?	21
3,3-diethyl-2-methylpentane	7.5×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	2.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[52897-16-2]	1.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
DSSAZLXYIQIXGW-UHFFFAOYSA-N	2.3×10^{-6}		Hilal et al. (2008)	Q	
	1.4×10^{-6}		Modarresi et al. (2005)	Q	247
	1.2×10^{-6}		Yao et al. (2002)	Q	229
	7.5×10^{-7}		Yaws (1999)	?	21
	1.1×10^{-6}		Yaws and Yang (1992)	?	21
2,4-dimethyl-3-(1-methylethyl)-pentane	9.1×10^{-7}		Yaws (2003)	X	237
$C_{10}H_{22}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
(2,4-dimethyl-3-isopropylpentane)	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
[13475-79-1]	1.0×10^{-6}		Hilal et al. (2008)	Q	
YVYHOOYMDHZALB-UHFFFAOYSA-N	1.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.2×10^{-6}		Yao et al. (2002)	Q	229
	9.2×10^{-7}		Yaws (1999)	?	21
	1.3×10^{-6}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
undecane	4.5×10^{-7}		Plyasunov and Shock (2000)	L	
$C_{11}H_{24}$	5.4×10^{-7}		Mackay and Shiu (1981)	L	
[1120-21-4]	5.1×10^{-6}		Duchowicz et al. (2020)	V	186
RSJKGSCJYJTIGS-UHFFFAOYSA-N	5.2×10^{-6}		HSDB (2015)	V	
	4.9×10^{-7}		Mackay et al. (2006a)	V	
	5.4×10^{-6}		Eastcott et al. (1988)	V	
	4.9×10^{-7}		Abraham (1984)	V	
	5.1×10^{-6}		Yaws (2003)	X	237
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	2.1×10^{-5}		Wang et al. (2017)	Q	80, 238
	1.2×10^{-6}		Wang et al. (2017)	Q	80, 239
	1.1×10^{-5}		Wang et al. (2017)	Q	80, 240
	4.4×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
	1.5×10^{-6}		Hilal et al. (2008)	Q	
	3.6×10^{-6}		Modarresi et al. (2007)	Q	67
	5.4×10^{-7}		Yaffe et al. (2003)	Q	248, 249
	3.4×10^{-6}		Yao et al. (2002)	Q	229, 267
	5.1×10^{-6}		Yaws (1999)	?	21
	5.4×10^{-6}		Yaws and Yang (1992)	?	21
2-methyldecane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	3.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[6975-98-0]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
CNPVJWYWYZMPDS-UHFFFAOYSA-N					
3-methyldecane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	2.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[13151-34-3]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
JJRUZTXRDDMYGM-UHFFFAOYSA-N					
4-methyldecane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	2.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[2847-72-5]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
DVWZNKLWPILULD-UHFFFAOYSA-N					
5-methyldecane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	2.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[13151-35-4]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
QUYFPNWYGLFQQU-UHFFFAOYSA-N					
2,2-dimethylnonane	9.7×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-14-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
WDSBVMLUILIJOW-UHFFFAOYSA-N					
2,3-dimethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[2884-06-2]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
IGJRNTLDWLTHCQ-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4-dimethylnonane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-24-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
JZUUOAUSQCXSTN-UHFFFAOYSA-N					
2,5-dimethylnonane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-27-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
NQUMJENPNGXAIH-UHFFFAOYSA-N					
2,6-dimethylnonane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-28-2]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
MGNGOEWESNDQAN-UHFFFAOYSA-N					
2,7-dimethylnonane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-29-3]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
QYQSPINNJUXEDY-UHFFFAOYSA-N					
2,8-dimethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-30-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
FZFRYQHIQUEAAV-UHFFFAOYSA-N					
3,3-dimethylnonane	9.5×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-15-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
HTRYNYZYFGHKDV-UHFFFAOYSA-N					
3,4-dimethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-22-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
PAXLEVPLFYBSQJ-UHFFFAOYSA-N					
3,5-dimethylnonane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-25-9]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
BAFVBVRBYKSWCE-UHFFFAOYSA-N					
3,6-dimethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-31-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
YHLBUWVGPXILSW-UHFFFAOYSA-N					
3,7-dimethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-32-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
YGPVLXJHRFZYJJ-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,4-dimethylnonane	9.9×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-18-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
HARRKRKVTQABSF-UHFFFAOYSA-N					
4,5-dimethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-23-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
JDNGDDOTBYZAGS-UHFFFAOYSA-N					
4,6-dimethylnonane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-26-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
JZKWOUUZMBTBDO-UHFFFAOYSA-N					
5,5-dimethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[6414-96-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
BEPKYSJVUZWKMP-UHFFFAOYSA-N					
3-ethylnonane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-11-3]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
FKJSIWPQZCKMIL-UHFFFAOYSA-N					
4-ethylnonane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[5911-05-7]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
UGCQDCMVAKKTQG-UHFFFAOYSA-N					
5-ethylnonane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-12-4]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
QPOVZYGNFWRMJE-UHFFFAOYSA-N					
2,2,3-trimethyloctane	9.0×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-26-6]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
XZPXMWMVWDSEMY-UHFFFAOYSA-N					
2,2,4-trimethyloctane	9.9×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[18932-14-4]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
IKMGZPRUMVFYBK-UHFFFAOYSA-N					
2,2,5-trimethyloctane	9.9×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62016-27-7]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
CSVNISDVBYGXME-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

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2,2,6-trimethyloctane	9.6×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-28-8]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
NBIHFQKVSFKHGH-UHFFFAOYSA-N					
2,2,7-trimethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62016-29-9]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
QGQAHVJOBYNMFN-UHFFFAOYSA-N					
2,3,3-trimethyloctane	8.7×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-30-2]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
KFYWDCDWVPXXCA-UHFFFAOYSA-N					
2,3,4-trimethyloctane	9.7×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-31-3]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
SJQAEXCGOLTHPG-UHFFFAOYSA-N					
2,3,5-trimethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-32-4]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
CEOHXVQAHFSSEG-UHFFFAOYSA-N					
2,3,6-trimethyloctane	9.7×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-33-5]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
MNFBUNLEXRMWOY-UHFFFAOYSA-N					
2,3,7-trimethyloctane	9.8×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-34-6]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
XJKKSYAVEVAGFX-UHFFFAOYSA-N					
2,4,4-trimethyloctane	9.9×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62016-35-7]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
CJXXTMYWNCYKHU-UHFFFAOYSA-N					
2,4,5-trimethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-36-8]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
UJYGOBMOHSFJQP-UHFFFAOYSA-N					
2,4,6-trimethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-37-9]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
XHNIFDXYGLPJLP-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4,7-trimethyloctane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62016-38-0]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
DUHKHXHIPOGMOW-UHFFFAOYSA-N					
2,5,5-trimethyloctane	9.8×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62016-39-1]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
DZKJZWAIBSEZKB-UHFFFAOYSA-N					
2,5,6-trimethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-14-2]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
VHBZECSWMWWTMQ-UHFFFAOYSA-N					
2,6,6-trimethyloctane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[54166-32-4]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
RUPXAIGHLDMSOL-UHFFFAOYSA-N					
3,3,4-trimethyloctane	8.7×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-40-4]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
IJVIFYHTPQSPSW-UHFFFAOYSA-N					
3,3,5-trimethyloctane	9.6×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-41-5]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
BEFCOJKHEMBPSK-UHFFFAOYSA-N					
3,3,6-trimethyloctane	9.2×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-42-6]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
CFESHXNQRRYSED-UHFFFAOYSA-N					
3,4,4-trimethyloctane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-43-7]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
WWCBWKZBTINVDE-UHFFFAOYSA-N					
3,4,5-trimethyloctane	9.6×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-44-8]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
BPFOUTQNEVQSFR-UHFFFAOYSA-N					
3,4,6-trimethyloctane	9.8×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-45-9]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
RMGAENUTYIFEJO-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,5,5-trimethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-94-8]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
FVYNWISHVUNIOZ-UHFFFAOYSA-N					
4,4,5-trimethyloctane	8.9×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-95-9]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
QGCXVKCDWOOWTQ-UHFFFAOYSA-N					
2-methyl-3-ethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-16-4]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
ITDXDXCBDQBZEB-UHFFFAOYSA-N					
2-methyl-4-ethyloctane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-17-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
ZYEQSLLHBOITAM-UHFFFAOYSA-N					
2-methyl-5-ethyloctane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-18-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
CQCKNPUKBOITAX-UHFFFAOYSA-N					
2-methyl-6-ethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-19-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
AZXGABNJUBNOHW-UHFFFAOYSA-N					
3-methyl-3-ethyloctane	9.1×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-16-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
DQNINFLTCGTQGU-UHFFFAOYSA-N					
3-methyl-4-ethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-20-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
BTRAURWAFYPYMW-UHFFFAOYSA-N					
3-methyl-5-ethyloctane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-21-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
LZFCEXJTLLKGPW-UHFFFAOYSA-N					
3-methyl-6-ethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-22-2]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
FTQLPWORENXYAZ-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methyl-3-ethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-23-3]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
LXRSBMFQRZTMNK-UHFFFAOYSA-N					
4-methyl-4-ethyloctane	9.7×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-19-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
IXZULXYHNRHENR-UHFFFAOYSA-N					
4-methyl-5-ethyloctane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-24-4]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
DTSHQAHKLUTGAR-UHFFFAOYSA-N					
4-methyl-6-ethyloctane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-25-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
NXUUVZOGBPCPDV-UHFFFAOYSA-N					
4-propyloctane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-13-5]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
VFAMBAFLNKONTN-UHFFFAOYSA-N					
4-isopropyloctane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-15-3]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
VSJAVEFYQMREHJ-UHFFFAOYSA-N					
2,2,3,3-tetramethylheptane	7.5×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-40-4]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
YPGGGWSLWOECQF-UHFFFAOYSA-N					
2,2,3,4-tetramethylheptane	8.6×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-41-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
HPKDRGPKZGWSND-UHFFFAOYSA-N					
2,2,3,5-tetramethylheptane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-42-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
KXNFNEAZTWCHIL-UHFFFAOYSA-N					
2,2,3,6-tetramethylheptane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-43-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
AQHGQPHAJYTMDJ-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,4,4-tetramethylheptane	8.6×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-44-8]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
JMRHVFQTDSCACD-UHFFFAOYSA-N					
2,2,4,5-tetramethylheptane	9.5×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-45-9]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
MPDBIZNQOUSUIN-UHFFFAOYSA-N					
2,2,4,6-tetramethylheptane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	7.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-46-0]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
XSMHBEAIQLABAO-UHFFFAOYSA-N					
2,2,5,5-tetramethylheptane	9.1×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-47-1]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
VQJNSRPWQMPDDO-UHFFFAOYSA-N					
2,2,5,6-tetramethylheptane	9.5×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-48-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
ZYJXKOJVCNGFSL-UHFFFAOYSA-N					
2,2,6,6-tetramethylheptane	9.5×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	7.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[40117-45-1]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
GKNMBVVJQTWDRT-UHFFFAOYSA-N					
2,3,3,4-tetramethylheptane	8.0×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-49-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
OHIUILFTBGSFAG-UHFFFAOYSA-N					
2,3,3,5-tetramethylheptane	8.6×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-50-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
XGCFPCZVDOZHLT-UHFFFAOYSA-N					
2,3,3,6-tetramethylheptane	8.7×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-51-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
ZVRALCAHDAJURU-UHFFFAOYSA-N					
2,3,4,4-tetramethylheptane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-52-8]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
SXHQWTUVNZIMTP-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4,5-tetramethylheptane	9.1×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-53-9]	9.6×10^{-7}		Gharagheizi et al. (2010)	Q	246
LGUFKOOYNDNVNP-UHFFFAOYSA-N					
2,3,4,6-tetramethylheptane	9.6×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-54-0]	9.6×10^{-7}		Gharagheizi et al. (2010)	Q	246
WOHJQOFSYZPITE-UHFFFAOYSA-N					
2,3,5,5-tetramethylheptane	9.1×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-55-1]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
QSBIXVGCKCYBBL-UHFFFAOYSA-N					
2,3,5,6-tetramethylheptane	9.5×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[52670-32-3]	9.6×10^{-7}		Gharagheizi et al. (2010)	Q	246
RAHGVMDMAJFLTP-UHFFFAOYSA-N					
2,4,4,5-tetramethylheptane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-56-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
QALMSCCHYDFGLF-UHFFFAOYSA-N					
2,4,4,6-tetramethylheptane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-57-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
DTMSZIVVBLZFEV-UHFFFAOYSA-N					
2,4,5,5-tetramethylheptane	8.6×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-58-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
JVYVKEOAYQAABU-UHFFFAOYSA-N					
3,3,4,4-tetramethylheptane	7.2×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-59-5]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
CFNIIBCZVLNKPV-UHFFFAOYSA-N					
3,3,4,5-tetramethylheptane	8.1×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-60-8]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
QVCSKDHUHWRVTA-UHFFFAOYSA-N					
3,3,5,5-tetramethylheptane	7.5×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-61-9]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
GALDMESQGNRJGE-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4,4,5-tetramethylheptane	7.8×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-62-0]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
CXIAIMLBUJNNJR-UHFFFAOYSA-N					
2,2-dimethyl-3-ethylheptane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61869-03-2]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
SBWMIVQVGGUMCE-UHFFFAOYSA-N					
2,2-dimethyl-4-ethylheptane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	8.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62016-46-0]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
BJOUMNMMNSZESV-UHFFFAOYSA-N					
2,2-dimethyl-5-ethylheptane	9.8×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62016-47-1]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
HVVFIKMZXFNXKA-UHFFFAOYSA-N					
2,3-dimethyl-3-ethylheptane	8.9×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-21-1]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
KQUHXOYVQZYOOF-UHFFFAOYSA-N					
2,3-dimethyl-4-ethylheptane	9.8×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-22-2]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
CNEPAGDSOHLVRW-UHFFFAOYSA-N					
2,3-dimethyl-5-ethylheptane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-23-3]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
BFCKNSGKYWMUNP-UHFFFAOYSA-N					
2,4-dimethyl-3-ethylheptane	9.8×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-24-4]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
OBCGEYFMJYXFJV-UHFFFAOYSA-N					
2,4-dimethyl-4-ethylheptane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-25-5]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
OETKSNKIFXLJDO-UHFFFAOYSA-N					
2,4-dimethyl-5-ethylheptane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-26-6]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
RZHNOEUMKYRHIX-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,5-dimethyl-3-ethylheptane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-27-7]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
DEZOXTLNRYCKNK-UHFFFAOYSA-N					
2,5-dimethyl-4-ethylheptane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-28-8]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
CUHCBWKQRDWQMN-UHFFFAOYSA-N					
2,5-dimethyl-5-ethylheptane	9.1×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-29-9]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
GPZDEXDVXFJVLH-UHFFFAOYSA-N					
2,6-dimethyl-3-ethylheptane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-30-2]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
BFXHSWDHLPKFSH-UHFFFAOYSA-N					
2,6-dimethyl-4-ethylheptane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-31-3]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
GBSGJLJGXHBTQQ-UHFFFAOYSA-N					
3,3-dimethyl-4-ethylheptane	8.9×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-32-4]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
QXJXAHFNWHEQEU-UHFFFAOYSA-N					
3,3-dimethyl-5-ethylheptane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-33-5]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
FLLHBJKGZIOYAA-UHFFFAOYSA-N					
3,4-dimethyl-3-ethylheptane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-34-6]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
HKSCZRRMBTUZLO-UHFFFAOYSA-N					
3,4-dimethyl-4-ethylheptane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-35-7]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
RMVWUAZCGGWZKA-UHFFFAOYSA-N					
3,4-dimethyl-5-ethylheptane	9.5×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-36-8]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
PCRCVFLPWIQGNJ-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,5-dimethyl-3-ethylheptane	8.9×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-37-9]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
FQOCKNRDCVODKW-UHFFFAOYSA-N					
3,5-dimethyl-4-ethylheptane	9.6×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-38-0]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
IKVNPWSSYMJDKE-UHFFFAOYSA-N					
4,4-dimethyl-3-ethylheptane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-39-1]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
YMWPSGKMCMMFSS-UHFFFAOYSA-N					
2-methyl-4-propylheptane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-96-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
AXOUMHTUGUFOKF-UHFFFAOYSA-N					
3-methyl-4-propylheptane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-97-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
WAMROSASDOIVDE-UHFFFAOYSA-N					
4-methyl-4-propylheptane	9.9×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-20-4]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
RDZFGBZTNOYNAH-UHFFFAOYSA-N					
2-methyl-3-isopropylheptane	9.9×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[6876-18-2]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
GECZBVJYUAPYFD-UHFFFAOYSA-N					
2-methyl-4-isopropylheptane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-98-2]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
ADLZFTVQXMDTCY-UHFFFAOYSA-N					
3-methyl-4-isopropylheptane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-99-3]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
SRECVVXQFXRBNI-UHFFFAOYSA-N					
4-methyl-4-isopropylheptane	8.9×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61869-00-9]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
LSJZMBVEVGYTAG-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3-diethylheptane	9.1×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-17-9]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
XATIZWAWQAIMQJ-UHFFFAOYSA-N					
3,4-diethylheptane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61869-01-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
UWOPVDFSBGDRJR-UHFFFAOYSA-N					
3,5-diethylheptane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61869-02-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
OBHTWTQZINRNAB-UHFFFAOYSA-N					
4,4-diethylheptane	9.6×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-21-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
WDTMGYSKSAMSPF-UHFFFAOYSA-N					
4-*tert*-butylheptane	9.6×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[60302-21-8]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
MDOHZJRFNISIIH-UHFFFAOYSA-N					
2,2,3,3,4-pentamethylhexane	6.6×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-85-7]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
RSEBTOONCGVAKN-UHFFFAOYSA-N					
2,2,3,3,5-pentamethylhexane	7.9×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-86-8]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
QGVXFIIZUSICQO-UHFFFAOYSA-N					
2,2,3,4,4-pentamethylhexane	6.5×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-87-9]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
HBVQLCKOFAUQGY-UHFFFAOYSA-N					
2,2,3,4,5-pentamethylhexane	8.2×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-88-0]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
LDUJDGROUWHEKU-UHFFFAOYSA-N					
2,2,3,5,5-pentamethylhexane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[14739-73-2]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
UKYAYXXQXKPIBL-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,4,4,5-pentamethylhexane	7.3×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[60302-23-0]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
JQFZWBZEZYOCQL-UHFFFAOYSA-N					
2,3,3,4,4-pentamethylhexane	6.4×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-89-1]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
GHRPCKCGHFDDOH-UHFFFAOYSA-N					
2,3,3,4,5-pentamethylhexane	7.5×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[52670-33-4]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
STMIMOZUYGUOQZ-UHFFFAOYSA-N					
2,2,3-trimethyl-3-ethylhexane	7.5×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-72-2]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
HUAYVWMWWLHZAB-UHFFFAOYSA-N					
2,2,3-trimethyl-4-ethylhexane	8.6×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-73-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
ZSUMTZIXJNZKBI-UHFFFAOYSA-N					
2,2,4-trimethyl-3-ethylhexane	8.7×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-74-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
UDUTWNYTAVENNO-UHFFFAOYSA-N					
2,2,4-trimethyl-4-ethylhexane	7.7×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-75-5]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
YFQDCXGMLYJDSG-UHFFFAOYSA-N					
2,2,5-trimethyl-3-ethylhexane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-76-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
GJVFOLLEVKEKMU-UHFFFAOYSA-N					
2,2,5-trimethyl-4-ethylhexane	9.9×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-77-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
UKTBERWYLDSZDQ-UHFFFAOYSA-N					
2,3,3-trimethyl-4-ethylhexane	7.9×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-78-8]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
DNDCULLMOLSZER-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4-trimethyl-3-ethylhexane	7.6×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-79-9]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
XCNOKZUAQAZTAJ-UHFFFAOYSA-N					
2,3,4-trimethyl-4-ethylhexane	8.2×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-80-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
HNNSQDJQJRTMMW-UHFFFAOYSA-N					
2,3,5-trimethyl-3-ethylhexane	8.6×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-81-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
VYVPEEFLIYVOTH-UHFFFAOYSA-N					
2,3,5-trimethyl-4-ethylhexane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-82-4]	9.6×10^{-7}		Gharagheizi et al. (2010)	Q	246
LDKMZLRIVWGQRW-UHFFFAOYSA-N					
2,4,4-trimethyl-3-ethylhexane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-83-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
MTYPKDRKJRWXKB-UHFFFAOYSA-N					
3,3,4-trimethyl-4-ethylhexane	6.8×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-84-6]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
ADDYWUNUHVKQGT-UHFFFAOYSA-N					
2,2-dimethyl-3-isopropylhexane	9.1×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-63-1]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
VKABOTNMFKIVDN-UHFFFAOYSA-N					
2,3-dimethyl-3-isopropylhexane	8.2×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-64-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
XVWGUCNHEXRNJU-UHFFFAOYSA-N					
2,4-dimethyl-3-isopropylhexane	9.5×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-65-3]	9.6×10^{-7}		Gharagheizi et al. (2010)	Q	246
QRNSQXWPYPLHTL-UHFFFAOYSA-N					
2,5-dimethyl-3-isopropylhexane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-66-4]	9.6×10^{-7}		Gharagheizi et al. (2010)	Q	246
QKICRGDGSLQROM-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-3,3-diethylhexane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-67-5]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
QNRHKXCWHYUEKP-UHFFFAOYSA-N					
2-methyl-3,4-diethylhexane	9.8×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-68-6]	9.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
MWHIPTVSAPEYPC-UHFFFAOYSA-N					
2-methyl-4,4-diethylhexane	9.0×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-69-7]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
UNPXTJSCIHOMKB-UHFFFAOYSA-N					
3-methyl-3,4-diethylhexane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-70-0]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
ZFMWIWWLOKHXHC-UHFFFAOYSA-N					
3-methyl-4,4-diethylhexane	8.1×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-71-1]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
CUHCCZRBXHOAMW-UHFFFAOYSA-N					
2,2,3,3,4,4-hexamethylpentane	5.0×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[60302-27-4]	7.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
JKJQSSSRSKPVEM-UHFFFAOYSA-N					
2,2,3,4-tetramethyl-3-ethylpentane	6.5×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-93-7]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
HBSINJYUKWVYBC-UHFFFAOYSA-N					
2,2,4,4-tetramethyl-3-ethylpentane	6.9×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[3178-30-1]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
FNWCWFQEEKFGHB-UHFFFAOYSA-N					
2,2,4-trimethyl-3-isopropylpentane	8.7×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	9.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[61868-90-4]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
SZPCILWZDHUKLW-UHFFFAOYSA-N					
2,3,4-trimethyl-3-isopropylpentane	7.1×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-91-5]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
FHBFVPOXLRZZPP-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2-dimethyl-3,3-diethylpentane	6.8×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[60302-28-5]	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
KCQSYGZVYTYSLG-UHFFFAOYSA-N					
2,4-dimethyl-3,3-diethylpentane	7.5×10^{-7}		Yaws (2003)	X	237
$C_{11}H_{24}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-92-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
VVQOQVXGUMJNET-UHFFFAOYSA-N					
dodecane	1.2×10^{-6}		Plyasunov and Shock (2000)	L	
$C_{12}H_{26}$	1.3×10^{-6}		Mackay and Shiu (1981)	L	
[112-40-3]	1.2×10^{-6}		Duchowicz et al. (2020)	V	186
SNRUBQQJIBEYMU-UHFFFAOYSA-N	1.2×10^{-6}		HSDB (2015)	V	
	1.2×10^{-6}		Mackay et al. (2006a)	V	
	1.3×10^{-6}		Eastcott et al. (1988)	V	
	1.2×10^{-6}		Abraham (1984)	V	
	1.2×10^{-6}		Yaws (2003)	X	258
	1.2×10^{-6}		Yaws (2003)	X	237
	3.0×10^{-6}		Dupeux et al. (2022)	Q	259
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	1.7×10^{-5}		Wang et al. (2017)	Q	80, 238
	8.5×10^{-7}		Wang et al. (2017)	Q	80, 239
	5.3×10^{-6}		Wang et al. (2017)	Q	80, 240
	5.1×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-6}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-7}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
	1.1×10^{-6}		Hilal et al. (2008)	Q	
	3.1×10^{-6}		Modarresi et al. (2007)	Q	67
	1.2×10^{-6}		Yaws (1999)	?	21
	1.4×10^{-6}		Yaws and Yang (1992)	?	21
2-methylundecane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	4.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[31807-55-3]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
GTJOHISYCKPIMT-UHFFFAOYSA-N					
3-methylundecane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	4.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[1002-43-3]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
HTZWVZNRDDOFEI-UHFFFAOYSA-N					
4-methylundecane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	2.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[2980-69-0]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
KNMXZGDUJVOTOC-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5-methylundecane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	2.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[1632-70-8]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
QULNVKABFWNUCW-UHFFFAOYSA-N					
6-methylundecane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	2.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-33-9]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
VPYZCUCKYWHJGX-UHFFFAOYSA-N					
2,2-dimethyldecane	9.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	3.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-37-3]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
WBWYXWILSHQILH-UHFFFAOYSA-N					
2,3-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	2.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-44-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
ZCTGYLNFWOQVHV-UHFFFAOYSA-N					
2,4-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[2801-84-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
OJAFXEXESSNPMH-UHFFFAOYSA-N					
2,5-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-50-4]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
DQHKBYZSYRJBMD-UHFFFAOYSA-N					
2,6-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	2.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[13150-81-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
DHJGXZWEQBKLNV-UHFFFAOYSA-N					
2,7-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	2.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-51-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
RVQIXUWWPOTVNP-UHFFFAOYSA-N					
2,8-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	2.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-52-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
KSRGGHUVCVWVDW-UHFFFAOYSA-N					
2,9-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	5.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[1002-17-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
HWISDPDDDUZJAW-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3-dimethyldecane	9.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-38-4]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
URERYYDSQOIHQK-UHFFFAOYSA-N					
3,4-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-45-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
NRBMEEDORZDRIT-UHFFFAOYSA-N					
3,5-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-48-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
XXSUEVGKGOUJMD-UHFFFAOYSA-N					
3,6-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-53-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
NQWFSCYWTXQNGG-UHFFFAOYSA-N					
3,7-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-54-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
VDAVEASVPZDNQB-UHFFFAOYSA-N					
3,8-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-55-9]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
KMAHIPNGGSOJSM-UHFFFAOYSA-N					
4,4-dimethyldecane	9.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-39-9]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
WZCACTKWHXCWFZ-UHFFFAOYSA-N					
4,5-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-46-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
QZFIIEYSHODCSV-UHFFFAOYSA-N					
4,6-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-49-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
TVGNRLXIJXKVGD-UHFFFAOYSA-N					
4,7-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-56-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
GCKWUFQALHAZDH-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5,5-dimethyldecane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[17453-92-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
RNXSOUOIPAWOAC-UHFFFAOYSA-N					
5,6-dimethyldecane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[1636-43-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
NCJIZIYQFWXMFZ-UHFFFAOYSA-N					
3-ethyldecane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	2.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[17085-96-0]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
ZBDDVSBBCGZQDV-UHFFFAOYSA-N					
4-ethyldecane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[1636-44-8]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
IGTKVLJTIZALGL-UHFFFAOYSA-N					
5-ethyldecane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-36-2]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
BCQLAHKMMOGIIS-UHFFFAOYSA-N					
2,2,3-trimethylnonane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[55499-04-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
XXNUJUNKYOZLAJ-UHFFFAOYSA-N					
2,2,4-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-50-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
YYYAICGYFLHBIN-UHFFFAOYSA-N					
2,2,5-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-51-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
ZIXRFABUOOUIMA-UHFFFAOYSA-N					
2,2,6-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-52-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
BUTMZMIZSWINDK-UHFFFAOYSA-N					
2,2,7-trimethylnonane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-53-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
PXOURNMYVAOUML-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,8-trimethylnonane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-54-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
WXUAVABOZJOELJ-UHFFFAOYSA-N					
2,3,3-trimethylnonane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-55-8]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
RSUFJUIYLXRYFG-UHFFFAOYSA-N					
2,3,4-trimethylnonane	9.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-56-9]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
RRZRZLRUYPZYEH-UHFFFAOYSA-N					
2,3,5-trimethylnonane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-57-0]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
IESSJVKAXJWJFD-UHFFFAOYSA-N					
2,3,6-trimethylnonane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-58-1]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
AUXUELQPRQTQBE-UHFFFAOYSA-N					
2,3,7-trimethylnonane	9.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-59-2]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
GGUGBCMHEULHJS-UHFFFAOYSA-N					
2,3,8-trimethylnonane	9.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-60-5]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
GQHCJRDJABETBJ-UHFFFAOYSA-N					
2,4,4-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-61-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
RRLKOZCPQXMIIJ-UHFFFAOYSA-N					
2,4,5-trimethylnonane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-62-7]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
NZAPYIGNIYRJNJ-UHFFFAOYSA-N					
2,4,6-trimethylnonane	9.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-10-5]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
QCQMRLDBNMVKOZ-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4,7-trimethylnonane	9.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-11-6]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
OHBDIVOYUFLOTO-UHFFFAOYSA-N					
2,4,8-trimethylnonane	9.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[49542-74-7]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
PZXMOJBYRFSNJH-UHFFFAOYSA-N					
2,5,5-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-12-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
ZRRKWMYBHUMSTG-UHFFFAOYSA-N					
2,5,6-trimethylnonane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-13-8]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
KXHDWXIQHWSOHI-UHFFFAOYSA-N					
2,5,7-trimethylnonane	9.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-14-9]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
KMBPYTMBXFKXON-UHFFFAOYSA-N					
2,5,8-trimethylnonane	9.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[49557-09-7]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
YYZRNFMGAQMLJJ-UHFFFAOYSA-N					
2,6,6-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-15-0]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
MTPVPWZHWOHMQT-UHFFFAOYSA-N					
2,6,7-trimethylnonane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-16-1]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
PGLYQCHTCUBASV-UHFFFAOYSA-N					
2,7,7-trimethylnonane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-17-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
RCTMUTWYOMEASD-UHFFFAOYSA-N					
3,3,4-trimethylnonane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-18-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
RNCRKMFELJSFRA-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3,5-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-19-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
KRWQPUYFIGHZNF-UHFFFAOYSA-N					
3,3,6-trimethylnonane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-20-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
GPSMOBMYMZBKGT-UHFFFAOYSA-N					
3,3,7-trimethylnonane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-21-8]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
NZYGFHSHEQXPFT-UHFFFAOYSA-N					
3,4,4-trimethylnonane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-22-9]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
UYNWXBDPBKCTRS-UHFFFAOYSA-N					
3,4,5-trimethylnonane	9.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-23-0]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
PFVDUOFPBLPHEQ-UHFFFAOYSA-N					
3,4,6-trimethylnonane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-24-1]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
VSRUKIVBXBGRDU-UHFFFAOYSA-N					
3,4,7-trimethylnonane	9.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[27802-85-3]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
HQIBDLHPQGDJEW-UHFFFAOYSA-N					
3,5,5-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-25-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
MUVSDRJGHVLJQX-UHFFFAOYSA-N					
3,5,6-trimethylnonane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-26-3]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
HMCPPWBQUPZETF-UHFFFAOYSA-N					
3,5,7-trimethylnonane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-27-4]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
LLVWEFHXQBAEJX-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,6,6-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-28-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
CBDYLMAJISNHBH-UHFFFAOYSA-N					
4,4,5-trimethylnonane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-29-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
QLJZSYCAASGFGU-UHFFFAOYSA-N					
4,4,6-trimethylnonane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-30-9]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
KBTTWWLCACXOSV-UHFFFAOYSA-N					
4,5,5-trimethylnonane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-31-0]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
QVDLUCCOJXIINS-UHFFFAOYSA-N					
4,5,6-trimethylnonane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62211-85-2]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
BBEKERHGCOZOIX-UHFFFAOYSA-N					
2-methyl-3-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-73-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
NVCDNLWOUSWNRQ-UHFFFAOYSA-N					
2-methyl-4-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-37-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
GRYPXYDXCQOVAY-UHFFFAOYSA-N					
2-methyl-5-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-38-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
WZWWJMDOQQIPJZ-UHFFFAOYSA-N					
2-methyl-6-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-39-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
GBMUYXDAAUUNLY-UHFFFAOYSA-N					
2-methyl-7-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-40-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
PHPGTUZXJVCCKP-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-3-ethylnonane	9.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-39-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
MJZXPSBAAXOUJF-UHFFFAOYSA-N					
3-methyl-4-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-41-2]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
ZELDGOVWPZHVJS-UHFFFAOYSA-N					
3-methyl-5-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-42-3]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
GDUZVOIDJDZQBC-UHFFFAOYSA-N					
3-methyl-6-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-43-4]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
WSMCXXNPFLZSMY-UHFFFAOYSA-N					
3-methyl-7-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-44-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
FSGFZSLYTXQNCW-UHFFFAOYSA-N					
4-methyl-3-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-45-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
AUMKRFNJSTUECA-UHFFFAOYSA-N					
4-methyl-4-ethylnonane	9.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[17312-40-2]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
LXQCGRFCISXKCQ-UHFFFAOYSA-N					
4-methyl-5-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-46-7]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
BDJIXOFXGLDYLN-UHFFFAOYSA-N					
4-methyl-6-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-47-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
SULZKBWLMOBACQ-UHFFFAOYSA-N					
4-methyl-7-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-48-9]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
HYIBWPIYSSTZLB-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5-methyl-3-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-49-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
ZBALIHDUORTBQR-UHFFFAOYSA-N					
5-methyl-4-ethylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[1632-71-9]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
HKUUNAOHRKAJIY-UHFFFAOYSA-N					
5-methyl-5-ethylnonane	9.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[14531-16-9]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
DZSBQMNPPIKBNF-UHFFFAOYSA-N					
4-propylnonane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[6165-37-3]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
QLKPGWNXMMBQMG-UHFFFAOYSA-N					
5-propylnonane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[998-35-6]	1.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
ISHSSTRAYNPQFX-UHFFFAOYSA-N					
4-isopropylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-71-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
BXYKZQOGHMLDIE-UHFFFAOYSA-N					
5-isopropylnonane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-72-9]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
ALZCRHWYCQKCQK-UHFFFAOYSA-N					
2,2,3,3-tetramethyloctane	6.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-74-8]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
UXQAEOWCSOPBLF-UHFFFAOYSA-N					
2,2,3,4-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-75-9]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
HEJULKHHKGYPNT-UHFFFAOYSA-N					
2,2,3,5-tetramethyloctane	8.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-76-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
MRBTZFDZTJYCAO-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,3,6-tetramethyloctane	7.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-77-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
YRSBZJIBIXVOME-UHFFFAOYSA-N					
2,2,3,7-tetramethyloctane	7.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-78-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
CPEHPCZXBBEYOL-UHFFFAOYSA-N					
2,2,4,4-tetramethyloctane	7.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-79-3]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
TYUFTNSABIBNRY-UHFFFAOYSA-N					
2,2,4,5-tetramethyloctane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-80-6]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
SNJCVPBJFQJMFW-UHFFFAOYSA-N					
2,2,4,6-tetramethyloctane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-81-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
ODZRFEPMTHWMBK-UHFFFAOYSA-N					
2,2,4,7-tetramethyloctane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-82-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
QHDQKPZLRKHEHV-UHFFFAOYSA-N					
2,2,5,5-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	5.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-83-9]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
RJJMZKVKQLGGDK-UHFFFAOYSA-N					
2,2,5,6-tetramethyloctane	8.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-84-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
BQUVPJLOJUCQGM-UHFFFAOYSA-N					
2,2,5,7-tetramethyloctane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-19-3]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
ISTINYWNHRBEDQ-UHFFFAOYSA-N					
2,2,6,6-tetramethyloctane	7.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-20-6]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
BANZIZHQGFRTMI-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,6,7-tetramethyloctane	8.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-21-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
ZSXJNQURTCJFGP-UHFFFAOYSA-N					
2,2,7,7-tetramethyloctane	7.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[1071-31-4]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
QZUFNKONEPLWBC-UHFFFAOYSA-N					
2,3,3,4-tetramethyloctane	7.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-22-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
ITTRGXLKGDMYDX-UHFFFAOYSA-N					
2,3,3,5-tetramethyloctane	7.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-23-9]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
RVOIBAZQSHFKMM-UHFFFAOYSA-N					
2,3,3,6-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-24-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
MBJHOSHYIFXEPL-UHFFFAOYSA-N					
2,3,3,7-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-25-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
WWQBXZREQWIXFF-UHFFFAOYSA-N					
2,3,4,4-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-26-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
MELCVUZPHQRNTK-UHFFFAOYSA-N					
2,3,4,5-tetramethyloctane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-27-3]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
AMIZVDCCXDQOHL-UHFFFAOYSA-N					
2,3,4,6-tetramethyloctane	8.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-28-4]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
OYZWSGWTBSWCLN-UHFFFAOYSA-N					
2,3,4,7-tetramethyloctane	8.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-29-5]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
YUCNZDFGMLKYFT-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,5,5-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-30-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
RQOLUXQWYAKKTG-UHFFFAOYSA-N					
2,3,5,6-tetramethyloctane	8.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-31-9]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
IPYLOMHOPWIUFA-UHFFFAOYSA-N					
2,3,5,7-tetramethyloctane	8.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-32-0]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
AIUMUUQTYGQPMV-UHFFFAOYSA-N					
2,3,6,6-tetramethyloctane	7.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-33-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
CVRMZIOMFWYAPV-UHFFFAOYSA-N					
2,3,6,7-tetramethyloctane	8.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[52670-34-5]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
FZCGYGCYZRXLDY-UHFFFAOYSA-N					
2,4,4,5-tetramethyloctane	8.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-34-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
OBWRJGVWBWXXAO-UHFFFAOYSA-N					
2,4,4,6-tetramethyloctane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-35-3]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
UQCGTRPILZWACX-UHFFFAOYSA-N					
2,4,4,7-tetramethyloctane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	5.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[35866-96-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
QYUWMFZODNLLRJ-UHFFFAOYSA-N					
2,4,5,5-tetramethyloctane	8.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-36-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
OMFWIGPPTXTQHH-UHFFFAOYSA-N					
2,4,5,6-tetramethyloctane	8.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-37-5]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
YJMGKHXCSVEVKG-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4,5,7-tetramethyloctane	9.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[2217-17-6]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
PWYLDJLMYGOPSR-UHFFFAOYSA-N					
2,4,6,6-tetramethyloctane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-38-6]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
VVEPRQWGSASPPP-UHFFFAOYSA-N					
2,5,5,6-tetramethyloctane	7.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-39-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
DLCPMTDXNVOOLU-UHFFFAOYSA-N					
2,5,6,6-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-40-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
SQOVOQLOSFZJGI-UHFFFAOYSA-N					
3,3,4,4-tetramethyloctane	6.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-41-1]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
VXEUNQVVVNDDTL-UHFFFAOYSA-N					
3,3,4,5-tetramethyloctane	7.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-42-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
FATMBSLXTUXZBP-UHFFFAOYSA-N					
3,3,4,6-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-43-3]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
VCXMKRQQDPQALS-UHFFFAOYSA-N					
3,3,5,5-tetramethyloctane	7.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-44-4]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
UJLDJWNVZROTLS-UHFFFAOYSA-N					
3,3,5,6-tetramethyloctane	7.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-45-5]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
AQPSWWWUVHSZJK-UHFFFAOYSA-N					
3,3,6,6-tetramethyloctane	7.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-46-6]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
PAEUGKMMSQUAGH-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4,4,5-tetramethyloctane	7.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-47-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
HWNTXBYEGXKWKG-UHFFFAOYSA-N					
3,4,4,6-tetramethyloctane	7.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-19-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
LNRFUGUGPGLBLV-UHFFFAOYSA-N					
3,4,5,5-tetramethyloctane	7.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-20-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
NCNZUEBQNGRARF-UHFFFAOYSA-N					
3,4,5,6-tetramethyloctane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-21-1]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
NADJQGPTQSFIHB-UHFFFAOYSA-N					
4,4,5,5-tetramethyloctane	6.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-22-2]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
INTYEXUWOYUVGJ-UHFFFAOYSA-N					
2,2-dimethyl-3-ethyloctane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-95-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
LIZQPVRBTUZZCL-UHFFFAOYSA-N					
2,2-dimethyl-4-ethyloctane	9.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-96-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
PEGJIJFSOTZJFH-UHFFFAOYSA-N					
2,2-dimethyl-5-ethyloctane	8.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-97-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
ACWGGQUVVQOZPJ-UHFFFAOYSA-N					
2,2-dimethyl-6-ethyloctane	8.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-98-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
SHNILIMSRTWRKG-UHFFFAOYSA-N					
2,3-dimethyl-3-ethyloctane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-99-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
NDFHPGVSCVJNFR-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-dimethyl-4-ethyloctane $C_{12}H_{26}$ [62184-00-3] DCBIYDZULXWXTQ-UHFFFAOYSA-N	9.3×10^{-7} 8.4×10^{-7} 9.2×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2,3-dimethyl-5-ethyloctane $C_{12}H_{26}$ [62184-01-4] NPUNZBBVZZNRNS-UHFFFAOYSA-N	9.5×10^{-7} 7.7×10^{-7} 9.2×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2,3-dimethyl-6-ethyloctane $C_{12}H_{26}$ [62184-02-5] BWSXPPUMTZVKPA-UHFFFAOYSA-N	9.3×10^{-7} 8.9×10^{-7} 9.2×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2,4-dimethyl-3-ethyloctane $C_{12}H_{26}$ [62184-03-6] QYHDQDAUJCPVFJ-UHFFFAOYSA-N	9.3×10^{-7} 8.4×10^{-7} 9.2×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2,4-dimethyl-4-ethyloctane $C_{12}H_{26}$ [62184-04-7] XAKSPVTVTMAMDT-UHFFFAOYSA-N	8.8×10^{-7} 7.1×10^{-7} 8.7×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2,4-dimethyl-5-ethyloctane $C_{12}H_{26}$ [62184-05-8] JHDZOLPKXSWZKD-UHFFFAOYSA-N	9.5×10^{-7} 7.5×10^{-7} 9.2×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2,4-dimethyl-6-ethyloctane $C_{12}H_{26}$ [62184-06-9] VGDSKYYXZZCASQ-UHFFFAOYSA-N	9.6×10^{-7} 7.2×10^{-7} 9.2×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2,5-dimethyl-3-ethyloctane $C_{12}H_{26}$ [62184-07-0] BCQWMBQACXNHGP-UHFFFAOYSA-N	9.5×10^{-7} 7.7×10^{-7} 9.2×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2,5-dimethyl-4-ethyloctane $C_{12}H_{26}$ [62184-08-1] IMMDGMKEESKIQT-UHFFFAOYSA-N	9.6×10^{-7} 7.2×10^{-7} 9.2×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2,5-dimethyl-5-ethyloctane $C_{12}H_{26}$ [62184-09-2] BVAIFAWSJOPLJD-UHFFFAOYSA-N	8.6×10^{-7} 7.5×10^{-7} 8.7×10^{-7}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,5-dimethyl-6-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-50-0]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
CYTDZGRTFHXLQS-UHFFFAOYSA-N					
2,6-dimethyl-3-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-51-1]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
WAFCPUFGSNTFSP-UHFFFAOYSA-N					
2,6-dimethyl-4-ethyloctane	9.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-52-2]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
JIOQMQLJPQDNFA-UHFFFAOYSA-N					
2,6-dimethyl-5-ethyloctane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-53-3]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
ZBMWKURVBLDBAH-UHFFFAOYSA-N					
2,6-dimethyl-6-ethyloctane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-54-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
DGFWFJRTTJTVEQ-UHFFFAOYSA-N					
2,7-dimethyl-3-ethyloctane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-55-5]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
XEMFRSYZKNPRTA-UHFFFAOYSA-N					
2,7-dimethyl-4-ethyloctane	9.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-56-6]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
KSVMIUVYLYZDMT-UHFFFAOYSA-N					
3,3-dimethyl-4-ethyloctane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-57-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
BKNJDUXGYCILJT-UHFFFAOYSA-N					
3,3-dimethyl-5-ethyloctane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-58-8]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
GQTCKTISADWVNV-UHFFFAOYSA-N					
3,3-dimethyl-6-ethyloctane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-59-9]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
DDRNTRVXHMVVLA-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4-dimethyl-3-ethyloctane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62212-28-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
AOQVLRSMPNHJPF-UHFFFAOYSA-N					
3,4-dimethyl-4-ethyloctane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-60-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
WBKPODGAYHVUMM-UHFFFAOYSA-N					
3,4-dimethyl-5-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-61-3]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
LEPWFUNEXVKPDO-UHFFFAOYSA-N					
3,4-dimethyl-6-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-62-4]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
DPDGQUDZYGOBAM-UHFFFAOYSA-N					
3,5-dimethyl-3-ethyloctane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-63-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
QYJKERUDQYOWRC-UHFFFAOYSA-N					
3,5-dimethyl-4-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-64-6]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
OMAJEXDENFMCIN-UHFFFAOYSA-N					
3,5-dimethyl-5-ethyloctane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-65-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
OLBJDMSGRVKJMF-UHFFFAOYSA-N					
3,5-dimethyl-6-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-66-8]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
LLHGAWREVJAITE-UHFFFAOYSA-N					
3,6-dimethyl-3-ethyloctane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-67-9]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
MNXPIOFJFYQCKE-UHFFFAOYSA-N					
3,6-dimethyl-4-ethyloctane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-68-0]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
RTVRGBUFZDOPIH-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

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4,4-dimethyl-3-ethyloctane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-69-1]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
RHSANRLUOZFJDW-UHFFFAOYSA-N					
4,4-dimethyl-5-ethyloctane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-70-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
BETVNWPSZXTJLK-UHFFFAOYSA-N					
4,4-dimethyl-6-ethyloctane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-71-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
UGEWSKWSWHZABT-UHFFFAOYSA-N					
4,5-dimethyl-3-ethyloctane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-72-6]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
MNDPOEACQSQPCJ-UHFFFAOYSA-N					
4,5-dimethyl-4-ethyloctane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-73-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
MOEUNMMPAYEJOZ-UHFFFAOYSA-N					
3,3-diethyloctane	9.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[17302-40-8]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
DGJISSKLLWWXTG-UHFFFAOYSA-N					
3,4-diethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-92-0]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
HILZBOWVGZXYGQ-UHFFFAOYSA-N					
3,5-diethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-93-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
DSYIMNMBWBEOHY-UHFFFAOYSA-N					
3,6-diethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-94-2]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
UTCTYSTYZOAAOS-UHFFFAOYSA-N					
4,4-diethyloctane	9.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[17312-42-4]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
FTEQKVNFZNDQJG-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,5-diethyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[1636-41-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
XRVCHXCONYJHLU-UHFFFAOYSA-N					
2-methyl-4-propyloctane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-33-2]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
FJPVBTBEYVNWCA-UHFFFAOYSA-N					
2-methyl-5-propyloctane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-34-3]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
NYBDGQCIJCAIJL-UHFFFAOYSA-N					
3-methyl-4-propyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-35-4]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
CTXPEFTVFFFIBQ-UHFFFAOYSA-N					
3-methyl-5-propyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-36-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
VOSHMCRSZWNTLJ-UHFFFAOYSA-N					
4-methyl-4-propyloctane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[17312-41-3]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
RNKCZSBPRRHTOZ-UHFFFAOYSA-N					
4-methyl-5-propyloctane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-85-1]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
MVUWSCFPURGAJF-UHFFFAOYSA-N					
2-methyl-3-isopropyloctane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[13287-19-9]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
KBIUKRVYBYJVSS-UHFFFAOYSA-N					
2-methyl-4-isopropyloctane	9.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-86-2]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
NRRICFUUPCDSKW-UHFFFAOYSA-N					
2-methyl-5-isopropyloctane	9.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-87-3]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
OPKVPKXVSDEXOZ-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-4-isopropyloctane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-88-4]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
UXTHXSNAZBLVOD-UHFFFAOYSA-N					
3-methyl-5-isopropyloctane	9.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-89-5]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
VEJPAYNPRZYJNN-UHFFFAOYSA-N					
4-methyl-4-isopropyloctane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-90-8]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
KCNISWXEVSJYRS-UHFFFAOYSA-N					
4-methyl-5-isopropyloctane	9.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62183-91-9]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
HEFVKUUZAXCMQX-UHFFFAOYSA-N					
4-*tert*-butyloctane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-32-1]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
RWILNGDOCMDMJW-UHFFFAOYSA-N					
2,2,4,6,6-pentamethylheptane	7.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	4.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[13475-82-6]	1.1×10^{-6}		Zhang et al. (2010)	Q	287, 288
VKPSKYDESGTTFR-UHFFFAOYSA-N	2.3×10^{-7}		Zhang et al. (2010)	Q	287, 289
	2.4×10^{-5}		Zhang et al. (2010)	Q	287, 290
	5.1×10^{-6}		Zhang et al. (2010)	Q	287, 291
	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
2,2,3,3,4-pentamethylheptane	6.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-80-5]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
NTDYBHYVUCYILC-UHFFFAOYSA-N					
2,2,3,3,5-pentamethylheptane	6.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-81-6]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
ZLCPPJIFAFIYPV-UHFFFAOYSA-N					
2,2,3,3,6-pentamethylheptane	6.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-82-7]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
LYTFNNQFUUFUDH-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,3,4,4-pentamethylheptane	6.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-83-8]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
SUFPUVGFEWPIFA-UHFFFAOYSA-N					
2,2,3,4,5-pentamethylheptane	7.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-84-9]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
XYDYIKVIGCXDLV-UHFFFAOYSA-N					
2,2,3,4,6-pentamethylheptane	7.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-85-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
XRJGBYMRUIWAJP-UHFFFAOYSA-N					
2,2,3,5,5-pentamethylheptane	6.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-86-1]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
OSZLORKBJVWZNT-UHFFFAOYSA-N					
2,2,3,5,6-pentamethylheptane	7.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-87-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
MHJUEZDXDYXCPA-UHFFFAOYSA-N					
2,2,3,6,6-pentamethylheptane	7.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-88-3]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
SLGYOGBODYIQGW-UHFFFAOYSA-N					
2,2,4,4,5-pentamethylheptane	6.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-61-5]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
XRGPEBQZXVFCRE-UHFFFAOYSA-N					
2,2,4,4,6-pentamethylheptane	7.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-62-6]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
NOFQKTWPZFUCOO-UHFFFAOYSA-N					
2,2,4,5,5-pentamethylheptane	7.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-63-7]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
JGOKXUSMFJOVQT-UHFFFAOYSA-N					
2,2,4,5,6-pentamethylheptane	7.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-64-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
JVESFBBBMJIZLO-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,5,5,6-pentamethylheptane	7.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-65-9]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
FMJMMNPKKCFHTH-UHFFFAOYSA-N					
2,3,3,4,4-pentamethylheptane	6.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62199-66-0]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
VBOBCKMZHQJDQA-UHFFFAOYSA-N					
2,3,3,4,5-pentamethylheptane	7.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-67-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
OLZJEASBDLLWCY-UHFFFAOYSA-N					
2,3,3,4,6-pentamethylheptane	7.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-68-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
YENAHMOHMFYKPC-UHFFFAOYSA-N					
2,3,3,5,5-pentamethylheptane	6.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-69-3]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
DTLBRJVRUQMSQN-UHFFFAOYSA-N					
2,3,3,5,6-pentamethylheptane	7.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[52670-35-6]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
SZQDOCSTKXRXAR-UHFFFAOYSA-N					
2,3,4,4,5-pentamethylheptane	7.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-70-6]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
CHHJLGDSEYTKKE-UHFFFAOYSA-N					
2,3,4,4,6-pentamethylheptane	7.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-71-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
DHXWMADSONSWTL-UHFFFAOYSA-N					
2,3,4,5,5-pentamethylheptane	7.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-72-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
BDFJISGXUJUYCX-UHFFFAOYSA-N					
2,3,4,5,6-pentamethylheptane	7.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[27574-98-7]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
YIKFFSNUOIJPSI-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4,4,5,5-pentamethylheptane	6.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-73-9]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
TXGUYEKSMHZHSB-UHFFFAOYSA-N					
3,3,4,4,5-pentamethylheptane	6.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62199-74-0]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
YFXNIDIHYOGTEN-UHFFFAOYSA-N					
3,3,4,5,5-pentamethylheptane	6.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62199-75-1]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
NZIFKVSORPBQSX-UHFFFAOYSA-N					
2,2,3-trimethyl-3-ethylheptane	6.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-04-6]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
CVXGCQXACVZXQR-UHFFFAOYSA-N					
2,2,3-trimethyl-4-ethylheptane	7.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-05-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
COHRBFNOOUABCT-UHFFFAOYSA-N					
2,2,3-trimethyl-5-ethylheptane	8.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-06-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
OOIGDPTZPWRGHN-UHFFFAOYSA-N					
2,2,4-trimethyl-3-ethylheptane	8.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-07-9]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
TYGUUZVWCBYDKW-UHFFFAOYSA-N					
2,2,4-trimethyl-4-ethylheptane	7.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-08-0]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
XMUXASPVOBQLPC-UHFFFAOYSA-N					
2,2,4-trimethyl-5-ethylheptane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-09-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
QADOHJKDWMLCQT-UHFFFAOYSA-N					
2,2,5-trimethyl-3-ethylheptane	8.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-10-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
SUDWTPMZYLBGKW-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,5-trimethyl-4-ethylheptane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-11-5]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
GDPLKYYKURLRKJ-UHFFFAOYSA-N					
2,2,5-trimethyl-5-ethylheptane	7.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-12-6]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
KJWMMFYTYSUWMH-UHFFFAOYSA-N					
2,2,6-trimethyl-3-ethylheptane	8.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-13-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
RIIDJOQRWGTQEN-UHFFFAOYSA-N					
2,2,6-trimethyl-4-ethylheptane	8.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	5.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-14-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
QGYSVVWKEDKPTP-UHFFFAOYSA-N					
2,2,6-trimethyl-5-ethylheptane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-15-9]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
LYZRWXZZVRWJHX-UHFFFAOYSA-N					
2,3,3-trimethyl-4-ethylheptane	7.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-16-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
VIIXOXRHJWHIBP-UHFFFAOYSA-N					
2,3,3-trimethyl-5-ethylheptane	7.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-17-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
JHGOLBUJAIJLCX-UHFFFAOYSA-N					
2,3,4-trimethyl-3-ethylheptane	7.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62199-18-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
YZXMDESZKHUODO-UHFFFAOYSA-N					
2,3,4-trimethyl-4-ethylheptane	7.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-55-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
QDWZIZQKVLESDK-UHFFFAOYSA-N					
2,3,4-trimethyl-5-ethylheptane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-56-5]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
URFFXJPJMCMXFR-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,5-trimethyl-3-ethylheptane	7.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-57-6]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
QHACFORXSGHTJG-UHFFFAOYSA-N					
2,3,5-trimethyl-4-ethylheptane	8.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-58-7]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
UEZAASCWBAVHRO-UHFFFAOYSA-N					
2,3,5-trimethyl-5-ethylheptane	7.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-59-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
LTSLSBVPXXAMBM-UHFFFAOYSA-N					
2,3,6-trimethyl-3-ethylheptane	7.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-60-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
KOVQAKVRXODFNL-UHFFFAOYSA-N					
2,3,6-trimethyl-4-ethylheptane	8.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-61-2]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
RBVKVRIWSQSXPO-UHFFFAOYSA-N					
2,3,6-trimethyl-5-ethylheptane	8.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-62-3]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
JXCQTSFHNKTOLJ-UHFFFAOYSA-N					
2,4,4-trimethyl-3-ethylheptane	7.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-63-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
BNFUBMCCIACHFX-UHFFFAOYSA-N					
2,4,4-trimethyl-5-ethylheptane	8.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-64-5]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
YSCJXRHNKUXHLH-UHFFFAOYSA-N					
2,4,5-trimethyl-3-ethylheptane	8.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-65-6]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
JFKSTTDMBQAPCT-UHFFFAOYSA-N					
2,4,5-trimethyl-4-ethylheptane	7.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-66-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
HSVLOEWHJNAWLC-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4,5-trimethyl-5-ethylheptane	7.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-67-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
JAUBFUIZENVVAG-UHFFFAOYSA-N					
2,4,6-trimethyl-3-ethylheptane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-68-9]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
KQBJYFJWQOUHCI-UHFFFAOYSA-N					
2,4,6-trimethyl-4-ethylheptane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-69-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
LPNPQCHEMXFBSW-UHFFFAOYSA-N					
2,5,5-trimethyl-3-ethylheptane	8.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-70-3]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
MARFNXCIPCRAJU-UHFFFAOYSA-N					
2,5,5-trimethyl-4-ethylheptane	8.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-71-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
HGYOEMXZYDBOKQ-UHFFFAOYSA-N					
3,3,4-trimethyl-4-ethylheptane	6.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62198-72-5]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
QLOXTBGCIUOWIG-UHFFFAOYSA-N					
3,3,4-trimethyl-5-ethylheptane	7.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-73-6]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
CUWOOQVXUDOHOC-UHFFFAOYSA-N					
3,3,5-trimethyl-4-ethylheptane	7.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-74-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
QXCHZKHHIUTBOU-UHFFFAOYSA-N					
3,3,5-trimethyl-5-ethylheptane	6.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-75-8]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
GCWLDOMARVHVOZ-UHFFFAOYSA-N					
3,4,4-trimethyl-3-ethylheptane	6.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62198-76-9]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
SIIFYRMARKBLER-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4,4-trimethyl-5-ethylheptane	7.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-77-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
XSLWCLUAFIVTLD-UHFFFAOYSA-N					
3,4,5-trimethyl-3-ethylheptane	7.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-78-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
ZHILUIHUWKDTTM-UHFFFAOYSA-N					
3,4,5-trimethyl-4-ethylheptane	7.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62198-79-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
SZOKDASFURUJDF-UHFFFAOYSA-N					
2,2-dimethyl-4-propylheptane	9.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	5.8×10^{-7}		Gharagheizi et al. (2012)	Q	
DWEXNJRCPKKJBQ-UHFFFAOYSA-N	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
2,3-dimethyl-4-propylheptane	9.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-30-2]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
AZUDVOIXPNEOLR-UHFFFAOYSA-N					
2,4-dimethyl-4-propylheptane	8.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-31-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
FDVJFPZZPSPQAO-UHFFFAOYSA-N					
2,5-dimethyl-4-propylheptane	9.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-32-4]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
PJXVVWKRCASATD-UHFFFAOYSA-N					
2,6-dimethyl-4-propylheptane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	5.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-33-5]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
UFJZYHSURMZROL-UHFFFAOYSA-N					
3,3-dimethyl-4-propylheptane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-34-6]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
XVWBLUKOUJTCDO-UHFFFAOYSA-N					
3,4-dimethyl-4-propylheptane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-35-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
UGSAJWKYCFFZRD-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,5-dimethyl-4-propylheptane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-36-8]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
GKVRDSIZILZQJE-UHFFFAOYSA-N					
2,2-dimethyl-3-isopropylheptane	8.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-37-9]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
XPOSVKCTMHOWTN-UHFFFAOYSA-N					
2,2-dimethyl-4-isopropylheptane	8.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	5.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-38-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
HFRVMJCEWUXCMP-UHFFFAOYSA-N					
2,3-dimethyl-3-isopropylheptane	7.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-39-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
IAWDNHPMOJTEEN-UHFFFAOYSA-N					
2,3-dimethyl-4-isopropylheptane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-40-4]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
GEQDAUMUCVOARW-UHFFFAOYSA-N					
2,4-dimethyl-3-isopropylheptane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-41-5]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
MWVRZCOXSIAHLW-UHFFFAOYSA-N					
2,4-dimethyl-4-isopropylheptane	8.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-42-6]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
MTPOSRQPOBWFQC-UHFFFAOYSA-N					
2,5-dimethyl-3-isopropylheptane	8.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-43-7]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
XSKMFUBSJXETFW-UHFFFAOYSA-N					
2,5-dimethyl-4-isopropylheptane	9.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-44-8]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
OOYWQZAQFKOCKA-UHFFFAOYSA-N					
2,6-dimethyl-3-isopropylheptane	8.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-45-9]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
NOAGKIODSFDOTA-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,6-dimethyl-4-isopropylheptane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	5.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[35866-89-8]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
BIBHNAJLMRUJLS-UHFFFAOYSA-N					
3,3-dimethyl-4-isopropylheptane	7.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-46-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
MACIOLXBYDNTTI-UHFFFAOYSA-N					
3,4-dimethyl-4-isopropylheptane	7.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-47-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
QFKXRROMVRXZIF-UHFFFAOYSA-N					
3,5-dimethyl-4-isopropylheptane	8.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-89-4]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
XJRRTENBDSNHQB-UHFFFAOYSA-N					
2-methyl-3,3-diethylheptane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62198-90-7]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
VBKOVPDJLQIMSZ-UHFFFAOYSA-N					
2-methyl-3,4-diethylheptane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-91-8]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
PRSHREOBBOOUSO-UHFFFAOYSA-N					
2-methyl-3,5-diethylheptane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-92-9]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
KZTGLPPJUZINLQ-UHFFFAOYSA-N					
2-methyl-4,4-diethylheptane	8.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-93-0]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
VJTVFYMTOXDIID-UHFFFAOYSA-N					
2-methyl-4,5-diethylheptane	9.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-94-1]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
SRLQJPCYGKMUSM-UHFFFAOYSA-N					
2-methyl-5,5-diethylheptane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-95-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
XPAWKGLXSPHNAN-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-3,4-diethylheptane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-96-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
VRVVWJIPKQWWJB-UHFFFAOYSA-N					
3-methyl-3,5-diethylheptane	8.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-97-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
RGRSPNWZJFXFAN-UHFFFAOYSA-N					
3-methyl-4,4-diethylheptane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62198-98-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
WSBKWCXGZHVUHW-UHFFFAOYSA-N					
3-methyl-4,5-diethylheptane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62198-99-6]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
NVBVLQDXCRDBBU-UHFFFAOYSA-N					
3-methyl-5,5-diethylheptane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-00-2]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
JOJSCBROPYJHJX-UHFFFAOYSA-N					
4-methyl-3,3-diethylheptane	8.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62199-01-3]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
KGSWPEXUAXYDMO-UHFFFAOYSA-N					
4-methyl-3,4-diethylheptane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-02-4]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
RAFABRWSQNCWEY-UHFFFAOYSA-N					
4-methyl-3,5-diethylheptane	9.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-03-5]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
XUVBJZPYCGZQDK-UHFFFAOYSA-N					
2-methyl-4-*tert*-butylheptane	8.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-23-3]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
HIHQJZLWJQHTEJ-UHFFFAOYSA-N					
3-methyl-4-*tert*-butylheptane	8.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-24-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
IKKVFRPBQQTTKP-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methyl-4-*tert*-butylheptane	7.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.7×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-25-5]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
JABLMQZBFVBNBS-UHFFFAOYSA-N					
3-ethyl-4-propylheptane	1.0×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-26-6]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
FPODIYZXVCXXQE-UHFFFAOYSA-N					
4-ethyl-4-propylheptane	9.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[17312-43-5]	1.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
JTZJHTZCYBYCSZ-UHFFFAOYSA-N					
3-ethyl-4-isopropylheptane	9.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-27-7]	9.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
VENQCMDSFBOTMS-UHFFFAOYSA-N					
4-ethyl-4-isopropylheptane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-28-8]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
IKRHMKIYGHBTGZ-UHFFFAOYSA-N					
2,2,3,3,4,4-hexamethylhexane	4.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[62185-11-9]	6.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
ACZDZCRQHVWGEF-UHFFFAOYSA-N					
2,2,3,3,4,5-hexamethylhexane	5.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.1×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-12-0]	7.4×10^{-7}		Gharagheizi et al. (2010)	Q	246
IFHVEHXJQMYGHH-UHFFFAOYSA-N					
2,2,3,3,5,5-hexamethylhexane	5.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[60302-24-1]	6.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
YFGLJPQISFJQSO-UHFFFAOYSA-N					
2,2,3,4,4,5-hexamethylhexane	5.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62185-13-1]	7.4×10^{-7}		Gharagheizi et al. (2010)	Q	246
QJVUKMHIEDVCDT-UHFFFAOYSA-N					
2,2,3,4,5,5-hexamethylhexane	6.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-14-2]	7.4×10^{-7}		Gharagheizi et al. (2010)	Q	246
NXZMBOYMQLHOPD-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3,4,4,5-hexamethylhexane	5.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[52670-36-7]	7.4×10^{-7}		Gharagheizi et al. (2010)	Q	246
GRVNDHRZJGSRDC-UHFFFAOYSA-N					
2,2,3,3-tetramethyl-4-ethylhexane	6.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-98-9]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
CRTTYRRLFPCOTC-UHFFFAOYSA-N					
2,2,3,4-tetramethyl-3-ethylhexane	6.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62184-99-0]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
SYWRGACXWPDDMM-UHFFFAOYSA-N					
2,2,3,4-tetramethyl-4-ethylhexane	6.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62185-00-6]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
WVLMCSYUMSZJQJ-UHFFFAOYSA-N					
2,2,3,5-tetramethyl-3-ethylhexane	6.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-01-7]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
CHURHVBNTYCJDL-UHFFFAOYSA-N					
2,2,3,5-tetramethyl-4-ethylhexane	7.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-02-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
GYAMSLKQDQYJGT-UHFFFAOYSA-N					
2,2,4,4-tetramethyl-3-ethylhexane	6.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-03-9]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
HWHADLCAKCOTRI-UHFFFAOYSA-N					
2,2,4,5-tetramethyl-3-ethylhexane	7.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.0×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-04-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
KZHIDSBQFJFWDV-UHFFFAOYSA-N					
2,2,4,5-tetramethyl-4-ethylhexane	6.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-05-1]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
HAVVVIZEMKFOFL-UHFFFAOYSA-N					
2,2,5,5-tetramethyl-3-ethylhexane	7.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	5.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-06-2]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
GJJUHGLRQQDIFN-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3,4-tetramethyl-4-ethylhexane	6.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62185-07-3]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
YVKQGHGRZXUTNK-UHFFFAOYSA-N					
2,3,3,5-tetramethyl-4-ethylhexane	7.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.5×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-08-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
AMMSTTMNZHWREI-UHFFFAOYSA-N					
2,3,4,4-tetramethyl-3-ethylhexane	6.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62185-09-5]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
VYCKEOSFJUAFGK-UHFFFAOYSA-N					
2,3,4,5-tetramethyl-3-ethylhexane	6.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-10-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
IBPLCPRMAQRHHK-UHFFFAOYSA-N					
2,2,3-trimethyl-3-isopropylhexane	6.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.6×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-79-5]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
UTCSLOLKGOKPGW-UHFFFAOYSA-N					
2,2,4-trimethyl-3-isopropylhexane	7.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-80-8]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
VEMACPZMOMAUAN-UHFFFAOYSA-N					
2,2,5-trimethyl-3-isopropylhexane	8.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	5.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-81-9]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
GZFAXOCUKPGWEA-UHFFFAOYSA-N					
2,2,5-trimethyl-4-isopropylhexane	8.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	5.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-82-0]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
QFLYTOVYLBZBJC-UHFFFAOYSA-N					
2,3,4-trimethyl-3-isopropylhexane	6.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62199-83-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
SXELEUFFBZGXIC-UHFFFAOYSA-N					
2,3,5-trimethyl-3-isopropylhexane	7.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-84-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
GUMUKRVQSSIBJO-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,5-trimethyl-4-isopropylhexane	8.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-85-3]	9.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
VBRDSJSWPGXVIR-UHFFFAOYSA-N					
2,4,4-trimethyl-3-isopropylhexane	7.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.4×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-86-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
UGPHXQWIHGYHOH-UHFFFAOYSA-N					
2,2-dimethyl-3,4-diethylhexane	8.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-89-7]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
ZAKPEOVUOZWBNO-UHFFFAOYSA-N					
2,2-dimethyl-4,4-diethylhexane	6.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-89-8]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
CYPRMBGQWCLJBN-UHFFFAOYSA-N					
2,3-dimethyl-3,4-diethylhexane	7.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62184-90-1]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
BUUBMKJJLVCTKU-UHFFFAOYSA-N					
2,3-dimethyl-4,4-diethylhexane	7.5×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62184-91-2]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
YNHBDJNMYMZVLM-UHFFFAOYSA-N					
2,4-dimethyl-3,3-diethylhexane	7.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-92-3]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
OXAROVXPKXMTIV-UHFFFAOYSA-N					
2,4-dimethyl-3,4-diethylhexane	7.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-93-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
AUVJTUXGNKLTIN-UHFFFAOYSA-N					
2,5-dimethyl-3,3-diethylhexane	8.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-94-5]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
XHDPVTDRZGCNFV-UHFFFAOYSA-N					
2,5-dimethyl-3,4-diethylhexane	8.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62184-95-6]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
WCPAKUFSQFCWTQ-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3-dimethyl-4,4-diethylhexane	6.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62184-96-7]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
XFUAJHJJXMVZCQ-UHFFFAOYSA-N					
3,4-dimethyl-3,4-diethylhexane	6.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[62184-97-8]	7.5×10^{-7}		Gharagheizi et al. (2010)	Q	246
NTQKWVJMJSYRDX-UHFFFAOYSA-N					
2,2-dimethyl-3-*tert*-butylhexane	6.4×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	8.3×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-76-2]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
VZAYJUSYQVNGBC-UHFFFAOYSA-N					
2-methyl-3-ethyl-3-isopropylhexane	8.3×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	9.2×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-77-3]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
TXYYDQJNRQJTOW-UHFFFAOYSA-N					
2-methyl-4-ethyl-3-isopropylhexane	9.7×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	6.8×10^{-7}		Gharagheizi et al. (2012)	Q	
[62199-78-4]	8.9×10^{-7}		Gharagheizi et al. (2010)	Q	246
JXHSGKIMXDNKIS-UHFFFAOYSA-N					
3,3,4-triethylhexane	8.2×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62199-87-5]	8.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
YGNQREHYYJPYLX-UHFFFAOYSA-N					
2,2,3,4,4-pentamethyl-3-ethylpentane	4.9×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[66576-21-4]	6.7×10^{-7}		Gharagheizi et al. (2010)	Q	246
IZNAUALMSCRPBS-UHFFFAOYSA-N					
2,2,3,4-tetramethyl-3-isopropylpentane	5.6×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62185-17-5]	7.4×10^{-7}		Gharagheizi et al. (2010)	Q	246
OKGFCJOAXUYCBG-UHFFFAOYSA-N					
2,2,4,4-tetramethyl-3-isopropylpentane	6.0×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	7.9×10^{-7}		Gharagheizi et al. (2012)	Q	
[62185-18-6]	7.4×10^{-7}		Gharagheizi et al. (2010)	Q	246
BYIFHEDQKBAFSW-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,4-trimethyl-3,3-diethylpentane	6.1×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62185-15-3]	7.2×10^{-7}		Gharagheizi et al. (2010)	Q	246
GIKXQMPMOJVRDN-UHFFFAOYSA-N					
2,4-dimethyl-3-ethyl-3-isopropylpentane	6.8×10^{-7}		Yaws (2003)	X	237
$C_{12}H_{26}$	1.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[62185-16-4]	8.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
ASDDXPPGGPFNIL-UHFFFAOYSA-N					
tridecane	3.4×10^{-6}		Duchowicz et al. (2020)	V	186
$C_{13}H_{28}$	1.4×10^{-6}		Yaws (2003)	X	237
[629-50-5]	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
IIYFAKIEWZDVMP-UHFFFAOYSA-N	5.9×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
	7.9×10^{-7}		Hilal et al. (2008)	Q	
	1.5×10^{-6}		Yaws (1999)	?	21
	4.3×10^{-6}		Yaws and Yang (1992)	?	21
2-methyldodecane	1.5×10^{-6}		Yaws (2003)	X	237
$C_{13}H_{28}$	4.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[1560-97-0]	1.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
HGEMCUOAMCILCP-UHFFFAOYSA-N					
3-methyldodecane	1.5×10^{-6}		Yaws (2003)	X	237
$C_{13}H_{28}$	4.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-57-1]	1.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
GRJUENNHVNYCHD-UHFFFAOYSA-N					
2,2-dimethylundecane	1.1×10^{-6}		Yaws (2003)	X	237
$C_{13}H_{28}$	3.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-64-0]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
QDKSGHXRHXVMPF-UHFFFAOYSA-N					
2,3-dimethylundecane	1.3×10^{-6}		Yaws (2003)	X	237
$C_{13}H_{28}$	4.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-77-5]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
QSSUTSOGIQHRIU-UHFFFAOYSA-N					
2,4-dimethylundecane	1.2×10^{-6}		Yaws (2003)	X	237
$C_{13}H_{28}$	2.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[17312-80-0]	1.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
WMZNFELFMFOGCC-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tetradecane	9.3×10^{-7}		Plyasunov and Shock (2000)	L	
$C_{14}H_{30}$	1.1×10^{-6}		Duchowicz et al. (2020)	V	186
[629-59-4]	1.1×10^{-6}		HSDB (2015)	V	
BGHCVCJVXZWKCC-UHFFFAOYSA-N	2.6×10^{-6}		Eastcott et al. (1988)	V	
	7.4×10^{-6}		Abraham (1984)	V	
	7.2×10^{-6}		Yaws (2003)	X	237
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	6.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	3.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
	5.6×10^{-7}		Hilal et al. (2008)	Q	
	2.9×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	2.2×10^{-6}		Yao et al. (2002)	Q	229
	7.2×10^{-6}		Yaws (1999)	?	21
	8.7×10^{-6}		Yaws and Yang (1992)	?	21
2-methyltridecane	2.4×10^{-6}		Yaws (2003)	X	237
$C_{14}H_{30}$	5.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[1560-96-9]	2.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
CJBFZKZYIPBBTO-UHFFFAOYSA-N					
3-methyltridecane	2.5×10^{-6}		Yaws (2003)	X	237
$C_{14}H_{30}$	5.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[6418-41-3]	2.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
NLHRRMKILFRDGV-UHFFFAOYSA-N					
2,2-dimethyldodecane	1.6×10^{-6}		Yaws (2003)	X	237
$C_{14}H_{30}$	4.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[49598-54-1]	1.8×10^{-6}		Gharagheizi et al. (2010)	Q	246
ATWISEHEXAEGKB-UHFFFAOYSA-N					
2,3-dimethyldodecane	2.1×10^{-6}		Yaws (2003)	X	237
$C_{14}H_{30}$	5.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[6117-98-2]	1.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
QBIXLGJCVGNDBJ-UHFFFAOYSA-N					
2,4-dimethyldodecane	1.6×10^{-6}		Yaws (2003)	X	237
$C_{14}H_{30}$	3.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[6117-99-3]	1.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
AFELDWXNIFIYOC-UHFFFAOYSA-N					
pentadecane	7.8×10^{-7}		Duchowicz et al. (2020)	V	186
$C_{15}H_{32}$	7.6×10^{-7}		HSDB (2015)	V	
[629-62-9]	1.1×10^{-5}		Yaws (2003)	X	237
YCOZIPAWZNQLMR-UHFFFAOYSA-N	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	7.1×10^{-6}		Gharagheizi et al. (2012)	Q	
	7.9×10^{-6}		Gharagheizi et al. (2010)	Q	246
	4.0×10^{-7}		Hilal et al. (2008)	Q	
	1.1×10^{-5}		Yaws (1999)	?	21
	2.1×10^{-5}		Yaws and Yang (1992)	?	21

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyltetradecane	4.9×10^{-6}		Yaws (2003)	X	237
$C_{15}H_{32}$	5.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[1560-95-8]	4.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
KUVMKLCGXIYSNH-UHFFFAOYSA-N					
3-methyltetradecane	5.1×10^{-6}		Yaws (2003)	X	237
$C_{15}H_{32}$	5.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[18435-22-8]	4.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
HXUYUZCPGPKNGS-UHFFFAOYSA-N					
2,2-dimethyltridecane	2.9×10^{-6}		Yaws (2003)	X	237
$C_{15}H_{32}$	4.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61869-04-3]	3.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
NVEUWWMNWPNXOC-UHFFFAOYSA-N					
2,3-dimethyltridecane	4.3×10^{-6}		Yaws (2003)	X	237
$C_{15}H_{32}$	5.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[18435-20-6]	3.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
SWUJSLXRUPXTQB-UHFFFAOYSA-N					
2,4-dimethyltridecane	2.6×10^{-6}		Yaws (2003)	X	237
$C_{15}H_{32}$	3.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-05-1]	3.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
JDFJCABQSZLDMZ-UHFFFAOYSA-N					
hexadecane	2.1×10^{-5}		Duchowicz et al. (2020)	V	186
$C_{16}H_{34}$	2.6×10^{-6}		Eastcott et al. (1988)	V	
[544-76-3]	2.7×10^{-5}		Abraham (1984)	V	
DCAYPVUWAIABOU-UHFFFAOYSA-N	2.1×10^{-5}		Yaws (2003)	X	237
	4.4×10^{-4}		Duchowicz et al. (2020)	Q	
	7.2×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
	2.9×10^{-7}		Hilal et al. (2008)	Q	
	2.1×10^{-5}		Yaws (1999)	?	21
	4.3×10^{-5}		Yaws and Yang (1992)	?	21
2-methylpentadecane	1.2×10^{-5}		Yaws (2003)	X	237
$C_{16}H_{34}$	5.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[1560-93-6]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
BANXPJUEBPWEOT-UHFFFAOYSA-N					
3-methylpentadecane	1.2×10^{-5}		Yaws (2003)	X	237
$C_{16}H_{34}$	6.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[2882-96-4]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
FWXKCXJPHSAYMK-UHFFFAOYSA-N					
2,2-dimethyltetradecane	6.5×10^{-6}		Yaws (2003)	X	237
$C_{16}H_{34}$	4.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[59222-86-5]	7.9×10^{-6}		Gharagheizi et al. (2010)	Q	246
VCAMXEBNASZVEZ-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-dimethyltetradecane	1.1×10^{-5}		Yaws (2003)	X	237
$C_{16}H_{34}$	6.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[18435-23-9]	7.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
ZQRVEWIJXCRTFW-UHFFFAOYSA-N					
2,4-dimethyltetradecane	5.1×10^{-6}		Yaws (2003)	X	237
$C_{16}H_{34}$	3.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-06-2]	7.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
NWTLFDYNCLTSAR-UHFFFAOYSA-N					
heptadecane	2.2×10^{-7}		Hilal et al. (2008)	Q	
$C_{17}H_{36}$	2.1×10^{-4}		Yaws (1999)	?	21
[629-78-7]	1.8×10^{-4}		Yaws and Yang (1992)	?	21
NDJKXXJCMXVBJW-UHFFFAOYSA-N					
octadecane	1.6×10^{-6}		Eastcott et al. (1988)	V	
$C_{18}H_{38}$	7.8×10^{-4}		Abraham (1984)	V	
[593-45-3]	1.5×10^{-7}		Hilal et al. (2008)	Q	
RZJRJXONCZWCBN-UHFFFAOYSA-N	6.1×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	3.6×10^{-4}		Yaws (1999)	?	21
	1.1×10^{-3}		Yaws and Yang (1992)	?	21
nonadecane	1.3×10^{-7}		Hilal et al. (2008)	Q	
$C_{19}H_{40}$	9.3×10^{-4}		Yaws (1999)	?	21
[629-92-5]	3.4×10^{-3}		Yaws and Yang (1992)	?	21
LQERIDTXQFOHKA-UHFFFAOYSA-N					
eicosane	5.0×10^{-6}		Eastcott et al. (1988)	V	
$C_{20}H_{42}$	1.4×10^{-2}		Abraham (1984)	V	
[112-95-8]	9.7×10^{-8}		Hilal et al. (2008)	Q	
CBFCDTFDPHXCNY-UHFFFAOYSA-N	2.3×10^{-3}		Yaws (1999)	?	21
	3.0×10^{-2}		Yaws and Yang (1992)	?	21
heneicosane	7.3×10^{-8}		Hilal et al. (2008)	Q	
$C_{21}H_{44}$					
[629-94-7]					
FNAZRRHPUDJQCJ-UHFFFAOYSA-N					
docosane	5.4×10^{-8}		Hilal et al. (2008)	Q	
$C_{22}H_{46}$					
[629-97-0]					
HOWGUJZVBDQJKV-UHFFFAOYSA-N					
tricosane	4.1×10^{-8}		Hilal et al. (2008)	Q	
$C_{23}H_{48}$					
[638-67-5]					
FIGVVZUWCLSUEI-UHFFFAOYSA-N					

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tetracosane $C_{24}H_{50}$ [646-31-1] POOSGDOYLQNASK-UHFFFAOYSA-N	3.1×10^{-8}		Hilal et al. (2008)	Q	
pentacosane $C_{25}H_{52}$ [629-99-2] YKNWIILGEFFOPE-UHFFFAOYSA-N	1.5×10^{-8}		Hilal et al. (2008)	Q	
hexacosane $C_{26}H_{54}$ [630-01-3] HMSWAIKSFDFLKN-UHFFFAOYSA-N	5.0×10^{-5} 1.3×10^{2} 1.1×10^{-8}		Eastcott et al. (1988) Abraham (1984) Hilal et al. (2008)	V V Q	
heptacosane $C_{27}H_{56}$ [593-49-7] BJQWYEJQWHSSCJ-UHFFFAOYSA-N	7.7×10^{-9}		Hilal et al. (2008)	Q	
octacosane $C_{28}H_{58}$ [630-02-4] ZYURHZPYMFLWSH-UHFFFAOYSA-N	5.6×10^{-9}		Hilal et al. (2008)	Q	
nonacosane $C_{29}H_{60}$ [630-03-5] IGGUPRCHHJZPBS-UHFFFAOYSA-N	4.0×10^{-9}		Hilal et al. (2008)	Q	
triacontane $C_{30}H_{62}$ [638-68-6] JXTPJDDICSTXJX-UHFFFAOYSA-N	2.9×10^{-9}		Hilal et al. (2008)	Q	
dotriacontane $C_{32}H_{66}$ [544-85-4] QHMGJGNTMQDRQA-UHFFFAOYSA-N	1.5×10^{-9}		Hilal et al. (2008)	Q	
pentatriacontane $C_{35}H_{72}$ [630-07-9] VHQQPFLOGSTQPC-UHFFFAOYSA-N	5.8×10^{-10}		Hilal et al. (2008)	Q	
hexatriacontane $C_{36}H_{74}$ [630-06-8] YDLYQMBWCWFRAI-UHFFFAOYSA-N	8.6×10^{8}		Abraham (1984)	V	

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Table A2.1: Alkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
octatriacontane $C_{38}H_{78}$ [7194-85-6] BVKCQBBZBGYNOP-UHFFFAOYSA-N	2.2×10^{-10}		Hilal et al. (2008)	Q	

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A2.2 Cycloalkanes

Table A2.2: Cycloalkanes

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyclopropane	1.2×10^{-4}	2800	Plyasunov and Shock (2000)	L	
C_3H_6	1.1×10^{-4}	1600	Wilhelm et al. (1977)	L	
[75-19-4]	8.1×10^{-5}		Steward et al. (1973)	L	14
LVZWSLJZHVFIQJ-UHFFFAOYSA-N	1.1×10^{-4}	2300	Allott et al. (1973)	L	
	7.8×10^{-5}		Guitart et al. (1989)	M	14
	1.1×10^{-4}	2000	Saidman et al. (1966)	M	
	1.2×10^{-5}		Duchowicz et al. (2020)	V	186
	1.2×10^{-5}		HSDB (2015)	V	
	1.3×10^{-4}		Irmann (1965)	V	
	1.3×10^{-4}		Yaws (2003)	X	237, 294
	1.1×10^{-4}		Hayer et al. (2022)	Q	20
	3.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.6×10^{-5}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-5}		Raventos-Duran et al. (2010)	Q	271, 243
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.4×10^{-4}		Hilal et al. (2008)	Q	
	2.3×10^{-5}		Modarresi et al. (2007)	Q	67
		2500	Kühne et al. (2005)	Q	
	1.2×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	7.3×10^{-5}		English and Carroll (2001)	Q	230, 231
	3.9×10^{-5}		Katritzky et al. (1998)	Q	
	9.0×10^{-5}		Nirmalakhandan et al. (1997)	Q	
		2200	Kühne et al. (2005)	?	
	1.3×10^{-4}		Yaws (1999)	?	21, 294
	1.1×10^{-4}	1600	Yaws et al. (1999)	?	21
	1.3×10^{-4}		Yaws and Yang (1992)	?	21, 294
	1.1×10^{-4}		Abraham et al. (1990)	?	
cyclobutane	1.3×10^{-6}		Hayer et al. (2022)	Q	20
C_4H_8	7.0×10^{-5}		HSDB (2015)	Q	99
[287-23-0]					
PMPVIKIVABFJJI-UHFFFAOYSA-N					
cyclopentane	5.8×10^{-5}	3500	Brockbank (2013)	L	1
C_5H_{10}	5.5×10^{-5}	3200	Plyasunov and Shock (2000)	L	
[287-92-3]	5.4×10^{-5}		Mackay and Shiu (1981)	L	
RGSFGYAAUTVSQA-UHFFFAOYSA-N	6.5×10^{-5}	3400	Hansen et al. (1993)	M	281
	5.6×10^{-5}		Mackay et al. (2006a)	V	
	5.2×10^{-5}		Mackay et al. (1993)	V	
	5.5×10^{-5}		Hwang et al. (1992)	V	
	5.4×10^{-5}		Eastcott et al. (1988)	V	
	5.3×10^{-5}		Hine and Mookerjee (1975)	V	
	5.6×10^{-5}		McAuliffe (1963)	V	
	5.3×10^{-5}		Yaws (2003)	X	258

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.2×10^{-5}		Yaws (2003)	X	237
	6.2×10^{-5}		Dupeux et al. (2022)	Q	259
	4.9×10^{-5}		Keshavarz et al. (2022)	Q	
	3.6×10^{-3}		Duchowicz et al. (2020)	Q	184
	5.2×10^{-5}		HSDB (2015)	Q	99
	3.0×10^{-5}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	5.8×10^{-5}		Gharagheizi et al. (2010)	Q	246
	1.1×10^{-4}		Hilal et al. (2008)	Q	
	1.2×10^{-5}		Modarresi et al. (2007)	Q	67
		3200	Kühne et al. (2005)	Q	
	3.1×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	4.8×10^{-5}		Yao et al. (2002)	Q	229
	3.8×10^{-5}		English and Carroll (2001)	Q	230, 231
	3.5×10^{-5}		Katritzky et al. (1998)	Q	
	4.3×10^{-5}		Suzuki et al. (1992)	Q	232
	5.7×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	6.5×10^{-5}		Duchowicz et al. (2020)	?	185, 21
		4300	Kühne et al. (2005)	?	
	5.3×10^{-5}		Yaws (1999)	?	21
	5.2×10^{-5}		Yaws and Yang (1992)	?	21
	5.3×10^{-5}		Abraham et al. (1990)	?	
	5.3×10^{-5}		Abraham (1979)	?	
cyclohexane C_6H_{12} [110-82-7] XDTMQSROBMDMFD-UHFFFAOYSA-N	5.1×10^{-5}	3900	Brockbank (2013)	L	1, 295
	5.3×10^{-5}	4000	Plyasunov and Shock (2000)	L	
	5.6×10^{-5}		Mackay and Shiu (1981)	L	
	3.2×10^{-4}	5400	Hiatt (2013)	M	
	8.0×10^{-5}		Helburn et al. (2008)	M	
	5.2×10^{-5}	4500	Dewulf et al. (1999)	M	296
	6.0×10^{-5}		Hansen et al. (1993)	M	297
	5.4×10^{-5}	3800	Kolb et al. (1992)	M	277
	3.4×10^{-5}		Guitart et al. (1989)	M	14
	5.5×10^{-5}	3200	Ashworth et al. (1988)	M	278
	5.4×10^{-5}	3400	Tsonopoulos and Wilson (1983)	M	1
	5.4×10^{-5}	3800	Tucker et al. (1981)	M	
	5.3×10^{-5}		Mackay et al. (2006a)	V	
	5.1×10^{-5}		Mackay et al. (1993)	V	
	6.0×10^{-5}		Hwang et al. (1992)	V	
	5.4×10^{-5}		Eastcott et al. (1988)	V	
	5.1×10^{-5}		Hine and Mookerjee (1975)	V	
	5.6×10^{-5}		McAuliffe (1963)	V	
	5.4×10^{-5}	4000	Plyasunov et al. (2001)	T	
		4000	Gill et al. (1976)	T	
	5.0×10^{-5}		Yaws (2003)	X	258
	5.1×10^{-5}		Yaws (2003)	X	237

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.2×10^{-5}	710	Goldstein (1982)	X	298
	6.7×10^{-5}		Dupeux et al. (2022)	Q	259
	6.6×10^{-5}		Keshavarz et al. (2022)	Q	
	3.6×10^{-3}		Duchowicz et al. (2020)	Q	299
	1.6×10^{-4}		Wang et al. (2017)	Q	80, 238
	9.6×10^{-5}		Wang et al. (2017)	Q	80, 239
	1.5×10^{-4}		Wang et al. (2017)	Q	80, 240
	2.7×10^{-5}		Gharagheizi et al. (2012)	Q	
	5.0×10^{-5}		Gharagheizi et al. (2010)	Q	246
	9.5×10^{-5}		Hilal et al. (2008)	Q	
	2.3×10^{-5}		Modarresi et al. (2007)	Q	67
		3600	Kühne et al. (2005)	Q	
	5.8×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	3.4×10^{-5}		Yao et al. (2002)	Q	229
	2.7×10^{-5}		English and Carroll (2001)	Q	230, 274
	3.4×10^{-5}		Katritzky et al. (1998)	Q	
	3.4×10^{-5}		Suzuki et al. (1992)	Q	232
	4.5×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	6.6×10^{-5}		Duchowicz et al. (2020)	?	185, 21
		3900	Kühne et al. (2005)	?	
	5.1×10^{-5}		Yaws (1999)	?	21
	3.1×10^{-5}		Abraham and Weathersby (1994)	?	21
	5.1×10^{-5}		Yaws and Yang (1992)	?	21
	5.1×10^{-5}		Abraham et al. (1990)	?	
	5.1×10^{-5}		Abraham (1979)	?	
methylcyclopentane	2.8×10^{-5}		Brockbank (2013)	L	
$C_5H_9CH_3$	2.8×10^{-5}	5500	Plyasunov and Shock (2000)	L	
[96-37-7]	2.7×10^{-5}		Mackay and Shiu (1981)	L	
GDOPTJXRTPNYNR-UHFFFAOYSA-N	2.7×10^{-5}		Duchowicz et al. (2020)	V	186
	2.7×10^{-5}		HSDB (2015)	V	
	2.8×10^{-5}		Mackay et al. (2006a)	V	
	2.7×10^{-5}		Mackay et al. (1993)	V	
	2.7×10^{-5}		Eastcott et al. (1988)	V	
	2.7×10^{-5}		Hine and Mookerjee (1975)	V	
	2.9×10^{-5}		McAuliffe (1963)	V	
	2.8×10^{-5}		Yaws (2003)	X	237
	1.4×10^{-3}		Duchowicz et al. (2020)	Q	
	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	271, 243
	4.9×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	3.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
	4.4×10^{-5}		Hilal et al. (2008)	Q	
	1.1×10^{-5}		Modarresi et al. (2007)	Q	67
	2.9×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	2.6×10^{-5}		Yao et al. (2002)	Q	229
	2.7×10^{-5}		English and Carroll (2001)	Q	230, 231

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	3.6×10^{-5}		Katritzky et al. (1998)	Q	
	3.1×10^{-5}		Suzuki et al. (1992)	Q	232
	3.9×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	2.8×10^{-5}		Yaws (1999)	?	21
	1.7×10^{-5}		Abraham and Weathersby (1994)	?	21
	2.8×10^{-5}		Yaws and Yang (1992)	?	21
cycloheptane	6.7×10^{-5}		Brockbank (2013)	L	
C_7H_{14}	1.0×10^{-4}	3100	Plyasunov and Shock (2000)	L	
[291-64-5]	1.1×10^{-4}		Duchowicz et al. (2020)	V	186
DMEGYFMYUHOHGS-UHFFFAOYSA-N	8.2×10^{-5}		Mackay et al. (2006a)	V	
	1.0×10^{-4}		Mackay et al. (1993)	V	
	1.1×10^{-4}		Cabani et al. (1981)	V	
	1.1×10^{-4}		Yaws (2003)	X	258
	1.1×10^{-4}		Yaws (2003)	X	237
	1.2×10^{-4}		Dupeux et al. (2022)	Q	259
	3.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.5×10^{-5}		HSDB (2015)	Q	99
	3.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	5.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
	5.1×10^{-5}		Hilal et al. (2008)	Q	
	8.3×10^{-6}		Modarresi et al. (2007)	Q	67
	1.1×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	3.2×10^{-5}		Katritzky et al. (1998)	Q	
	1.1×10^{-4}		Yaws (1999)	?	21
	1.6×10^{-3}		Hoff et al. (1993)	?	21
	1.1×10^{-4}		Yaws and Yang (1992)	?	21
methylcyclohexane	2.6×10^{-5}	4500	Brockbank (2013)	L	1
$C_6H_{11}CH_3$	2.4×10^{-5}		Plyasunov and Shock (2000)	L	
[108-87-2]	2.5×10^{-5}		Mackay and Shiu (1981)	L	
UAEPNZWRGJTJPN-UHFFFAOYSA-N	3.2×10^{-4}	5300	Hiatt (2013)	M	
	1.5×10^{-4}		Ramachandran et al. (1996)	M	
	9.6×10^{-5}	9400	Hansen et al. (1993)	M	281
	5.0×10^{-6}		Abraham and Acree (2007)	V	
	2.5×10^{-5}		Mackay et al. (2006a)	V	
	2.3×10^{-5}		Mackay et al. (1993)	V	
	2.3×10^{-5}		Meylan and Howard (1991)	V	
	2.6×10^{-5}		Eastcott et al. (1988)	V	
	2.3×10^{-5}		Hine and Mookerjee (1975)	V	
	2.7×10^{-5}		McAuliffe (1963)	V	
	2.3×10^{-5}		Yaws (2003)	X	237
	8.9×10^{-5}		Keshavarz et al. (2022)	Q	
	1.4×10^{-3}		Duchowicz et al. (2020)	Q	299
	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	

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Table A2.2: Cycloalkanes (. . . continued)

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	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	271, 243
	3.9×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	2.4×10^{-5}		Gharagheizi et al. (2010)	Q	246
	3.5×10^{-5}		Hilal et al. (2008)	Q	
	2.1×10^{-5}		Modarresi et al. (2007)	Q	67
		3900	Kühne et al. (2005)	Q	
	2.5×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	2.7×10^{-5}		Yao et al. (2002)	Q	229
	1.9×10^{-5}		English and Carroll (2001)	Q	230, 260
	3.5×10^{-5}		Katritzky et al. (1998)	Q	
	8.6×10^{-5}		Russell et al. (1992)	Q	279
	2.3×10^{-5}		Suzuki et al. (1992)	Q	232
	2.9×10^{-5}		Meylan and Howard (1991)	Q	
	3.1×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	2.3×10^{-5}		Duchowicz et al. (2020)	?	185, 21
		3100	Kühne et al. (2005)	?	
	2.3×10^{-5}		Yaws (1999)	?	21
	2.3×10^{-5}		Yaws and Yang (1992)	?	21
methylcyclohexane-d14 $C_6D_{11}CD_3$ [10120-28-2] UAEPNZWRGJTJPN-OBYKGMMLSA-N	3.1×10^{-4}	5600	Hiatt (2013)	M	
ethylcyclopentane C_7H_{14} [1640-89-7] IFTRQJLVEBNKJK-UHFFFAOYSA-N	1.8×10^{-5}		Yaws (2003)	X	237
	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	246
	2.4×10^{-5}		Yao et al. (2002)	Q	229
	1.8×10^{-5}		Yaws (1999)	?	21
1,1-dimethylcyclopentane C_7H_{14} [1638-26-2] QWHNJUXXYKPLQM-UHFFFAOYSA-N	2.3×10^{-5}		Yaws (2003)	X	237
	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	246
	1.7×10^{-5}		Yao et al. (2002)	Q	229
	2.3×10^{-5}		Yaws (1999)	?	21
cis-1,2-dimethylcyclopentane C_7H_{14} [1192-18-3] RIRARCHMRDHZAR-KNVOCYPGSA-N	1.9×10^{-5}		Yaws (2003)	X	237
	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	246
	1.9×10^{-5}		Yaws (1999)	?	21
cis-1,3-dimethylcyclopentane C_7H_{14} [2532-58-3] XAZKFISIRYLAEE-KNVOCYPGSA-N	2.2×10^{-5}		Yaws (2003)	X	237
	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	246
	2.2×10^{-5}		Yaws (1999)	?	21

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
trans-1,2-dimethylcyclopentane	2.2×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[822-50-4]	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	246
RIRARCHMRDHZAR-RNFRBKRXSA-N	2.2×10^{-5}		Yaws (1999)	?	21
trans-1,3-dimethylcyclopentane	2.2×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[1759-58-6]	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	246
XAZKFISIRYLAEE-RNFRBKRXSA-N	2.2×10^{-5}		Yaws (1999)	?	21
cyclooctane	7.3×10^{-5}	4800	Brockbank (2013)	L	1
C_8H_{16}	9.3×10^{-5}	3800	Plyasunov and Shock (2000)	L	
[292-64-8]	6.9×10^{-5}	4700	Dohányosová et al. (2004)	M	300
WJTCGQSWYFHTAC-UHFFFAOYSA-N	6.9×10^{-5}		Mackay et al. (2006a)	V	
	9.3×10^{-5}		Mackay et al. (1993)	V	
	9.5×10^{-5}		Cabani et al. (1981)	V	
	9.7×10^{-5}		Yaws (2003)	X	237
	3.1×10^{-5}		Gharagheizi et al. (2012)	Q	
	9.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
	7.5×10^{-5}		Hilal et al. (2008)	Q	
	7.4×10^{-6}		Modarresi et al. (2007)	Q	67
		4300	Kühne et al. (2005)	Q	
		5000	Kühne et al. (2005)	?	
	9.8×10^{-5}		Hoff et al. (1993)	?	21
	9.5×10^{-5}		Yaws and Yang (1992)	?	21
methylcycloheptane	2.1×10^{-5}		Hilal et al. (2008)	Q	
C_8H_{16}					
[4126-78-7]					
GYNNXHKOJHMOHS-UHFFFAOYSA-N					
1,1-dimethylcyclohexane	1.8×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	8.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[590-66-9]	1.6×10^{-5}		Gharagheizi et al. (2010)	Q	246
QEGNUYASOUJEHD-UHFFFAOYSA-N	2.0×10^{-5}		Yao et al. (2002)	Q	229
	1.8×10^{-5}		Yaws (1999)	?	21
1,2-dimethylcyclohexane	2.8×10^{-5}		Duchowicz et al. (2020)	V	186
$C_6H_{10}(CH_3)_2$	2.1×10^{-5}		Mackay et al. (1993)	V	
[583-57-3]	5.5×10^{-4}		Duchowicz et al. (2020)	Q	
KVZJLSYJROEPSQ-UHFFFAOYSA-N	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	271, 243
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	1.4×10^{-5}		Hilal et al. (2008)	Q	
	3.1×10^{-5}		Katritzky et al. (1998)	Q	
	1.7×10^{-5}		Suzuki et al. (1992)	Q	232
	2.3×10^{-5}		Nirmalakhandan and Speece (1988)	Q	

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Table A2.2: Cycloalkanes (. . . continued)

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cis-1,2-dimethylcyclohexane	2.6×10^{-5}	4600	Brockbank (2013)	L	1
$C_6H_{10}(CH_3)_2$	2.8×10^{-5}		Plyasunov and Shock (2000)	L	
[2207-01-4]	2.8×10^{-5}		Mackay and Shiu (1981)	L	
KVZJLSYJROEPSQ-OCAPTIKFSA-N	2.7×10^{-5}	4600	Dohányosová et al. (2004)	M	301
	2.8×10^{-5}		Duchowicz et al. (2020)	V	186
	4.6×10^{-6}		Abraham and Acree (2007)	V	
	2.8×10^{-5}		Mackay et al. (2006a)	V	
	2.8×10^{-5}		Meylan and Howard (1991)	V	
	2.8×10^{-5}		Eastcott et al. (1988)	V	
	2.8×10^{-5}		Hine and Mookerjee (1975)	V	
	2.8×10^{-5}		Yaws (2003)	X	237
	5.5×10^{-4}		Duchowicz et al. (2020)	Q	
	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	246
	2.3×10^{-5}		Modarresi et al. (2007)	Q	67
		4300	Kühne et al. (2005)	Q	
	2.9×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	1.4×10^{-5}		English and Carroll (2001)	Q	230, 231
	4.3×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	2.2×10^{-5}		Meylan and Howard (1991)	Q	
		4900	Kühne et al. (2005)	?	
	2.8×10^{-5}		Yaws (1999)	?	21
	2.8×10^{-5}		Yaws and Yang (1992)	?	21
trans-1,2-dimethylcyclohexane	1.6×10^{-5}	4000	Brockbank (2013)	L	1
$C_6H_{10}(CH_3)_2$	1.6×10^{-5}	4300	Dohányosová et al. (2004)	M	302
[6876-23-9]	1.8×10^{-5}		Duchowicz et al. (2020)	V	186
KVZJLSYJROEPSQ-HTQZYQBOSA-N	5.7×10^{-6}		Abraham and Acree (2007)	V	
	1.3×10^{-5}		Mackay et al. (1993)	V	
	1.6×10^{-5}		Yaws (2003)	X	237
	5.5×10^{-4}		Duchowicz et al. (2020)	Q	
	9.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	246
		4300	Kühne et al. (2005)	Q	
		4600	Kühne et al. (2005)	?	
	1.6×10^{-5}		Yaws (1999)	?	21
	2.1×10^{-5}		Yaws and Yang (1992)	?	21
			Haynes (2014)	W	303
cis-1,3-dimethylcyclohexane	1.8×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	8.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[638-04-0]	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	246
SGVUHPSBDNVHKL-OCAPTIKFSA-N	1.8×10^{-5}		Yaws (1999)	?	21
trans-1,3-dimethylcyclohexane	1.7×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	9.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[2207-03-6]	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	246
SGVUHPSBDNVHKL-HTQZYQBOSA-N	1.7×10^{-5}		Yaws (1999)	?	21

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
1,4-dimethylcyclohexane $C_6H_{10}(CH_3)_2$ [589-90-2] QRMPKOFEUHIBNM-UHFFFAOYSA-N	1.5×10^{-5}		Hilal et al. (2008)	Q	
cis-1,4-dimethylcyclohexane C_8H_{16} [624-29-3] QRMPKOFEUHIBNM-OCAPTIKFSA-N	1.7×10^{-5}		Yaws (2003)	X	237
	9.8×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	246
	1.7×10^{-5}		Yaws (1999)	?	21
trans-1,4-dimethylcyclohexane $C_6H_{10}(CH_3)_2$ [2207-04-7] QRMPKOFEUHIBNM-ZKCHVHJHSA-N	1.1×10^{-5}		Plyasunov and Shock (2000)	L	
	1.1×10^{-5}		Mackay and Shiu (1981)	L	
	1.1×10^{-5}		Duchowicz et al. (2020)	V	186
	1.1×10^{-5}		Mackay et al. (2006a)	V	
	1.1×10^{-5}		Mackay et al. (1993)	V	
	1.1×10^{-5}		Eastcott et al. (1988)	V	
	1.1×10^{-5}		Yaws (2003)	X	237
	5.5×10^{-4}		Duchowicz et al. (2020)	Q	
	8.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	246
	2.9×10^{-5}		Yaffe et al. (2003)	Q	248, 272
	1.4×10^{-5}		English and Carroll (2001)	Q	230, 231
	2.2×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	1.1×10^{-5}		Yaws (1999)	?	21
	1.1×10^{-5}		Yaws and Yang (1992)	?	21
ethylcyclohexane C_8H_{16} [1678-91-7] IIEWJVIFRVWJOD-UHFFFAOYSA-N	2.1×10^{-5}	4100	Brockbank (2013)	L	1, 304
	2.0×10^{-5}	4400	Dohányosová et al. (2004)	M	305
	3.1×10^{-5}	4600	Heidman et al. (1985)	M	1
	3.3×10^{-5}		Duchowicz et al. (2020)	V	186
	7.3×10^{-6}		Abraham and Acree (2007)	V	
	1.5×10^{-5}		Yaws (2003)	X	237
	1.4×10^{-3}		Duchowicz et al. (2020)	Q	
	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
	2.3×10^{-5}		Hilal et al. (2008)	Q	
		4300	Kühne et al. (2005)	Q	
	3.3×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	3.5×10^{-5}		Yao et al. (2002)	Q	229, 267
	3.4×10^{-5}		Katritzky et al. (1998)	Q	
		4700	Kühne et al. (2005)	?	
	1.5×10^{-5}		Yaws (1999)	?	21

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1,2-trimethylcyclopentane	1.3×10^{-5}		Yaws (2003)	X	237
$C_5H_7(CH_3)_3$	8.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[4259-00-1]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
WINCSBAYCULVDU-UHFFFAOYSA-N	6.9×10^{-6}		Hilal et al. (2008)	Q	
1,1,3-trimethylcyclopentane	6.2×10^{-6}		Plyasunov and Shock (2000)	L	
$C_5H_7(CH_3)_3$	6.3×10^{-6}		Mackay and Shiu (1981)	L	
[4516-69-2]	6.3×10^{-6}		Mackay et al. (2006a)	V	
OBKHYUIZSOIEPG-UHFFFAOYSA-N	6.3×10^{-6}		Mackay et al. (1993)	V	
	6.3×10^{-6}		Eastcott et al. (1988)	V	
	1.5×10^{-5}		Yaws (2003)	X	237
	6.2×10^{-6}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	271, 243
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
	6.2×10^{-6}		Yaffe et al. (2003)	Q	248, 249
1,*cis*-2,*cis*-3-trimethylcyclopentane	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	8.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[2613-69-6]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
VCWNHOPGKQCXIQ-RNLVFQAGSA-N					
1,*cis*-2,*trans*-3-trimethylcyclopentane	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	7.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[15890-40-1]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
VCWNHOPGKQCXIQ-JIGDXULJSA-N					
1,*trans*-2,*cis*-3-trimethylcyclopentane	1.4×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	6.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[19374-46-0]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
VCWNHOPGKQCXIQ-RNFRBKRXSA-N					
1,*cis*-2,*cis*-4-trimethylcyclopentane	1.3×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	7.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[2613-72-1]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
PNUFYSGVPVMNRN-RNLVFQAGSA-N					
1,*cis*-2,*trans*-4-trimethylcyclopentane	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	7.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[4850-28-6]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
PNUFYSGVPVMNRN-WHUPJOBBSA-N					

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
1,*trans*-2,*cis*-4-trimethylcyclopentane	1.4×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	6.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[16883-48-0]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
PNUFYSGVPVMNRN-HTQZYQBOSA-N					
1-methyl-1-ethylcyclopentane	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	9.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[16747-50-5]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
LETYIFNDQBJGPJ-UHFFFAOYSA-N	1.5×10^{-5}		Yao et al. (2002)	Q	229
	1.1×10^{-5}		Yaws (1999)	?	21
1-methyl-*cis*-2-ethylcyclopentane	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[930-89-2]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
BSKOLJVTLRLTHE-SFYZADRCSA-N					
1-methyl-*trans*-2-ethylcyclopentane	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	9.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[930-90-5]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
BSKOLJVTLRLTHE-HTQZYQBOSA-N					
1-methyl-*cis*-3-ethylcyclopentane	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	9.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[2613-66-3]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
PQXAPVOKLYINEI-SFYZADRCSA-N					
1-methyl-*trans*-3-ethylcyclopentane	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	9.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[2613-65-2]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
PQXAPVOKLYINEI-HTQZYQBOSA-N					
propylcyclopentane	1.1×10^{-5}		Plyasunov and Shock (2000)	L	
$C_5H_9C_3H_7$	1.1×10^{-5}		Mackay and Shiu (1981)	L	
[2040-96-2]	1.1×10^{-5}		Duchowicz et al. (2020)	V	186
KDIAMAVWIJYWHN-UHFFFAOYSA-N	1.1×10^{-5}		Mackay et al. (2006a)	V	
	1.1×10^{-5}		Mackay et al. (1993)	V	
	1.1×10^{-5}		Eastcott et al. (1988)	V	
	1.1×10^{-5}		Yaws (2003)	X	237
	1.4×10^{-3}		Duchowicz et al. (2020)	Q	
	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
	2.0×10^{-5}		Hilal et al. (2008)	Q	
	1.1×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	2.5×10^{-5}		Yao et al. (2002)	Q	229

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Table A2.2: Cycloalkanes (. . . continued)

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	3.2×10^{-5}		Katritzky et al. (1998)	Q	
	2.5×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	1.1×10^{-5}		Yaws (1999)	?	21
	1.1×10^{-5}		Yaws and Yang (1992)	?	21
isopropylcyclopentane	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[3875-51-2]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
TVSBRLGQVHJIKT-UHFFFAOYSA-N					
5,5-dimethylbicyclo[2.1.1]hexane	3.1×10^{-4}		Wang et al. (2017)	Q	80, 238
C_8H_{14}	1.7×10^{-5}		Wang et al. (2017)	Q	80, 239
(MCM:C8BC)	2.1×10^{-4}		Wang et al. (2017)	Q	80, 240
WZXMVFMYGAOEAT-UHFFFAOYSA-N					
1,1,2-trimethylcyclohexane	9.0×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	8.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[7094-26-0]	9.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
MEBONNVPKOBPEA-UHFFFAOYSA-N					
1,1,3-trimethylcyclohexane	9.3×10^{-6}		Plyasunov and Shock (2000)	L	
C_9H_{18}	9.5×10^{-6}		Mackay et al. (2006a)	V	
[3073-66-3]	9.5×10^{-6}		Mackay et al. (1993)	V	
PYOLJOJPIPCRDP-UHFFFAOYSA-N	1.2×10^{-5}		Yaws (2003)	X	237
	6.2×10^{-6}		Gharagheizi et al. (2012)	Q	
	9.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
1,1,4-trimethylcyclohexane	1.1×10^{-5}		Yaws (2003)	X	237
C_9H_{18}	5.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[7094-27-1]	9.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
UIWORXHEVNIOJG-UHFFFAOYSA-N					
1,*cis*-2,*cis*-3-trimethylcyclohexane	5.6×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	8.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[1839-88-9]	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	246
DQTVJLHNWPRPPH-AYMMMOKOSA-N					
1,*cis*-2,*trans*-3-trimethylcyclohexane	6.2×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	8.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[7667-55-2]	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	246
DQTVJLHNWPRPPH-BRPSZJMVSA-N					
1,*cis*-2,*cis*-4-trimethylcyclohexane	6.2×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	7.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[1678-80-4]	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	246
VCJPCEVERINRSG-YIZRAAEISA-N					

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,*cis*-2,*trans*-4-trimethylcyclohexane	6.7×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	7.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[7667-58-5]	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	246
VCJPCEVERINRSG-HLTSFMKQSA-N					
cis,*cis*-1,3,5-trimethylcyclohexane	1.7×10^{-5}		Yaws (2003)	X	237
C_9H_{18}	5.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[1795-27-3]	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	246
ODNRTOSCFYDTKF-AYMMMOKOSA-N					
cis,*trans*-1,3,5-trimethylcyclohexane	1.6×10^{-5}		Yaws (2003)	X	237
C_9H_{18}	6.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[1795-26-2]	6.1×10^{-6}		Gharagheizi et al. (2012)	Q	
ODNRTOSCFYDTKF-FBJIGQNJSA-N	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	246
1,*trans*-2,*cis*-3-trimethylcyclohexane	7.8×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	6.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[1678-81-5]	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	246
DQTVJLHNWPRPPH-HTQZYQBOSA-N					
1,*trans*-2,*cis*-4-trimethylcyclohexane	7.1×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	6.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[7667-59-6]	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	246
VCJPCEVERINRSG-DJLDLDEBSA-N					
1,*trans*-2,*trans*-4-trimethylcyclohexane	7.8×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	6.1×10^{-6}		Gharagheizi et al. (2012)	Q	
[7667-60-9]	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	246
VCJPCEVERINRSG-IWSPIJDZSA-N					
1-methyl-1-ethylcyclohexane	8.1×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[4926-90-3]	1.0×10^{-5}		Gharagheizi et al. (2010)	Q	246
YPJRYQGOKHKNKZ-UHFFFAOYSA-N					
1-methyl-*cis*-2-ethylcyclohexane	9.7×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[4923-77-7]	8.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
XARGIVYWQPXRTC-BDAKNGLRSA-N					
1-methyl-*cis*-3-ethylcyclohexane	1.1×10^{-5}		Yaws (2003)	X	237
C_9H_{18}	7.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[19489-10-2]	8.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
UDDVMPHNQKRNNS-BDAKNGLRSA-N					

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methyl-*cis*-4-ethylcyclohexane	1.2×10^{-5}		Yaws (2003)	X	237
C_9H_{18}	8.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[4926-78-7]	8.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
CYISMTMRBPPERU-DTORHVGOSA-N					
1-methyl-*trans*-2-ethylcyclohexane	1.0×10^{-5}		Yaws (2003)	X	237
C_9H_{18}	8.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[4923-78-8]	8.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
XARGIVYWQPXRTC-RKDXNWHRSA-N					
1-methyl-*trans*-3-ethylcyclohexane	1.1×10^{-5}		Yaws (2003)	X	237
C_9H_{18}	8.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[4926-76-5]	8.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
UDDVMPHNQKRNNS-RKDXNWHRSA-N					
1-methyl-*trans*-4-ethylcyclohexane	8.4×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	7.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[6236-88-0]	8.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
CYISMTMRBPPERU-KYZUINATSA-N					
propylcyclohexane	9.6×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[1678-92-8]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
DEDZSLCZHWTGOR-UHFFFAOYSA-N	4.9×10^{-5}		Yao et al. (2002)	Q	229
	9.6×10^{-6}		Yaws (1999)	?	21
isopropylcyclohexane	9.4×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[696-29-7]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
GWESVXSMPKAFAS-UHFFFAOYSA-N	2.7×10^{-5}		Yao et al. (2002)	Q	229, 267
	9.4×10^{-6}		Yaws (1999)	?	21
1,1,2,2-tetramethylcyclopentane	8.0×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	5.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[52688-89-8]	8.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
YXDMSFJDVHXFCV-UHFFFAOYSA-N					
cis-1,1,2,3-tetramethylcyclopentane	7.2×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	5.8×10^{-6}		Gharagheizi et al. (2012)	Q	
CXCBKSYSKZEEJB-YUMQZZPRSA-N	8.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
trans-1,1,2,3-tetramethylcyclopentane	8.4×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	4.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-70-0]	8.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
CXCBKSYSKZEEJB-SFYZADRCSA-N					

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cis-1,1,2,4-tetramethylcyclopentane	8.4×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	4.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-71-1]	8.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
AVBGIJNNMIBMQG-SFYZADRCSA-N					
trans-1,1,2,4-tetramethylcyclopentane	8.4×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	4.6×10^{-6}		Gharagheizi et al. (2012)	Q	
AVBGIJNNMIBMQG-YUMQZZPRSA-N	8.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
1,1,3,3-tetramethylcyclopentane	1.1×10^{-5}		Yaws (2003)	X	237
C_9H_{18}	3.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[50876-33-0]	8.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
YWYCGTZNHWYQBD-UHFFFAOYSA-N					
cis-1,1,3,4-tetramethylcyclopentane	8.0×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	5.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[53907-60-1]	8.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
OWHFMVURUNNXMJ-OCAPTIKFSA-N					
trans-1,1,3,4-tetramethylcyclopentane	9.9×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	3.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[20309-77-7]	8.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
OWHFMVURUNNXMJ-HTQZYQBOSA-N					
cis-1,2,2,3-tetramethylcyclopentane	7.2×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	5.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[18938-68-6]	8.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
DHLYDHNCPUAVHP-OCAPTIKFSA-N					
trans-1,2,2,3-tetramethylcyclopentane	7.2×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	5.8×10^{-6}		Gharagheizi et al. (2012)	Q	
DHLYDHNCPUAVHP-YUMQZZPRSA-N	8.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
1,*cis*-2,*cis*-3,*cis*-4-tetramethylcyclopentane	6.3×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	6.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[2532-65-2]	7.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
INYXDKODFMWKER-FNCVBFRFSA-N					
1,*cis*-2,*cis*-3,*trans*-4-tetramethylcyclopentane	7.2×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	7.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
[2532-69-6]					
INYXDKODFMWKER-BGZDPUMWSA-N					

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,*cis*-2,*trans*-3,*cis*-4-tetramethylcyclopentane	8.2×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	4.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[2532-68-5]	7.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
INYXDKODFMWKER-BZNPZCIMSA-N					
1,*trans*-2,*cis*-3,*trans*-4-tetramethylcyclopentane	8.8×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	3.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[2532-67-4]	7.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
INYXDKODFMWKER-HXFLIBJXSA-N					
1,*trans*-2,*trans*-3,*cis*-4-tetramethylcyclopentane	8.2×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	4.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[19907-40-5]	7.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
INYXDKODFMWKER-OJOKCITNSA-N					
1,1-dimethyl-2-ethylcyclopentane	7.7×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	6.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[54549-80-3]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
RXPIHZJWAFCHEJ-UHFFFAOYSA-N					
1,1-dimethyl-3-ethylcyclopentane	8.3×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	5.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-61-9]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
WXHYOGXBESCULU-UHFFFAOYSA-N					
1,*cis*-2-dimethyl-1-ethylcyclopentane	6.9×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	7.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-63-1]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
DRWDWIMYUGHJBR-DTWKUNHWSA-N					
1,*trans*-2-dimethyl-1-ethylcyclopentane	6.9×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	7.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-62-0]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
DRWDWIMYUGHJBR-RKDXNWHRSA-N					
1,*cis*-2-dimethyl-*cis*-3-ethylcyclopentane	6.0×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	8.0×10^{-6}		Gharagheizi et al. (2012)	Q	
UMUGNPFWQJAOJI-HLTSFMKQSA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
1,*trans*-2-dimethyl-*trans*-3-ethylcyclopentane	6.7×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	6.6×10^{-6}		Gharagheizi et al. (2012)	Q	
UMUGNPFWQJAOJI-HRDYMLBCSA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,*cis*-2-dimethyl-*trans*-3-ethylcyclopentane	6.7×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	6.6×10^{-6}		Gharagheizi et al. (2012)	Q	
UMUGNPFWQJAOJI-IWSPIJDZSA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
1,*trans*-2-dimethyl-*cis*-3-ethylcyclopentane	7.7×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	5.4×10^{-6}		Gharagheizi et al. (2012)	Q	
UMUGNPFWQJAOJI-VGMNWLOBSA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
1,*cis*-2-dimethyl-*cis*-4-ethylcyclopentane	6.5×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	7.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-64-2]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
QKXQNQVXTYSGKS-BRPSZJMVSA-N					
1,*cis*-2-dimethyl-*trans*-4-ethylcyclopentane	6.5×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	7.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-65-3]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
QKXQNQVXTYSGKS-AYMMMOKOSA-N					
1,*trans*-2-dimethyl-*cis*-4-ethylcyclopentane	7.4×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	5.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-66-4]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
QKXQNQVXTYSGKS-HTQZYQBOSA-N					
1,*cis*-3-dimethyl-1-ethylcyclopentane	8.0×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	5.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-68-6]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
OAWOMHRJVJMDLZ-DTWKUNHWSA-N					
1,*trans*-3-dimethyl-1-ethylcyclopentane	8.0×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	5.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-67-5]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
OAWOMHRJVJMDLZ-RKDXNWHRSA-N					
1,*cis*-3-dimethyl-*cis*-2-ethylcyclopentane	6.0×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	8.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[19903-00-5]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
JREISGVVJTVFBL-AYMMMOKOSA-N					
1,*cis*-3-dimethyl-*trans*-2-ethylcyclopentane	7.8×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	5.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[19902-98-8]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
JREISGVVJTVFBL-BRPSZJMVSA-N					

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,*trans*-3-dimethyl-*cis*-2-ethylcyclopentane	6.9×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	6.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[19902-99-9]	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
JREISGVVJTVFBL-HTQZYQBOSA-N					
1,*cis*-3-dimethyl-*cis*-4-ethylcyclopentane	6.7×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	6.6×10^{-6}		Gharagheizi et al. (2012)	Q	
VMCXXGFUCWAIIN-YIZRAAEISA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
1,*cis*-3-dimethyl-*trans*-4-ethylcyclopentane	7.8×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	5.2×10^{-6}		Gharagheizi et al. (2012)	Q	
VMCXXGFUCWAIIN-DJLDLDEBSA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
1,*trans*-3-dimethyl-*cis*-4-ethylcyclopentane	3.5×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	2.5×10^{-5}		Gharagheizi et al. (2012)	Q	
VMCXXGFUCWAIIN-CIUDSAMLSA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
1,*trans*-3-dimethyl-*trans*-4-ethylcyclopentane	6.7×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	6.6×10^{-6}		Gharagheizi et al. (2012)	Q	
VMCXXGFUCWAIIN-XHNCKOQMSA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
1-methyl-1-propylcyclopentane	7.2×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	8.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[16631-63-3]	7.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
HICYLMKNNFKEMK-UHFFFAOYSA-N					
1-methyl-*cis*-2-propylcyclopentane	6.4×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	8.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[932-43-4]	6.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
ADQJFBQXLAAVQA-BDAKNGLRSA-N					
1-methyl-*trans*-2-propylcyclopentane	7.1×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	7.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[932-44-5]	6.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
ADQJFBQXLAAVQA-RKDXNWHRSA-N					
1-methyl-*cis*-3-propylcyclopentane	6.9×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	7.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[2443-04-1]	6.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
HRSBIYASWAILIF-BDAKNGLRSA-N					

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methyl-*trans*-3-propylcyclopentane	6.9×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	7.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[2443-03-0]	6.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
HRSBIYASWAILIF-RKDXNWHRSA-N					
1-methyl-1-isopropylcyclopentane	6.5×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	8.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[61828-00-0]	7.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
XFMQGDWBNOQLEG-UHFFFAOYSA-N					
1-methyl-*cis*-2-isopropylcyclopentane	6.5×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	7.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-01-7]	7.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
CGWXYEIWDQDFIU-RKDXNWHRSA-N					
1-methyl-*trans*-2-isopropylcyclopentane	7.3×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	6.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[61828-01-1]	7.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
CGWXYEIWDQDFIU-BDAKNGLRSA-N					
1-methyl-*cis*-3-isopropylcyclopentane	7.2×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	6.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61828-02-2]	7.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
CDTDMKCVKCGRPD-BDAKNGLRSA-N					
1-methyl-*trans*-3-isopropylcyclopentane	7.2×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	6.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[61828-03-3]	7.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
CDTDMKCVKCGRPD-RKDXNWHRSA-N					
1,1-diethylcyclopentane	6.7×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	9.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[2721-38-2]	7.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
DPGQSDLGKGLNHC-UHFFFAOYSA-N					
1,*cis*-2-diethylcyclopentane	6.3×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	8.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[932-39-8]	6.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
JKMYLSLBFNMSFP-DTORHVGOSA-N					
1,*trans*-2-diethylcyclopentane	6.9×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	7.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[932-40-1]	6.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
JKMYLSLBFNMSFP-RKDXNWHRSA-N					

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,*cis*-3-diethylcyclopentane	6.7×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	8.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-59-5]	6.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
RUUVWUNHERVOAY-DTORHVGOSA-N					
1,*trans*-3-diethylcyclopentane	6.7×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	8.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[62016-60-8]	6.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
RUUVWUNHERVOAY-RKDXNWHRSA-N					
butylcyclopentane	6.5×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[2040-95-1]	8.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
ZAGHKONXGGSVDV-UHFFFAOYSA-N	6.5×10^{-6}		Yaws (1999)	?	21
isobutylcyclopentane	7.2×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	8.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[3788-32-7]	8.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
DPUYDFJBHDYVQM-UHFFFAOYSA-N					
sec-butylcyclopentane	6.5×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	9.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[4850-32-2]	8.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
DCEHVBLXWODXCW-UHFFFAOYSA-N					
tert-butylcyclopentane	6.7×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	7.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[3875-52-3]	7.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
BFWVYBVSRYIDHI-UHFFFAOYSA-N					
octahydro-1H-indene	8.8×10^{-5}		Hilal et al. (2008)	Q	
C_9H_{16}					
[496-10-6]					
BNRNAKTVFSZAFA-UHFFFAOYSA-N					
butylcyclohexane	7.2×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{20}$	8.5×10^{-6}		Gharagheizi et al. (2012)	Q	
[1678-93-9]	9.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
GGBJHURWWWLEQH-UHFFFAOYSA-N	7.2×10^{-6}		Yaws (1999)	?	21
pentylcyclopentane	5.3×10^{-6}		Plyasunov and Shock (2000)	L	
$C_{10}H_{20}$	5.4×10^{-6}		Mackay and Shiu (1981)	L	
[3741-00-2]	5.4×10^{-6}		Mackay et al. (2006a)	V	
HPQURZRDYMUHJI-UHFFFAOYSA-N	5.4×10^{-6}		Mackay et al. (1993)	V	
	5.4×10^{-6}		Eastcott et al. (1988)	V	
	5.2×10^{-6}		Yaws (2003)	X	237
	8.1×10^{-6}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-6}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	7.0×10^{-6}		Gharagheizi et al. (2010)	Q	246

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Table A2.2: Cycloalkanes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.2×10^{-6}		Hilal et al. (2008)	Q	
	5.8×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	1.6×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	5.4×10^{-6}		Yaws and Yang (1992)	?	21
decahydronaphthalene	7.2×10^{-5}	4100	Ashworth et al. (1988)	M	278
$C_{10}H_{18}$	2.1×10^{-5}		Duchowicz et al. (2020)	V	186
(decalin)	2.1×10^{-5}		HSDB (2015)	V	
[91-17-8]	4.4×10^{-3}		Duchowicz et al. (2020)	Q	
NNBZCPXTIHJBJL-UHFFFAOYSA-N	6.5×10^{-5}		Hilal et al. (2008)	Q	
		4500	Kühne et al. (2005)	Q	
	2.1×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	6.5×10^{-5}		Katritzky et al. (1998)	Q	
		4100	Kühne et al. (2005)	?	
(*Z*)-bicyclo[4.4.0]decane	4.3×10^{-4}		Mackay et al. (1993)	V	
$C_{10}H_{18}$	6.1×10^{-5}		Yaws (2003)	X	237
(*cis*-decahydronaphthalene; *cis*-decalin)	4.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[493-01-6]	8.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
NNBZCPXTIHJBJL-AOOOYVTPSA-N	6.1×10^{-5}		Yaws (1999)	?	21
(*E*)-bicyclo[4.4.0]decane	2.7×10^{-4}		Mackay et al. (1993)	V	
$C_{10}H_{18}$	3.9×10^{-5}		Yaws (2003)	X	237
(*trans*-decahydronaphthalene; *trans*-decalin)	2.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[493-02-7]	8.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
NNBZCPXTIHJBJL-MGCOHNPYSA-N	4.0×10^{-5}		Yaws (1999)	?	21
2,6,6-trimethylbicyclo[3.1.1]heptane $C_{10}H_{18}$ (dihydropinene) [473-55-2] XOKSLPVRUOBDEW-UHFFFAOYSA-N	2.8×10^{-5}		HSDB (2015)	Q	99
tricyclene $C_{10}H_{16}$ [508-32-7] RRBYUSWBLVXTQN-UHFFFAOYSA-N	4.9×10^{-5}		Plyasunov and Shock (2000)	L	
hexylcyclopentane	5.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{22}$	6.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[4457-00-5]	6.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
LKHGKBBAJAFMSQ-UHFFFAOYSA-N					
pentylcyclohexane	7.1×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{22}$	6.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[4292-92-6]	9.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
HLTMUYBTNSVOFY-UHFFFAOYSA-N					

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyclododecane $C_{12}H_{24}$ [294-62-2] DDTBPAQBQHZRDW-UHFFFAOYSA-N	6.4×10^{-6}		HSDB (2015)	Q	99
heptylcyclopentane $C_{12}H_{24}$ [5617-42-5] BOFNAOHMSHEKQL-UHFFFAOYSA-N	6.6×10^{-6} 9.8×10^{-6} 7.3×10^{-6}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
hexylcyclohexane $C_{12}H_{24}$ [4292-75-5] QHWAQXOSHHKCFK-UHFFFAOYSA-N	8.8×10^{-6} 7.4×10^{-6} 1.1×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
1,1'-bicyclohexyl $C_{12}H_{22}$ [92-51-3] WVIIMZNLDWSIRH-UHFFFAOYSA-N	3.1×10^{-5}		Hilal et al. (2008)	Q	
heptylcyclohexane $C_{13}H_{26}$ [5617-41-4] MSTLSCNJAHAQNU-UHFFFAOYSA-N	1.4×10^{-5} 1.3×10^{-5} 1.7×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
octylcyclopentane $C_{13}H_{26}$ [1795-20-6] HARXDULSBROLME-UHFFFAOYSA-N	1.1×10^{-5} 1.8×10^{-5} 1.0×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
octylcyclohexane $C_{14}H_{28}$ [1795-15-9] FBXWCEKQCVOOLT-UHFFFAOYSA-N	3.1×10^{-5} 2.1×10^{-5} 3.3×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
nonylcyclopentane $C_{14}H_{28}$ [2882-98-6] GDCYEUOAZVKNHT-UHFFFAOYSA-N	2.3×10^{-5} 2.0×10^{-5} 1.8×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
octahydro-1,1,2,3,3-pentamethyl-1H-indene $C_{14}H_{26}$ [33704-60-8] TUALLFJCLUYJEN-UHFFFAOYSA-N	9.0×10^{-6} 1.1×10^{-6} 6.5×10^{-4} 3.5×10^{-5}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
nonylcyclohexane $C_{15}H_{30}$ [2883-02-5] CLMFECCMAVQYQA-UHFFFAOYSA-N	8.7×10^{-5} 2.2×10^{-5} 8.7×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246

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Table A2.2: Cycloalkanes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
decylcyclopentane	6.4×10^{-5}		Yaws (2003)	X	237
$C_{15}H_{30}$	2.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[1795-21-7]	4.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
WOUVLFFZQCUYOL-UHFFFAOYSA-N					
decylcyclohexane	3.7×10^{-4}		Yaws (1999)	?	21
$C_{16}H_{32}$					
[1795-16-0]					
STWFZICHPLEOIC-UHFFFAOYSA-N					
1,1'-(2-methylpentane-2,4-diyl)dicyclohexane	2.9×10^{-6}		Zhang et al. (2010)	Q	287, 288
$C_{18}H_{34}$	2.1×10^{-6}		Zhang et al. (2010)	Q	287, 289
[38970-72-8]	1.1×10^{-3}		Zhang et al. (2010)	Q	287, 290
XUVKLBIJXLIPDZ-UHFFFAOYSA-N	1.9×10^{-5}		Zhang et al. (2010)	Q	287, 291
1,1':3',1"-tercyclohexane	6.7×10^{-6}		Zhang et al. (2010)	Q	287, 288
$C_{18}H_{32}$	1.5×10^{-5}		Zhang et al. (2010)	Q	287, 289
[1706-50-9]	1.7×10^{-3}		Zhang et al. (2010)	Q	287, 290
JBQRJHVXZMSLNH-UHFFFAOYSA-N	9.0×10^{-5}		Zhang et al. (2010)	Q	287, 291

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A2.3 Aliphatic alkenes and cycloalkenes

Table A2.3: Aliphatic alkenes and cycloalkenes

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethene	5.9×10^{-5}	2200	Burkholder et al. (2019)	L	1
C_2H_4	5.9×10^{-5}	2200	Burkholder et al. (2015)	L	1
(ethylene)	5.9×10^{-5}	2200	Sander et al. (2011)	L	1
[74-85-1]	5.9×10^{-5}	2200	Sander et al. (2006)	L	1
VGGSQFUCUMXWEO-UHFFFAOYSA-N	4.8×10^{-5}	2000	Plyasunov and Shock (2000)	L	
	4.7×10^{-5}	2000	Hayduk (1994)	L	1
	4.6×10^{-5}		Mackay and Shiu (1981)	L	
	4.7×10^{-5}	1800	Wilhelm et al. (1977)	L	
	3.5×10^{-5}		Steward et al. (1973)	L	14
	4.6×10^{-5}	2200	Allott et al. (1973)	L	
	4.9×10^{-5}	2000	Maaßen (1995)	M	306
	4.8×10^{-5}	1900	Reichl (1995)	M	307
	4.7×10^{-5}		McAuliffe (1966)	M	
	4.7×10^{-5}	2000	Morrison and Billett (1952)	M	308
	4.8×10^{-5}		Orcutt and Seevers (1937a)	M	
	3.4×10^{-5}		Grollman (1929)	M	58
	4.8×10^{-5}	2300	Winkler (1906)	M	
	4.6×10^{-5}		Hine and Mookerjee (1975)	V	
	4.7×10^{-5}	1900	Wauchope and Haque (1972)	V	
	3.1×10^{-5}		Pierotti (1965)	T	
	4.7×10^{-5}		Yaws (2003)	X	237
	4.7×10^{-5}		Deno and Berkheimer (1960)	C	
	3.4×10^{-5}		Hayer et al. (2022)	Q	20
	2.0×10^{-5}		Keshavarz et al. (2022)	Q	
	4.0×10^{-3}		Duchowicz et al. (2020)	Q	299
	2.1×10^{-4}		Wang et al. (2017)	Q	80, 238
	2.6×10^{-5}		Wang et al. (2017)	Q	80, 239
	8.3×10^{-5}		Wang et al. (2017)	Q	80, 240
	4.6×10^{-5}		Li et al. (2014)	Q	241
	2.4×10^{-5}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	6.8×10^{-5}		Gharagheizi et al. (2010)	Q	246
	2.9×10^{-5}		Hilal et al. (2008)	Q	
	1.0×10^{-4}		Modarresi et al. (2007)	Q	67
		2700	Kühne et al. (2005)	Q	
	4.7×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	8.2×10^{-5}		English and Carroll (2001)	Q	230, 231
	1.5×10^{-5}		Katritzky et al. (1998)	Q	
	9.5×10^{-5}		Suzuki et al. (1992)	Q	232
	5.2×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	4.3×10^{-5}		Duchowicz et al. (2020)	?	185, 21
		1900	Kühne et al. (2005)	?	
	4.8×10^{-5}		Yaws (1999)	?	21

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.1×10^{-5}	2400	Yaws et al. (1999)	?	21
	3.9×10^{-5}		Abraham and Weathersby (1994)	?	21
	4.8×10^{-5}	2000	Dean and Lange (1999)	?	309, 23
	4.7×10^{-5}		Yaws and Yang (1992)	?	21
	4.6×10^{-5}		Abraham et al. (1990)	?	
	4.8×10^{-5}		Seinfeld (1986)	?	21
propene	5.6×10^{-5}	2600	Plyasunov and Shock (2000)	L	
C_3H_6	4.7×10^{-5}		Mackay and Shiu (1981)	L	
(propylene)	7.3×10^{-5}	3400	Wilhelm et al. (1977)	L	
[115-07-1]	5.4×10^{-5}	2700	Maaßen (1995)	M	310
QQONPFPTGQHPMA-UHFFFAOYSA-N	5.4×10^{-5}	2800	Reichl (1995)	M	311
	4.8×10^{-5}		McAuliffe (1966)	M	
	4.7×10^{-5}		Hine and Mookerjee (1975)	V	
	4.4×10^{-5}		Irmann (1965)	V	
	4.8×10^{-5}		Yaws (2003)	X	237
	9.2×10^{-5}		Deno and Berkheimer (1960)	C	
	6.5×10^{-5}		Hayer et al. (2022)	Q	20
	2.7×10^{-5}		Keshavarz et al. (2022)	Q	
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	299
	2.5×10^{-4}		Wang et al. (2017)	Q	80, 238
	2.7×10^{-5}		Wang et al. (2017)	Q	80, 239
	8.5×10^{-5}		Wang et al. (2017)	Q	80, 240
	2.9×10^{-5}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	6.6×10^{-5}		Gharagheizi et al. (2010)	Q	246
	3.4×10^{-5}		Hilal et al. (2008)	Q	
	5.9×10^{-5}		Modarresi et al. (2007)	Q	67
		3100	Kühne et al. (2005)	Q	
	5.1×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	1.0×10^{-4}		Yao et al. (2002)	Q	229
	6.2×10^{-5}		English and Carroll (2001)	Q	230, 231
	4.4×10^{-5}		Katritzky et al. (1998)	Q	
	6.9×10^{-5}		Suzuki et al. (1992)	Q	232
	4.1×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	4.6×10^{-5}		Irmann (1965)	Q	
	5.0×10^{-5}		Duchowicz et al. (2020)	?	185, 21
		3800	Kühne et al. (2005)	?	
	4.8×10^{-5}		Yaws (1999)	?	21
	6.8×10^{-5}	2800	Yaws et al. (1999)	?	21
	4.8×10^{-5}		Yaws and Yang (1992)	?	21
	4.3×10^{-5}		Abraham et al. (1990)	?	

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-butene	4.2×10^{-5}	3000	Plyasunov and Shock (2000)	L	
C_4H_8	1.3×10^{-4}	6400	Wilhelm et al. (1977)	L	
[106-98-9]	4.5×10^{-5}	3000	Serra and Palavra (2003)	M	312
VXNZUUAINFGPBY-UHFFFAOYSA-N	4.0×10^{-5}		McAuliffe (1966)	M	
	3.9×10^{-5}		Mackay et al. (2006a)	V	
	3.9×10^{-5}		Mackay et al. (1993)	V	
	3.9×10^{-5}		Hine and Mookerjee (1975)	V	
	4.1×10^{-5}		Irmann (1965)	V	
	4.0×10^{-5}		Yaws (2003)	X	237
	5.5×10^{-5}		Hayer et al. (2022)	Q	20
	3.6×10^{-5}		Keshavarz et al. (2022)	Q	
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	184
	2.2×10^{-4}		Wang et al. (2017)	Q	80, 238
	3.2×10^{-5}		Wang et al. (2017)	Q	80, 239
	8.5×10^{-5}		Wang et al. (2017)	Q	80, 240
	3.9×10^{-5}		Li et al. (2014)	Q	241
	3.1×10^{-5}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	4.6×10^{-5}		Gharagheizi et al. (2010)	Q	246
	3.4×10^{-5}		Hilal et al. (2008)	Q	
	5.7×10^{-5}		Modarresi et al. (2007)	Q	67
	6.0×10^{-6}		Modarresi et al. (2005)	Q	247
	3.9×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	7.1×10^{-5}		Yao et al. (2002)	Q	229
	4.7×10^{-5}		English and Carroll (2001)	Q	230, 231
	5.6×10^{-5}		Katritzky et al. (1998)	Q	
	5.2×10^{-5}		Suzuki et al. (1992)	Q	232
	3.4×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	4.1×10^{-5}		Irmann (1965)	Q	
	4.2×10^{-5}		Duchowicz et al. (2020)	?	185, 21
	4.0×10^{-5}		Yaws (1999)	?	21
	4.0×10^{-5}		Yaws and Yang (1992)	?	21
	3.9×10^{-5}		Abraham et al. (1990)	?	
			Mackay and Shiu (1981)	W	313
2-butene	5.1×10^{-5}		Hilal et al. (2008)	Q	
C_4H_8					
[107-01-7]					
IAQRGUVFOMOMEM-UHFFFAOYSA-N					

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cis-2-butene	5.5×10^{-5}		Irmann (1965)	V	
C_4H_8	4.1×10^{-5}		Yaws (2003)	X	237
[590-18-1]	3.6×10^{-5}		Keshavarz et al. (2022)	Q	
IAQRGUVFOMOMEM-ARJAWSKDSA-N	5.2×10^{-4}		Duchowicz et al. (2020)	Q	299
	3.2×10^{-4}		Wang et al. (2017)	Q	314, 80, 238
	5.4×10^{-5}		Wang et al. (2017)	Q	314, 80, 239
	6.0×10^{-5}		Wang et al. (2017)	Q	314, 80, 240
	3.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	5.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
	4.5×10^{-5}		Modarresi et al. (2007)	Q	67
	6.9×10^{-6}		Modarresi et al. (2005)	Q	247
	9.1×10^{-5}		Yao et al. (2002)	Q	229
	5.9×10^{-5}		Irmann (1965)	Q	
	4.3×10^{-5}		Duchowicz et al. (2020)	?	185, 21
	4.1×10^{-5}		Yaws (1999)	?	21
trans-2-butene	3.9×10^{-5}		Irmann (1965)	V	
C_4H_8	4.3×10^{-5}		Yaws (2003)	X	237
[624-64-6]	1.0×10^{-4}		Hayer et al. (2022)	Q	20
IAQRGUVFOMOMEM-ONEGZZNKSA-N	3.6×10^{-5}		Keshavarz et al. (2022)	Q	
	5.2×10^{-4}		Duchowicz et al. (2020)	Q	
	3.2×10^{-4}		Wang et al. (2017)	Q	314, 80, 238
	5.4×10^{-5}		Wang et al. (2017)	Q	314, 80, 239
	6.0×10^{-5}		Wang et al. (2017)	Q	314, 80, 240
	2.7×10^{-5}		Gharagheizi et al. (2012)	Q	
	5.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
	4.5×10^{-5}		Modarresi et al. (2007)	Q	67
	8.5×10^{-6}		Modarresi et al. (2005)	Q	247
	7.9×10^{-5}		Yao et al. (2002)	Q	229
	5.4×10^{-5}		Irmann (1965)	Q	
	4.4×10^{-5}		Duchowicz et al. (2020)	?	185, 21
	4.3×10^{-5}		Yaws (1999)	?	21
2-methylpropene	5.7×10^{-5}	3000	Plyasunov and Shock (2000)	L	
C_4H_8	5.6×10^{-5}	3000	Wilhelm et al. (1977)	L	
(isobutene)	4.8×10^{-5}		McAuliffe (1966)	M	
[115-11-7]	4.6×10^{-5}		Mackay et al. (2006a)	V	
VQTUBCCKSQIDNK-UHFFFAOYSA-N	4.6×10^{-5}		Mackay et al. (1993)	V	
	4.6×10^{-5}		Hine and Mookerjee (1975)	V	
	4.8×10^{-5}		Yaws (2003)	X	237
	6.1×10^{-5}		Hayer et al. (2022)	Q	20
	3.6×10^{-5}		Keshavarz et al. (2022)	Q	

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.1×10^{-4}		Duchowicz et al. (2020)	Q	299
	1.6×10^{-4}		Wang et al. (2017)	Q	80, 238
	3.9×10^{-5}		Wang et al. (2017)	Q	80, 239
	9.3×10^{-5}		Wang et al. (2017)	Q	80, 240
	2.0×10^{-5}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	6.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
	8.6×10^{-5}		Hilal et al. (2008)	Q	
	4.6×10^{-5}		Modarresi et al. (2007)	Q	67
		3400	Kühne et al. (2005)	Q	
	8.2×10^{-6}		Modarresi et al. (2005)	Q	247
	4.7×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	6.5×10^{-5}		Yao et al. (2002)	Q	229
	4.8×10^{-5}		English and Carroll (2001)	Q	230, 231
	5.3×10^{-5}		Katritzky et al. (1998)	Q	
	4.5×10^{-5}		Suzuki et al. (1992)	Q	232
	2.8×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	4.5×10^{-5}		Duchowicz et al. (2020)	?	185, 21
		3000	Kühne et al. (2005)	?	
	4.8×10^{-5}		Yaws (1999)	?	21
	5.6×10^{-5}	3000	Yaws et al. (1999)	?	21
	4.8×10^{-5}		Yaws and Yang (1992)	?	21
			Mackay and Shiu (1981)	W	313
1-pentene C_5H_{10} [109-67-1] YWAKXRMUMFPDSH-UHFFFAOYSA-N	3.0×10^{-5}		Brockbank (2013)	L	
	2.4×10^{-5}		Plyasunov and Shock (2000)	L	
	2.5×10^{-5}		Mackay and Shiu (1981)	L	
	2.5×10^{-5}		Duchowicz et al. (2020)	V	186
	2.5×10^{-5}		HSDB (2015)	V	
	2.5×10^{-5}		Mackay et al. (2006a)	V	
	2.5×10^{-5}		Mackay et al. (1993)	V	
	2.5×10^{-5}		Eastcott et al. (1988)	V	
	1.8×10^{-5}		Amoore and Buttery (1978)	V	
	2.4×10^{-5}		Hine and Mookerjee (1975)	V	
	2.7×10^{-5}		McAuliffe (1966)	V	24
	2.5×10^{-5}		Yaws (2003)	X	237
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.7×10^{-4}		Wang et al. (2017)	Q	80, 238
	2.3×10^{-5}		Wang et al. (2017)	Q	80, 239
	7.6×10^{-5}		Wang et al. (2017)	Q	80, 240
	3.0×10^{-5}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-5}		Raventos-Duran et al. (2010)	Q	271, 243
	3.1×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	3.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
	2.5×10^{-5}		Hilal et al. (2008)	Q	

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.7×10^{-5}		Modarresi et al. (2007)	Q	67
	5.4×10^{-6}		Modarresi et al. (2005)	Q	247
	2.5×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	5.1×10^{-5}		Yao et al. (2002)	Q	229
	3.6×10^{-5}		English and Carroll (2001)	Q	230, 260
	6.0×10^{-5}		Katritzky et al. (1998)	Q	
	4.0×10^{-5}		Suzuki et al. (1992)	Q	232
	2.7×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	2.5×10^{-5}		Yaws (1999)	?	21
	2.5×10^{-5}		Yaws and Yang (1992)	?	21
	2.4×10^{-5}		Abraham et al. (1990)	?	
2-pentene C_5H_{10} [109-68-2] QMMOXUPEWRXHJS-UHFFFAOYSA-N	4.1×10^{-5}		Plyasunov and Shock (2000)	L	
	4.1×10^{-5}		Duchowicz et al. (2020)	V	186
	4.4×10^{-5}		Eastcott et al. (1988)	V	
	5.2×10^{-4}		Duchowicz et al. (2020)	Q	
	3.6×10^{-5}		Hilal et al. (2008)	Q	
	4.7×10^{-5}		Yaffe et al. (2003)	Q	248, 272
	6.1×10^{-5}		Katritzky et al. (1998)	Q	
cis-2-pentene C_5H_{10} [627-20-3] QMMOXUPEWRXHJS-HYXAFXHYSA-N	4.4×10^{-5}		Brockbank (2013)	L	
	4.4×10^{-5}		Mackay and Shiu (1981)	L	
	4.4×10^{-5}		Duchowicz et al. (2020)	V	186
	4.4×10^{-5}		Yaws (2003)	X	237
	5.2×10^{-4}		Duchowicz et al. (2020)	Q	
	2.6×10^{-4}		Wang et al. (2017)	Q	314, 80, 238
	3.7×10^{-5}		Wang et al. (2017)	Q	314, 80, 239
	5.8×10^{-5}		Wang et al. (2017)	Q	314, 80, 240
	4.5×10^{-5}		HSDB (2015)	Q	99
	2.7×10^{-5}		Gharagheizi et al. (2012)	Q	
	3.6×10^{-5}		Gharagheizi et al. (2010)	Q	246
	5.4×10^{-6}		Modarresi et al. (2005)	Q	247
	4.7×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	7.3×10^{-5}		Yao et al. (2002)	Q	229
	4.4×10^{-5}		Yaws (1999)	?	21
	4.4×10^{-5}		Yaws and Yang (1992)	?	21
trans-2-pentene C_5H_{10} [646-04-8] QMMOXUPEWRXHJS-HWKANZROSA-N	4.3×10^{-5}		Brockbank (2013)	L	
	4.3×10^{-5}		Duchowicz et al. (2020)	V	186
	4.2×10^{-5}		Hine and Mookerjee (1975)	V	
	4.3×10^{-5}		Yaws (2003)	X	237
	5.2×10^{-4}		Duchowicz et al. (2020)	Q	
	2.6×10^{-4}		Wang et al. (2017)	Q	314, 80, 238
	3.7×10^{-5}		Wang et al. (2017)	Q	314, 80, 239

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.9×10^{-5}		Wang et al. (2017)	Q	314, 80, 240
	3.1×10^{-5}		HSDB (2015)	Q	99
	2.6×10^{-5}		Gharagheizi et al. (2012)	Q	
	3.6×10^{-5}		Gharagheizi et al. (2010)	Q	246
	1.0×10^{-5}		Modarresi et al. (2005)	Q	247
	6.7×10^{-5}		Yao et al. (2002)	Q	229
	3.6×10^{-5}		English and Carroll (2001)	Q	230, 231
	4.0×10^{-5}		Suzuki et al. (1992)	Q	232
	2.7×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	4.3×10^{-5}		Yaws (1999)	?	21
	4.3×10^{-5}		Yaws and Yang (1992)	?	21
2-methyl-1-butene C_5H_{10} [563-46-2] MHNNAWXXUZQSNM-UHFFFAOYSA-N	2.3×10^{-5}		Duchowicz et al. (2020)	V	186
	2.3×10^{-5}		HSDB (2015)	V	
	3.3×10^{-5}		Yaws (2003)	X	237
	5.1×10^{-4}		Duchowicz et al. (2020)	Q	
	1.5×10^{-4}		Wang et al. (2017)	Q	80, 238
	4.6×10^{-5}		Wang et al. (2017)	Q	80, 239
	8.7×10^{-5}		Wang et al. (2017)	Q	80, 240
	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
	3.8×10^{-5}		Gharagheizi et al. (2010)	Q	246
	4.2×10^{-6}		Modarresi et al. (2005)	Q	247
	5.1×10^{-5}		Yao et al. (2002)	Q	229, 267
	3.4×10^{-5}		Yaws (1999)	?	21
2-methyl-2-butene C_5H_{10} [513-35-9] BKOOMYPCSUNDGP-UHFFFAOYSA-N	5.7×10^{-5}	3500	Brockbank (2013)	L	1
	6.7×10^{-5}	3600	Plyasunov and Shock (2000)	L	
	4.4×10^{-5}		Duchowicz et al. (2020)	V	186
	7.4×10^{-5}		Mackay et al. (2006a)	V	
	4.4×10^{-5}		Hine and Mookerjee (1975)	V	
	3.4×10^{-5}		Yaws (2003)	X	237
	1.7×10^{-4}		Duchowicz et al. (2020)	Q	
	2.1×10^{-4}		Wang et al. (2017)	Q	80, 238
	6.0×10^{-5}		Wang et al. (2017)	Q	80, 239
	6.3×10^{-5}		Wang et al. (2017)	Q	80, 240
	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
	4.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
	7.5×10^{-5}		Hilal et al. (2008)	Q	
	9.7×10^{-6}		Modarresi et al. (2005)	Q	247
	4.7×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	5.4×10^{-5}		Yao et al. (2002)	Q	229
	4.8×10^{-5}		English and Carroll (2001)	Q	230, 274
	5.8×10^{-5}		Katritzky et al. (1998)	Q	
	3.6×10^{-5}		Suzuki et al. (1992)	Q	232
	2.3×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	3.5×10^{-5}		Yaws (1999)	?	21

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-1-butene	1.9×10^{-5}		Plyasunov and Shock (2000)	L	
C_5H_{10}	1.8×10^{-5}		Mackay and Shiu (1981)	L	
[563-45-1]	1.9×10^{-5}		McAuliffe (1966)	M	
YHQXBTXEYZIYOV-UHFFFAOYSA-N	1.8×10^{-5}		HSDB (2015)	V	
	1.8×10^{-5}		Mackay et al. (2006a)	V	
	1.8×10^{-5}		Mackay et al. (1993)	V	
	1.8×10^{-5}		Hine and Mookerjee (1975)	V	
	1.9×10^{-5}		Yaws (2003)	X	237
	2.1×10^{-4}		Wang et al. (2017)	Q	80, 238
	1.4×10^{-5}		Wang et al. (2017)	Q	80, 239
	6.9×10^{-5}		Wang et al. (2017)	Q	80, 240
	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	3.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
	1.5×10^{-5}		Hilal et al. (2008)	Q	
	3.7×10^{-5}		Modarresi et al. (2007)	Q	67
	7.2×10^{-6}		Modarresi et al. (2005)	Q	247
	1.8×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	2.6×10^{-5}		Yao et al. (2002)	Q	229
	3.6×10^{-5}		English and Carroll (2001)	Q	230, 231
	5.7×10^{-5}		Katritzky et al. (1998)	Q	
	3.6×10^{-5}		Suzuki et al. (1992)	Q	232
	2.3×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	1.9×10^{-5}		Yaws (1999)	?	21
	1.9×10^{-5}		Yaws and Yang (1992)	?	21
1-hexene	2.5×10^{-5}		Brockbank (2013)	L	
C_6H_{12}	2.3×10^{-5}	3900	Plyasunov and Shock (2000)	L	
[592-41-6]	2.4×10^{-5}		Mackay and Shiu (1981)	L	
LIKMAJRDDDTEIG-UHFFFAOYSA-N	2.4×10^{-5}		Duchowicz et al. (2020)	V	186
	2.4×10^{-5}		HSDB (2015)	V	
	2.4×10^{-5}		Mackay et al. (2006a)	V	
	2.4×10^{-5}		Mackay et al. (1993)	V	
	2.4×10^{-5}		Hwang et al. (1992)	V	
	2.4×10^{-5}		Eastcott et al. (1988)	V	
	2.4×10^{-5}		Hine and Mookerjee (1975)	V	
	2.7×10^{-5}		McAuliffe (1966)	V	24
	2.4×10^{-5}		Yaws (2003)	X	237
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.4×10^{-4}		Wang et al. (2017)	Q	80, 238
	1.7×10^{-5}		Wang et al. (2017)	Q	80, 239
	7.1×10^{-5}		Wang et al. (2017)	Q	80, 240
	2.8×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	245

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
	1.8×10^{-5}		Hilal et al. (2008)	Q	
	3.6×10^{-5}		Modarresi et al. (2007)	Q	67
		4100	Kühne et al. (2005)	Q	
	4.0×10^{-6}		Modarresi et al. (2005)	Q	247
	2.5×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	2.5×10^{-5}		Yao et al. (2002)	Q	229, 267
	2.7×10^{-5}		English and Carroll (2001)	Q	230, 231
	6.1×10^{-5}		Katritzky et al. (1998)	Q	
	3.1×10^{-5}		Suzuki et al. (1992)	Q	232
	2.1×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
		4000	Kühne et al. (2005)	?	
	3.3×10^{-5}		Yaws (1999)	?	21
	3.3×10^{-5}		Yaws and Yang (1992)	?	21
	2.8×10^{-5}		Abraham et al. (1990)	?	
cis-2-hexene	2.6×10^{-5}		Yaws (2003)	X	237
C_6H_{12}	2.3×10^{-4}		Wang et al. (2017)	Q	314, 80, 238
[7688-21-3]	2.4×10^{-5}		Wang et al. (2017)	Q	314, 80, 239
RYPKRALMXUUNKS-HYXAFXHYSA-N	5.0×10^{-5}		Wang et al. (2017)	Q	314, 80, 240
	2.3×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
	5.8×10^{-6}		Modarresi et al. (2005)	Q	247
	3.0×10^{-5}		Yao et al. (2002)	Q	229
	2.6×10^{-5}		Yaws (1999)	?	21
trans-2-hexene	2.6×10^{-5}		Yaws (2003)	X	237
C_6H_{12}	2.3×10^{-4}		Wang et al. (2017)	Q	314, 80, 238
[4050-45-7]	2.4×10^{-5}		Wang et al. (2017)	Q	314, 80, 239
RYPKRALMXUUNKS-HWKANZROSA-N	5.0×10^{-5}		Wang et al. (2017)	Q	314, 80, 240
	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
	5.6×10^{-6}		Modarresi et al. (2005)	Q	247
	3.2×10^{-5}		Yao et al. (2002)	Q	229
	2.7×10^{-5}		Yaws (1999)	?	21
cis-3-hexene	2.6×10^{-5}		Yaws (2003)	X	237
C_6H_{12}	2.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[7642-09-3]	2.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
ZQDPJFUHLCOCRG-WAYWQWQTSA-N	4.5×10^{-6}		Modarresi et al. (2005)	Q	247
	3.3×10^{-5}		Yao et al. (2002)	Q	229
	2.7×10^{-5}		Yaws (1999)	?	21

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
trans-3-hexene	2.6×10^{-5}		Yaws (2003)	X	237
C_6H_{12}	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[13269-52-8]	2.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
ZQDPJFUHLCOCRG-AATRIKPKSA-N	5.4×10^{-6}		Modarresi et al. (2005)	Q	247
	3.1×10^{-5}		Yao et al. (2002)	Q	229
	2.7×10^{-5}		Yaws (1999)	?	21
2-methyl-1-pentene	3.3×10^{-5}		Plyasunov and Shock (2000)	L	
C_6H_{12}	3.6×10^{-5}		Mackay and Shiu (1981)	L	
[763-29-1]	3.6×10^{-5}		Duchowicz et al. (2020)	V	186
WWUVJRULCWHUSA-UHFFFAOYSA-N	3.6×10^{-5}		Mackay et al. (2006a)	V	
	3.6×10^{-5}		Mackay et al. (1993)	V	
	3.6×10^{-5}		Eastcott et al. (1988)	V	
	3.4×10^{-5}		Cabani et al. (1981)	V	
	3.5×10^{-5}		Yaws (2003)	X	237
	5.1×10^{-4}		Duchowicz et al. (2020)	Q	
	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	271, 243
	3.1×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	2.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
	2.2×10^{-5}		Hilal et al. (2008)	Q	
	5.8×10^{-6}		Modarresi et al. (2005)	Q	247
	3.6×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	4.5×10^{-5}		Yao et al. (2002)	Q	229
	2.1×10^{-5}		English and Carroll (2001)	Q	230, 231
	1.9×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	3.6×10^{-5}		Yaws (1999)	?	21
	3.5×10^{-5}		Yaws and Yang (1992)	?	21
3-methyl-1-pentene	2.8×10^{-5}		Yaws (2003)	X	237
C_6H_{12}	2.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[760-20-3]	2.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
LDTAOIUHUHHCMU-UHFFFAOYSA-N	6.2×10^{-6}		Modarresi et al. (2005)	Q	247
	2.1×10^{-5}		Yao et al. (2002)	Q	229
	2.8×10^{-5}		Yaws (1999)	?	21
4-methyl-1-pentene	1.5×10^{-5}		Plyasunov and Shock (2000)	L	
C_6H_{12}	1.6×10^{-5}		Mackay and Shiu (1981)	L	
[691-37-2]	1.6×10^{-5}		Duchowicz et al. (2020)	V	186
WSSSPWUEQFSQQG-UHFFFAOYSA-N	1.6×10^{-5}		Mackay et al. (2006a)	V	
	1.6×10^{-5}		Mackay et al. (1993)	V	
	1.6×10^{-5}		Eastcott et al. (1988)	V	
	1.6×10^{-5}		Hine and Mookerjee (1975)	V	
	1.6×10^{-5}		Yaws (2003)	X	237
	6.1×10^{-4}		Duchowicz et al. (2020)	Q	
	2.3×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	244

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
	1.2×10^{-5}		Hilal et al. (2008)	Q	
	3.4×10^{-5}		Modarresi et al. (2007)	Q	67
	7.3×10^{-6}		Modarresi et al. (2005)	Q	247
	1.6×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	2.7×10^{-5}		Yao et al. (2002)	Q	229
	2.7×10^{-5}		English and Carroll (2001)	Q	230, 231
	5.8×10^{-5}		Katritzky et al. (1998)	Q	
	2.8×10^{-5}		Suzuki et al. (1992)	Q	232
	1.8×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	1.6×10^{-5}		Yaws (1999)	?	21
	1.6×10^{-5}		Yaws and Yang (1992)	?	21
2-methyl-2-pentene	2.6×10^{-5}		Yaws (2003)	X	237
C_6H_{12}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[625-27-4]	2.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
JMMZCWZIJXAGKW-UHFFFAOYSA-N	7.9×10^{-6}		Modarresi et al. (2005)	Q	247
	4.8×10^{-5}		Yao et al. (2002)	Q	229, 267
	2.7×10^{-5}		Yaws (1999)	?	21
cis-3-methyl-2-pentene	2.6×10^{-5}		Yaws (2003)	X	237
C_6H_{12}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[922-62-3]	2.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
BEQGRRJLJLVQAQ-XQRVVYSFSA-N	2.7×10^{-5}		Yaws (1999)	?	21
trans-3-methyl-2-pentene	2.6×10^{-5}		Yaws (2003)	X	237
C_6H_{12}	1.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[616-12-6]	2.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
BEQGRRJLJLVQAQ-GQCTYLIASA-N	5.5×10^{-6}		Modarresi et al. (2005)	Q	247
	3.9×10^{-5}		Yao et al. (2002)	Q	229
	2.6×10^{-5}		Yaws (1999)	?	21
cis-4-methyl-2-pentene	2.8×10^{-5}		Yaws (2003)	X	237
C_6H_{12}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[691-38-3]	2.8×10^{-5}		Gharagheizi et al. (2010)	Q	246
LGAQJENWWYGFSN-PLNGDYQASA-N	3.7×10^{-6}		Modarresi et al. (2005)	Q	247
	3.3×10^{-5}		Yao et al. (2002)	Q	229
	2.8×10^{-5}		Yaws (1999)	?	21
trans-4-methyl-2-pentene	2.8×10^{-5}		Yaws (2003)	X	237
C_6H_{12}	1.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[674-76-0]	2.8×10^{-5}		Gharagheizi et al. (2010)	Q	246
LGAQJENWWYGFSN-SNAWJCMRSA-N	5.0×10^{-6}		Modarresi et al. (2005)	Q	247
	3.1×10^{-5}		Yao et al. (2002)	Q	229
	2.8×10^{-5}		Yaws (1999)	?	21

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methylenepentane	2.7×10^{-5}		Yaws (2003)	X	237
C_6H_{12}	2.0×10^{-5}		Gharagheizi et al. (2012)	Q	
(2-ethyl-1-butene)	2.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
[760-21-4]	3.9×10^{-6}		Modarresi et al. (2005)	Q	247
RYKZRKKEYSRDNF-UHFFFAOYSA-N	4.3×10^{-5}		Yao et al. (2002)	Q	229
	2.7×10^{-5}		Yaws (1999)	?	21
2,3-dimethyl-1-butene	2.8×10^{-5}		Yaws (2003)	X	237
C_6H_{12}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[563-78-0]	2.9×10^{-5}		Gharagheizi et al. (2010)	Q	246
OWWIWYDDISJUMY-UHFFFAOYSA-N	1.7×10^{-5}		Hilal et al. (2008)	Q	
	6.0×10^{-6}		Modarresi et al. (2005)	Q	247
	1.9×10^{-5}		Yao et al. (2002)	Q	229
	2.8×10^{-5}		Yaws (1999)	?	21
3,3-dimethyl-1-butene	2.8×10^{-5}		Yaws (2003)	X	237
C_6H_{12}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[558-37-2]	2.6×10^{-5}		Gharagheizi et al. (2010)	Q	246
PKXHXOTZMFCXSH-UHFFFAOYSA-N	5.2×10^{-6}		Modarresi et al. (2005)	Q	247
	1.0×10^{-5}		Yao et al. (2002)	Q	229
	2.9×10^{-5}		Yaws (1999)	?	21
2,3-dimethyl-2-butene	2.5×10^{-5}		Yaws (2003)	X	237
C_6H_{12}	1.4×10^{-4}		Wang et al. (2017)	Q	80, 238
[563-79-1]	1.1×10^{-4}		Wang et al. (2017)	Q	80, 239
WGLLSSPDPJPLOR-UHFFFAOYSA-N	5.5×10^{-5}		Wang et al. (2017)	Q	80, 240
	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
	4.9×10^{-6}		Modarresi et al. (2005)	Q	247
	2.7×10^{-5}		Yao et al. (2002)	Q	229
	2.6×10^{-5}		Yaws (1999)	?	21
1-heptene	2.0×10^{-5}		Brockbank (2013)	L	
C_7H_{14}	2.5×10^{-5}		Plyasunov and Shock (2000)	L	
[592-76-7]	2.3×10^{-5}		Duchowicz et al. (2020)	V	186
ZGEGCLOFRBLKSE-UHFFFAOYSA-N	2.3×10^{-5}		HSDB (2015)	V	
	2.5×10^{-5}		Mackay et al. (2006a)	V	
	2.5×10^{-5}		Mackay et al. (1993)	V	
	2.5×10^{-5}		Yaws (2003)	X	237
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.6×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-5}		Gharagheizi et al. (2010)	Q	246
	1.3×10^{-5}		Hilal et al. (2008)	Q	
	3.3×10^{-5}		Modarresi et al. (2007)	Q	67
	3.2×10^{-6}		Modarresi et al. (2005)	Q	247
	2.2×10^{-5}		Yao et al. (2002)	Q	229
	2.1×10^{-5}		English and Carroll (2001)	Q	230, 231
	5.8×10^{-5}		Katritzky et al. (1998)	Q	
	1.7×10^{-5}		Nirmalakhandan et al. (1997)	Q	

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.5×10^{-5}		Yaws (1999)	?	21
	2.5×10^{-5}		Yaws and Yang (1992)	?	21
	2.4×10^{-5}		Abraham et al. (1990)	?	
2-heptene	2.3×10^{-5}		Plyasunov and Shock (2000)	L	
C_7H_{14}	2.4×10^{-5}		Duchowicz et al. (2020)	V	186
[592-77-8]	5.2×10^{-4}		Duchowicz et al. (2020)	Q	
OTTZHAVKAVGASB-UHFFFAOYSA-N	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	271, 243
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	1.7×10^{-5}		Hilal et al. (2008)	Q	
	2.6×10^{-5}		Modarresi et al. (2007)	Q	67
	2.1×10^{-5}		English and Carroll (2001)	Q	230, 274
cis-2-heptene	2.4×10^{-5}		Brockbank (2013)	L	
C_7H_{14}	1.5×10^{-5}		Yaws (2003)	X	237
[6443-92-1]	2.0×10^{-5}		Gharagheizi et al. (2012)	Q	
OTTZHAVKAVGASB-HYXAFXHYSA-N	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
	9.1×10^{-6}		Modarresi et al. (2005)	Q	247
	3.0×10^{-5}		Yao et al. (2002)	Q	229, 267
	1.5×10^{-5}		Yaws (1999)	?	21
trans-2-heptene	2.4×10^{-5}		Brockbank (2013)	L	
C_7H_{14}	2.4×10^{-5}		Mackay and Shiu (1981)	L	
[14686-13-6]	2.3×10^{-5}		Duchowicz et al. (2020)	V	186
OTTZHAVKAVGASB-HWKANZROSA-N	2.4×10^{-5}		Mackay et al. (1993)	V	
	2.4×10^{-5}		Eastcott et al. (1988)	V	
	2.4×10^{-5}		Hine and Mookerjee (1975)	V	
	1.5×10^{-5}		Yaws (2003)	X	237
	5.2×10^{-4}		Duchowicz et al. (2020)	Q	
	2.0×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
	2.5×10^{-5}		Modarresi et al. (2007)	Q	67
	4.4×10^{-6}		Modarresi et al. (2005)	Q	247
	2.8×10^{-5}		Yao et al. (2002)	Q	229
	1.7×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	2.4×10^{-5}		Suzuki et al. (1992)	Q	232
	1.5×10^{-5}		Yaws (1999)	?	21
cis-3-heptene	1.6×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[7642-10-6]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
WZHKDGJSXCTSCK-ALCCZGGFSA-N	3.8×10^{-6}		Modarresi et al. (2005)	Q	247
	3.1×10^{-5}		Yao et al. (2002)	Q	229
	1.6×10^{-5}		Yaws (1999)	?	21

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
trans-3-heptene	1.6×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[14686-14-7]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
WZHKDGJSXCTSCK-FNORWQNLSA-N	4.0×10^{-6}		Modarresi et al. (2005)	Q	247
	2.8×10^{-5}		Yao et al. (2002)	Q	229
	1.6×10^{-5}		Yaws (1999)	?	21
2-methyl-1-hexene	1.7×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[6094-02-6]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
IRUDSQHLKGNCGF-UHFFFAOYSA-N	3.2×10^{-6}		Modarresi et al. (2005)	Q	247
	2.4×10^{-5}		Yao et al. (2002)	Q	229
	1.7×10^{-5}		Yaws (1999)	?	21
2-methyl-2-hexene	1.6×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[2738-19-4]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
BWEKDYGHDCHWEN-UHFFFAOYSA-N					
2-methyl-*cis*-3-hexene	1.9×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[15840-60-5]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
IQANHWBWTVLDTP-WAYWQWQTSA-N					
2-methyl-*trans*-3-hexene	1.9×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[692-24-0]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
IQANHWBWTVLDTP-AATRIKPKSA-N					
3-methyl-1-hexene	1.9×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	2.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[3404-61-3]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
RITONZMLZWYPHW-UHFFFAOYSA-N	9.9×10^{-6}		Modarresi et al. (2005)	Q	247
	1.0×10^{-5}		Yao et al. (2002)	Q	229
	1.9×10^{-5}		Yaws (1999)	?	21
3-methyl-*cis*-2-hexene	1.6×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[10574-36-4]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
JZMUUSXQSKCZNO-ALCCZGGFSA-N					
3-methyl-*trans*-2-hexene	1.6×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[20710-38-7]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
JZMUUSXQSKCZNO-FNORWQNLSA-N					
3-methyl-*cis*-3-hexene	1.7×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[4914-89-0]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
FHHSSXNRVNXTBG-SREVYHEPSA-N					

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-*trans*-3-hexene	1.7×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[3899-36-3]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
FHHSSXNRVNXTBG-VOTSOKGWSA-N					
4-methyl-1-hexene	1.8×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	2.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[3769-23-1]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
SUWJESCICIOQHO-UHFFFAOYSA-N	4.8×10^{-6}		Modarresi et al. (2005)	Q	247
	1.3×10^{-5}		Yao et al. (2002)	Q	229, 267
	1.9×10^{-5}		Yaws (1999)	?	21
4-methyl-*cis*-2-hexene	1.9×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[3683-19-0]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
MBNDKEPQUVZHCM-XQRVVYSFSA-N					
4-methyl-*trans*-2-hexene	1.9×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[3683-22-5]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
MBNDKEPQUVZHCM-GQCTYLIASA-N					
5-methyl-1-hexene	1.9×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[3524-73-0]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
JIUFYGIESXPUPL-UHFFFAOYSA-N					
5-methyl-*cis*-2-hexene	1.8×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[13151-17-2]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
GHBKCPRDHLITSE-PLNGDYQASA-N					
5-methyl-*trans*-2-hexene	1.8×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[7385-82-2]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
GHBKCPRDHLITSE-SNAWJCMRSA-N					
2,3-dimethyl-1-pentene	1.9×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[3404-72-6]	1.8×10^{-5}		Gharagheizi et al. (2010)	Q	246
LIMAEKMEXJTSNI-UHFFFAOYSA-N					
2,3-dimethyl-2-pentene	1.5×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[10574-37-5]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
WFHALSLYRWWUGH-UHFFFAOYSA-N					
2,4-dimethyl-1-pentene	1.9×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[2213-32-3]	1.8×10^{-5}		Gharagheizi et al. (2010)	Q	246
LXQPBCHJNIOMQU-UHFFFAOYSA-N					

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4-dimethyl-2-pentene C_7H_{14} [625-65-0] VVCFYASOGFVJFN-UHFFFAOYSA-N	2.0×10^{-5} 9.9×10^{-6} 1.9×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
3,3-dimethyl-1-pentene C_7H_{14} [3404-73-7] TXBZITDWMURSEF-UHFFFAOYSA-N	2.1×10^{-5} 1.8×10^{-5} 1.8×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
3,4-dimethyl-1-pentene C_7H_{14} [7385-78-6] WFHXQNMTMDKVJG-UHFFFAOYSA-N	2.0×10^{-5} 2.0×10^{-5} 1.9×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
3,4-dimethyl-*cis*-2-pentene C_7H_{14} [4914-91-4] PPBWEVVDSRKEIK-ALCCZGGFSA-N	1.8×10^{-5} 1.2×10^{-5} 1.9×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
3,4-dimethyl-*trans*-2-pentene C_7H_{14} [4914-92-5] PPBWEVVDSRKEIK-FNORWQNLSA-N	1.7×10^{-5} 1.3×10^{-5} 1.9×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
4,4-dimethyl-1-pentene C_7H_{14} [762-62-9] KLCNJIQZXOQYTE-UHFFFAOYSA-N	2.1×10^{-5} 1.6×10^{-5} 1.8×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
4,4-dimethyl-*cis*-2-pentene C_7H_{14} [762-63-0] BIDIHFPLDRSAMB-WAYWQWQTSA-N	1.9×10^{-5} 1.4×10^{-5} 1.8×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
4,4-dimethyl-*trans*-2-pentene C_7H_{14} [690-08-4] BIDIHFPLDRSAMB-AATRIKPKSA-N	2.1×10^{-5} 1.2×10^{-5} 1.8×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2-ethyl-1-pentene C_7H_{14} [3404-71-5] TWCRBBJSQAZZQB-UHFFFAOYSA-N	1.6×10^{-5} 1.9×10^{-5} 1.5×10^{-5} 2.9×10^{-6} 2.4×10^{-5} 1.6×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Modarresi et al. (2005) Yao et al. (2002) Yaws (1999)	X Q Q Q Q ?	237 246 247 229 21

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-1-pentene	1.9×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[4038-04-4]	1.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
YPVPQMCSLFDIKA-UHFFFAOYSA-N	4.9×10^{-6}		Modarresi et al. (2005)	Q	247
	1.3×10^{-5}		Yao et al. (2002)	Q	229
	1.9×10^{-5}		Yaws (1999)	?	21
3-ethyl-2-pentene	1.6×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[816-79-5]	1.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
XMYFZAWUNVHVGI-UHFFFAOYSA-N					
3-methyl-2-ethyl-1-butene	1.9×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[7357-93-9]	1.8×10^{-5}		Gharagheizi et al. (2010)	Q	246
ADHCYQWFCLQBFG-UHFFFAOYSA-N					
2,3,3-trimethyl-1-butene	1.9×10^{-5}		Yaws (2003)	X	237
C_7H_{14}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[594-56-9]	1.9×10^{-5}		Gharagheizi et al. (2010)	Q	246
AUYRUAVCWOAHQN-UHFFFAOYSA-N	3.0×10^{-6}		Modarresi et al. (2005)	Q	247
	7.8×10^{-6}		Yao et al. (2002)	Q	229
	2.0×10^{-5}		Yaws (1999)	?	21
1-octene	1.6×10^{-5}		Brockbank (2013)	L	
C_8H_{16}	1.1×10^{-5}	4400	Plyasunov and Shock (2000)	L	
[111-66-0]	1.0×10^{-5}		Mackay and Shiu (1981)	L	
KWKAKUADMBZCLK-UHFFFAOYSA-N	1.6×10^{-5}		Duchowicz et al. (2020)	V	186
	1.6×10^{-5}		HSDB (2015)	V	
	1.0×10^{-5}		Mackay et al. (2006a)	V	
	1.0×10^{-5}		Mackay et al. (1993)	V	
	1.0×10^{-5}		Hwang et al. (1992)	V	
	1.0×10^{-5}		Meylan and Howard (1991)	V	
	1.0×10^{-5}		Eastcott et al. (1988)	V	
	1.0×10^{-5}		Hine and Mookerjee (1975)	V	
	1.5×10^{-5}		McAuliffe (1966)	V	24
	1.6×10^{-5}		Yaws (2003)	X	237
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-6}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
	9.2×10^{-6}		Hilal et al. (2008)	Q	
	2.6×10^{-5}		Modarresi et al. (2007)	Q	67
	2.1×10^{-6}		Modarresi et al. (2005)	Q	247
	1.1×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	1.9×10^{-5}		Yao et al. (2002)	Q	229
	1.6×10^{-5}		English and Carroll (2001)	Q	230, 231

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.7×10^{-5}		Katritzky et al. (1998)	Q	
	8.4×10^{-6}		Russell et al. (1992)	Q	279
	1.8×10^{-5}		Suzuki et al. (1992)	Q	232
	1.6×10^{-5}		Meylan and Howard (1991)	Q	
	1.3×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	1.6×10^{-5}		Yaws (1999)	?	21
	1.6×10^{-5}		Yaws and Yang (1992)	?	21
	1.6×10^{-5}		Abraham et al. (1990)	?	
cis-2-octene	8.3×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[7642-04-8]	9.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
ILPBINAXDRFYPL-HYXAFXHYSA-N					
trans-2-octene	8.3×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[13389-42-9]	9.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
ILPBINAXDRFYPL-HWKANZROSA-N	8.4×10^{-6}		Yaws (1999)	?	21
cis-3-octene	8.9×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[14850-22-7]	9.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
YCTDZYMMFQCTEO-ALCCZGGFSA-N					
trans-3-octene	8.6×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[14919-01-8]	9.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
YCTDZYMMFQCTEO-FNORWQNLSA-N	8.8×10^{-6}		Yaws (1999)	?	21
cis-4-octene	8.9×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[7642-15-1]	9.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
IRUCBBFNLDIMIK-FPLPWBNLSA-N					
trans-4-octene	8.9×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[14850-23-8]	9.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
IRUCBBFNLDIMIK-BQYQJAHWSA-N	9.1×10^{-6}		Yaws (1999)	?	21
2-methyl-1-heptene	9.6×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[15870-10-7]	9.8×10^{-6}		Gharagheizi et al. (2010)	Q	246
RCBGGJURENJHKV-UHFFFAOYSA-N					
2-methyl-2-heptene	8.9×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[627-97-4]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
WEPNJTDVIIKRIK-UHFFFAOYSA-N					

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-*cis*-3-heptene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[20488-34-0]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
CYEZJYAMLNTSKN-SREVYHEPSA-N					
2-methyl-*trans*-3-heptene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[692-96-6]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
CYEZJYAMLNTSKN-VOTSOKGWSA-N					
3-methyl-1-heptene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[4810-09-7]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
QDMFTFWKTYXBIW-UHFFFAOYSA-N					
3-methyl-*cis*-2-heptene	9.0×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[22768-19-0]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
OFKLSPUVNMOIJB-YVMONPNESA-N					
3-methyl-*trans*-2-heptene	9.0×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[22768-20-3]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
OFKLSPUVNMOIJB-VMPITWQZSA-N					
3-methyl-*cis*-3-heptene	9.2×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[22768-17-8]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
AAUHUDBDDBJONC-FPLPWBNLSA-N					
3-methyl-*trans*-3-heptene	9.2×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[22768-18-9]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
AAUHUDBDDBJONC-BQYQJAHWSA-N					
4-methyl-1-heptene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[13151-05-8]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
BFGOGLKYJXQPJZ-UHFFFAOYSA-N					
4-methyl-*cis*-2-heptene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[66225-16-9]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
SVGLFIBXFVQUQY-XQRVVYSFSA-N					
4-methyl-*trans*-2-heptene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[66225-17-0]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
SVGLFIBXFVQUQY-GQCTYLIASA-N					

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methyl-*cis*-3-heptene	9.0×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[14255-24-4]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
KKVVJQGDNYIIMN-VURMDHGXSA-N					
4-methyl-*trans*-3-heptene	9.0×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[13714-85-7]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
KKVVJQGDNYIIMN-SOFGYWHQSA-N					
5-methyl-1-heptene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[13151-04-7]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
WNEYWVBECXCQRT-UHFFFAOYSA-N					
5-methyl-*cis*-2-heptene	9.9×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[24608-84-2]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
VIHUHUGDEZCPDK-XQRVVYSFSA-N					
5-methyl-*trans*-2-heptene	9.9×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[24608-85-3]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
VIHUHUGDEZCPDK-GQCTYLIASA-N					
5-methyl-*cis*-3-heptene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[50422-80-5]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
YMNTZRCUPAYGLG-SREVYHEPSA-N					
5-methyl-*trans*-3-heptene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[53510-18-2]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
YMNTZRCUPAYGLG-VOTSOKGWSA-N					
6-methyl-1-heptene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[5026-76-6]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
DFVOXRAAHOJJBN-UHFFFAOYSA-N					
6-methyl-*cis*-2-heptene	1.0×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[66225-18-1]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
LXBJRNXXTAWCKU-PLNGDYQASA-N					
6-methyl-*trans*-2-heptene	1.0×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[51065-65-7]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
LXBJRNXXTAWCKU-SNAWJCMRSA-N					

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
6-methyl-*cis*-3-heptene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[66225-19-2]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
PMPISKBGRHSPEE-WAYWQWQTSA-N					
6-methyl-*trans*-3-heptene	1.0×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[66225-20-5]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
PMPISKBGRHSPEE-AATRIKPKSA-N					
2,2-dimethyl-*cis*-3-hexene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[690-92-6]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
JPLZSSHKQZJYTJ-SREVYHEPSA-N					
2,2-dimethyl-*trans*-3-hexene	1.4×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	9.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[690-93-7]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
JPLZSSHKQZJYTJ-VOTSOKGWSA-N					
2,3-dimethyl-1-hexene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[16746-86-4]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
LVLXQRZPKUFJJQ-UHFFFAOYSA-N					
2,3-dimethyl-2-hexene	9.1×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	7.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[7145-20-2]	9.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
RGYAVZGBAJFMIZ-UHFFFAOYSA-N					
2,3-dimethyl-*cis*-3-hexene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	9.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[59643-75-3]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
PRTXQHCLTIKAAJ-VURMDHGXSA-N					
2,3-dimethyl-*trans*-3-hexene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	9.2×10^{-6}		Gharagheizi et al. (2012)	Q	
[66225-30-7]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
PRTXQHCLTIKAAJ-SOFGYWHQSA-N					
2,4-dimethyl-1-hexene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[16746-87-5]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
PKVDGQHNRICJLA-UHFFFAOYSA-N					
2,4-dimethyl-2-hexene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	8.4×10^{-6}		Gharagheizi et al. (2012)	Q	
[14255-23-3]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
IZSBIPQYBGDXJZ-UHFFFAOYSA-N					

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4-dimethyl-*cis*-3-hexene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	8.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[37549-89-6]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
VFCHHMABGOYOQI-VURMDHGXSA-N					
2,4-dimethyl-*trans*-3-hexene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	7.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[61847-78-7]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
VFCHHMABGOYOQI-SOFGYWHQSA-N					
2,5-dimethyl-1-hexene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[6975-92-4]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
ISZWTVCVSJVEOL-UHFFFAOYSA-N					
2,5-dimethyl-2-hexene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	8.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[3404-78-2]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
VFZIUYUUQFYZBR-UHFFFAOYSA-N					
2,5-dimethyl-*cis*-3-hexene	1.3×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	9.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[10557-44-5]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
KNCMKWVOMRUHKZ-WAYWQWQTSA-N					
2,5-dimethyl-*trans*-3-hexene	1.4×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	9.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[692-70-6]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
KNCMKWVOMRUHKZ-AATRIKPKSA-N					
3,3-dimethyl-1-hexene	1.3×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[3404-77-1]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
RXYYKIMRVXDSFR-UHFFFAOYSA-N					
3,4-dimethyl-1-hexene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[16745-94-1]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
OWWRMMIWAOBBFK-UHFFFAOYSA-N					
3,4-dimethyl-*cis*-2-hexene	1.0×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	9.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[19550-81-3]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
FMNLVKMLDPGPRY-ALCCZGGFSA-N					
3,4-dimethyl-*trans*-2-hexene	1.0×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	9.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[19550-82-4]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
FMNLVKMLDPGPRY-FNORWQNLSA-N					

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4-dimethyl-*cis*-3-hexene	9.0×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	7.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[19550-87-9]	9.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
XTUXVDJHGIEBAA-FPLPWBNLSA-N					
3,4-dimethyl-*trans*-3-hexene	9.0×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	7.9×10^{-6}		Gharagheizi et al. (2012)	Q	
[19550-88-0]	9.0×10^{-6}		Gharagheizi et al. (2010)	Q	246
XTUXVDJHGIEBAA-BQYQJAHWSA-N					
3,5-dimethyl-1-hexene	1.3×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[7423-69-0]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
FEZKAPRRVNNJTK-UHFFFAOYSA-N					
3,5-dimethyl-*cis*-2-hexene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	8.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[66225-31-8]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
BQAZYKYBFAMHPG-YVMONPNESA-N					
3,5-dimethyl-*trans*-2-hexene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	8.7×10^{-6}		Gharagheizi et al. (2012)	Q	
[66225-12-5]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
BQAZYKYBFAMHPG-VMPITWQZSA-N					
4,4-dimethyl-1-hexene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[1647-08-1]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
SUJVAMIXNUAJEY-UHFFFAOYSA-N					
4,4-dimethyl-*cis*-2-hexene	1.3×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
OQEVAISXHCRQGF-ALCCZGGFSA-N	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
4,4-dimethyl-*trans*-2-hexene	1.3×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[19550-83-5]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
OQEVAISXHCRQGF-FNORWQNLSA-N					
4,5-dimethyl-1-hexene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[16106-59-5]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
UFWIBUBEFUNVNI-UHFFFAOYSA-N					
4,5-dimethyl-*cis*-2-hexene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[65036-71-7]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
OAVNNZUEVHDCKP-WAYWQWQTSA-N					

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,5-dimethyl-*trans*-2-hexene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[66225-14-7]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
OAVNNZUEVHDCKP-AATRIKPKSA-N					
5,5-dimethyl-1-hexene	1.4×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[7116-86-1]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
KZJIOVQKSAOPOP-UHFFFAOYSA-N					
5,5-dimethyl-*cis*-2-hexene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[39761-61-0]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
NWZJLSKAFZXSQH-WAYWQWQTSA-N					
5,5-dimethyl-*trans*-2-hexene	1.3×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[39782-43-9]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
NWZJLSKAFZXSQH-AATRIKPKSA-N					
2-ethyl-1-hexene	9.2×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	2.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[1632-16-2]	9.8×10^{-6}		Gharagheizi et al. (2010)	Q	246
XTVRLCUJHGUXCP-UHFFFAOYSA-N	9.4×10^{-6}		Yaws (1999)	?	21
3-ethyl-1-hexene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[3404-58-8]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
OLGHJTHQWQKJQQ-UHFFFAOYSA-N					
3-ethyl-3-hexene	1.0×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	9.6×10^{-6}		Gharagheizi et al. (2012)	Q	
[16789-51-8]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
AUJLDZJNMXNESO-UHFFFAOYSA-N					
3-ethyl-*cis*-2-hexene	9.2×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[36880-72-5]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
QEMJIDSLEPYRLM-YVMONPNESA-N					
3-ethyl-*trans*-2-hexene	9.2×10^{-6}		Yaws (2003)	X	237
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[66225-15-8]	9.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
QEMJIDSLEPYRLM-VMPITWQZSA-N					
4-ethyl-1-hexene	1.3×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[16746-85-3]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
OPMUAJRVOWSBTP-UHFFFAOYSA-N					

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-ethyl-*cis*-2-hexene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[54616-49-8]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
STHONQMAWQLWLX-DAXSKMNVSA-N					
4-ethyl-*trans*-2-hexene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[19781-63-6]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
STHONQMAWQLWLX-QPJJXVBHSA-N					
2,3,3-trimethyl-1-pentene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[560-23-6]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
TUSBCMPNIOJUBX-UHFFFAOYSA-N					
2,3,4-trimethyl-1-pentene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[565-76-4]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
FAWUHEYSSPPNSH-UHFFFAOYSA-N					
2,3,4-trimethyl-2-pentene	1.0×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	6.8×10^{-6}		Gharagheizi et al. (2012)	Q	
[565-77-5]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
SZFRZEBLZFTODC-UHFFFAOYSA-N					
2,4,4-trimethyl-1-pentene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.3×10^{-5}		HSDB (2015)	Q	99
[107-39-1]	9.0×10^{-6}		Gharagheizi et al. (2012)	Q	
FXNDIJDIPNCZQJ-UHFFFAOYSA-N	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
	2.6×10^{-6}		Modarresi et al. (2005)	Q	247
	1.1×10^{-5}		Yao et al. (2002)	Q	229
	1.2×10^{-5}		Yaws (1999)	?	21
2,4,4-trimethyl-2-pentene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.1×10^{-5}		HSDB (2015)	Q	99
[107-40-4]	6.8×10^{-6}		Gharagheizi et al. (2012)	Q	
LAAVYEUJEMRIGF-UHFFFAOYSA-N	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
	5.9×10^{-6}		Modarresi et al. (2005)	Q	247
	1.0×10^{-5}		Yao et al. (2002)	Q	229
	1.2×10^{-5}		Yaws (1999)	?	21
3,3,4-trimethyl-1-pentene	1.3×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[560-22-5]	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	246
LLFHCOGPDCJMKY-UHFFFAOYSA-N					
3,4,4-trimethyl-1-pentene	1.3×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[564-03-4]	1.4×10^{-5}		Gharagheizi et al. (2010)	Q	246
BOPVNOMJIDZBQB-UHFFFAOYSA-N					

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4,4-trimethyl-2-pentene C_8H_{16} [598-96-9] FZQMZRXKWHQJAG-UHFFFAOYSA-N	1.1×10^{-5}		HSDB (2015)	Q	99
3,4,4-trimethyl-*cis*-2-pentene C_8H_{16} [39761-64-3] FZQMZRXKWHQJAG-SREVYHEPSA-N	1.1×10^{-5} 8.9×10^{-6} 1.2×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
3,4,4-trimethyl-*trans*-2-pentene C_8H_{16} [39761-57-4] FZQMZRXKWHQJAG-VOTSOKGWSA-N	1.1×10^{-5} 8.9×10^{-6} 1.2×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2-methyl-3-ethyl-1-pentene C_8H_{16} [19780-66-6] HPHHYSWOBXEIRG-UHFFFAOYSA-N	1.1×10^{-5} 1.2×10^{-5} 1.1×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2-methyl-3-ethyl-2-pentene C_8H_{16} [19780-67-7] FQYUGAXHZSQHMU-UHFFFAOYSA-N	1.1×10^{-5} 6.8×10^{-6} 9.0×10^{-6}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
3-methyl-2-ethyl-1-pentene C_8H_{16} [3404-67-9] YXLCVBVDFKWWRW-UHFFFAOYSA-N	1.2×10^{-5} 1.2×10^{-5} 1.1×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
3-methyl-3-ethyl-1-pentene C_8H_{16} [6196-60-7] PHHHEKOJKDYRIN-UHFFFAOYSA-N	1.1×10^{-5} 1.9×10^{-5} 1.3×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
4-methyl-2-ethyl-1-pentene C_8H_{16} [3404-80-6] TVBQWTDYXVGWJL-UHFFFAOYSA-N	1.2×10^{-5} 1.2×10^{-5} 1.1×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
4-methyl-3-ethyl-1-pentene C_8H_{16} [61847-80-1] DTNALCAUPPLROB-UHFFFAOYSA-N	1.2×10^{-5} 1.6×10^{-5} 1.3×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
4-methyl-3-ethyl-*cis*-2-pentene C_8H_{16} [42067-48-1] DSTFDBMUTNIZGD-YVMONPNESA-N	1.0×10^{-5} 9.8×10^{-6} 1.1×10^{-5}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methyl-3-ethyl-*trans*-2-pentene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	9.3×10^{-6}		Gharagheizi et al. (2012)	Q	
[42067-49-2]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
DSTFDBMUTNIZGD-VMPITWQZSA-N					
2-propyl-1-pentene	1.0×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[15918-08-8]	9.8×10^{-6}		Gharagheizi et al. (2010)	Q	246
FYUUBXZYRPRIHC-UHFFFAOYSA-N					
2-isopropyl-1-pentene	1.1×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[16746-02-4]	1.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
QOUCFWFZPKWYRE-UHFFFAOYSA-N					
3,3-dimethyl-2-ethyl-1-butene	1.2×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[18231-53-3]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
KQRPZENSXZIOQO-UHFFFAOYSA-N					
3-methyl-2-isopropyl-1-butene	1.3×10^{-5}		Yaws (2003)	X	237
C_8H_{16}	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[111823-35-9]	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
GIBPFTYFAOOKOV-UHFFFAOYSA-N					
1-nonene	1.1×10^{-5}		Brockbank (2013)	L	
C_9H_{18}	1.2×10^{-5}		Plyasunov and Shock (2000)	L	
[124-11-8]	1.2×10^{-5}		Duchowicz et al. (2020)	V	186
JRZJOMJEPLMPRA-UHFFFAOYSA-N	1.2×10^{-5}		Mackay et al. (2006a)	V	
	1.2×10^{-5}		Mackay et al. (1993)	V	
	1.2×10^{-5}		Yaws (2003)	X	237
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
	8.9×10^{-6}		Gharagheizi et al. (2010)	Q	246
	6.5×10^{-6}		Hilal et al. (2008)	Q	
	1.1×10^{-5}		Yaffe et al. (2003)	Q	248, 272
	1.7×10^{-5}		Yao et al. (2002)	Q	229
	1.2×10^{-5}		English and Carroll (2001)	Q	230, 231
	1.0×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	1.2×10^{-5}		Yaws (1999)	?	21
	1.2×10^{-5}		Yaws and Yang (1992)	?	21
	1.2×10^{-5}		Abraham et al. (1990)	?	
2-methyl-1-octene	6.2×10^{-6}		Yaws (2003)	X	237
C_9H_{18}	1.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[4588-18-5]	6.9×10^{-6}		Gharagheizi et al. (2010)	Q	246
FBEDQPGLIKZGIN-UHFFFAOYSA-N					

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-decene	8.6×10^{-6}		Brockbank (2013)	L	
$C_{10}H_{20}$	1.8×10^{-5}		Duchowicz et al. (2020)	V	186
[872-05-9]	3.7×10^{-6}		HSDB (2015)	V	
AFFLGGQVNFXPEV-UHFFFAOYSA-N	3.3×10^{-6}		Mackay et al. (1993)	V	
	3.7×10^{-6}		Yaws (2003)	X	237
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.4×10^{-5}		Gharagheizi et al. (2012)	Q	
	7.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
	4.2×10^{-6}		Hilal et al. (2008)	Q	
	4.7×10^{-6}		Yaws (1999)	?	21
2-methyl-1-nonene	4.3×10^{-6}		Yaws (2003)	X	237
$C_{10}H_{20}$	1.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[2980-71-4]	5.2×10^{-6}		Gharagheizi et al. (2010)	Q	246
YLZQHQUVNZVGOK-UHFFFAOYSA-N					
1-undecene	4.5×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{22}$	6.7×10^{-6}		HSDB (2015)	Q	99
[821-95-4]	2.9×10^{-5}		Gharagheizi et al. (2012)	Q	
DCTOHCCUXLBQMS-UHFFFAOYSA-N	6.7×10^{-6}		Gharagheizi et al. (2010)	Q	246
	2.2×10^{-6}		Hilal et al. (2008)	Q	
	1.2×10^{-5}		Yao et al. (2002)	Q	229
	4.6×10^{-6}		Yaws (1999)	?	21
2-methyl-1-decene	3.4×10^{-6}		Yaws (2003)	X	237
$C_{11}H_{22}$	1.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[13151-27-4]	4.4×10^{-6}		Gharagheizi et al. (2010)	Q	246
HLMACKQLXSEXIY-UHFFFAOYSA-N					
1-dodecene	5.1×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{24}$	2.3×10^{-6}		HSDB (2015)	Q	99
[112-41-4]	3.4×10^{-5}		Gharagheizi et al. (2012)	Q	
CRSBERNSMYQZNG-UHFFFAOYSA-N	7.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
	1.5×10^{-6}		Hilal et al. (2008)	Q	
	9.9×10^{-6}		Yao et al. (2002)	Q	229
	5.2×10^{-6}		Yaws (1999)	?	21
2-methyl-1-undecene	3.4×10^{-6}		Yaws (2003)	X	237
$C_{12}H_{24}$	4.3×10^{-6}		Gharagheizi et al. (2010)	Q	246
[18516-37-5]					
SJVKHZYVCVKEGM-UHFFFAOYSA-N					
2,2,4,6,6-pentamethyl-3-heptene	3.6×10^{-6}		Zhang et al. (2010)	Q	287, 288
$C_{12}H_{24}$	5.2×10^{-7}		Zhang et al. (2010)	Q	287, 289
[123-48-8]	1.8×10^{-5}		Zhang et al. (2010)	Q	287, 290
NBUMCEJRJRRLCA-UHFFFAOYSA-N	1.5×10^{-5}		Zhang et al. (2010)	Q	287, 291

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-tridecene	5.8×10^{-6}		Yaws (2003)	X	258
$C_{13}H_{26}$	5.8×10^{-6}		Yaws (2003)	X	237
[2437-56-1]	9.4×10^{-6}		Dupeux et al. (2022)	Q	259
VQOXUMQBYILCKR-UHFFFAOYSA-N	3.8×10^{-6}		HSDB (2015)	Q	99
	3.9×10^{-5}		Gharagheizi et al. (2012)	Q	
	8.8×10^{-6}		Gharagheizi et al. (2010)	Q	246
	9.2×10^{-6}		Yao et al. (2002)	Q	229
	5.9×10^{-6}		Yaws (1999)	?	21
2-methyl-1-dodecene	4.1×10^{-6}		Yaws (2003)	X	237
$C_{13}H_{26}$	2.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[16435-49-7]	4.9×10^{-6}		Gharagheizi et al. (2010)	Q	246
PWRBDKMPAZFCSV-UHFFFAOYSA-N					
1-tetradecene	3.0×10^{-6}		Brockbank (2013)	L	
$C_{14}H_{28}$	1.4×10^{-5}		Yaws (2003)	X	237
[1120-36-1]	1.2×10^{-6}		HSDB (2015)	Q	99
HFDVRLIODXPAHB-UHFFFAOYSA-N	4.3×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
	1.5×10^{-5}		Yaws (1999)	?	21
2-tetradecene	7.5×10^{-6}		Yaws (2003)	X	237
$C_{14}H_{28}$	4.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[638-60-8]	4.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
OBDUMNZXAIUUTH-UHFFFAOYSA-N					
2-methyl-1-tridecene	8.9×10^{-6}		Yaws (2003)	X	237
$C_{14}H_{28}$	3.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[18094-01-4]	6.9×10^{-6}		Gharagheizi et al. (2010)	Q	246
VNBHQOHLCULRDN-UHFFFAOYSA-N					
1-pentadecene	2.2×10^{-6}		Brockbank (2013)	L	
$C_{15}H_{30}$	3.5×10^{-5}		Yaws (2003)	X	237
[13360-61-7]	4.7×10^{-5}		Gharagheizi et al. (2012)	Q	
PJLHTVIBELQURV-UHFFFAOYSA-N	2.6×10^{-5}		Gharagheizi et al. (2010)	Q	246
	8.7×10^{-5}		Yao et al. (2002)	Q	229, 267
	3.6×10^{-5}		Yaws (1999)	?	21
2-methyl-1-tetradecene	1.1×10^{-5}		Yaws (2003)	X	237
$C_{15}H_{30}$	2.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[52254-38-3]	1.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
WSNMNSLVXDWAFZ-UHFFFAOYSA-N					
1-hexadecene	5.7×10^{-5}		Yaws (2003)	X	237
$C_{16}H_{32}$	4.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[629-73-2]	6.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
GQEZCXVZFLOKMC-UHFFFAOYSA-N	5.8×10^{-5}		Yaws (1999)	?	21

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-1-pentadecene	2.5×10^{-5}		Yaws (2003)	X	237
$C_{16}H_{32}$	3.1×10^{-5}		Gharagheizi et al. (2012)	Q	
[29833-69-0]	2.8×10^{-5}		Gharagheizi et al. (2010)	Q	246
FWQJRKLMXMTXDY-UHFFFAOYSA-N					
2,4-dimethylpentadecane	1.1×10^{-5}		Yaws (2003)	X	237
$C_{17}H_{36}$	4.0×10^{-6}		Gharagheizi et al. (2012)	Q	
[61868-07-3]	2.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
TXGHMPJBDYZJLF-UHFFFAOYSA-N					
1,2-butadiene	1.2×10^{-4}		Yaws (2003)	X	237
C_4H_6	1.0×10^{-4}		HSDB (2015)	Q	99
[590-19-2]	1.5×10^{-4}		Gharagheizi et al. (2012)	Q	
QNRMTGGDHLBXQZ-UHFFFAOYSA-N	1.2×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.1×10^{-4}		Hilal et al. (2008)	Q	
	1.2×10^{-4}		Yaws (1999)	?	21
1,3-butadiene	1.4×10^{-4}	3200	Plyasunov and Shock (2000)	L	
C_4H_6	1.3×10^{-4}		Mackay and Shiu (1981)	L	
[106-99-0]	1.4×10^{-4}	4500	Wilhelm et al. (1977)	L	
KAKZBPTYRLMSJV-UHFFFAOYSA-N	1.4×10^{-4}		Ross and Hudson (1957)	M	
	1.3×10^{-4}		Duchowicz et al. (2020)	V	186
	1.3×10^{-4}		HSDB (2015)	V	
	1.3×10^{-4}		Mackay et al. (2006a)	V	
	3.9×10^{-6}		Lide and Frederikse (1995)	V	
	4.8×10^{-5}		Mackay et al. (1993)	V	
	5.0×10^{-5}		Hwang et al. (1992)	V	
	1.6×10^{-4}		Hine and Mookerjee (1975)	V	
	1.2×10^{-4}		Irmann (1965)	V	
	1.4×10^{-4}		Yaws (2003)	X	237
	1.5×10^{-4}		Irmann (1965)	C	
	1.5×10^{-4}		Hayer et al. (2022)	Q	20
	5.6×10^{-3}		Duchowicz et al. (2020)	Q	
	6.3×10^{-4}		Wang et al. (2017)	Q	80, 238
	1.4×10^{-4}		Wang et al. (2017)	Q	80, 239
	2.0×10^{-4}		Wang et al. (2017)	Q	80, 240
	2.7×10^{-4}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.4×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.8×10^{-4}		Hilal et al. (2008)	Q	
	1.8×10^{-4}		Modarresi et al. (2007)	Q	67
		3600	Kühne et al. (2005)	Q	
	1.3×10^{-5}		Modarresi et al. (2005)	Q	247
	1.3×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	2.5×10^{-4}		Yao et al. (2002)	Q	229
	1.3×10^{-4}		English and Carroll (2001)	Q	230, 274
	1.8×10^{-4}		Suzuki et al. (1992)	Q	232

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	9.2×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
		4100	Kühne et al. (2005)	?	
	1.4×10^{-4}		Yaws (1999)	?	21
	1.4×10^{-4}		Yaws and Yang (1992)	?	21
3-methyl-1,2-butadiene	1.1×10^{-4}		Yaws (2003)	X	237
C_5H_8	7.2×10^{-5}		Gharagheizi et al. (2012)	Q	
(2-methyl-2,3-butadiene)	9.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
[598-25-4]	1.0×10^{-5}		Modarresi et al. (2005)	Q	247
PAKGDPSCXSUALC-UHFFFAOYSA-N	1.1×10^{-4}		Yaws (1999)	?	21
2-methyl-1,3-butadiene	1.3×10^{-4}	2700	Plyasunov and Shock (2000)	L	
C_5H_8	1.3×10^{-4}		Mackay and Shiu (1981)	L	
(isoprene)	3.0×10^{-4}		Schuhfried et al. (2015)	M	
[78-79-5]	3.4×10^{-4}	4400	Leng et al. (2013)	M	
RRHGJUQNOFWUDK-UHFFFAOYSA-N	1.2×10^{-4}	4400	Ooki and Yokouchi (2011)	M	70
	2.9×10^{-4}		Karl et al. (2003)	M	28
	1.3×10^{-4}		Duchowicz et al. (2020)	V	186
	1.3×10^{-4}		Martins et al. (2017)	V	315
	1.3×10^{-4}		HSDB (2015)	V	
	1.3×10^{-4}		Mackay et al. (2006a)	V	
	1.3×10^{-4}		Copolovici and Niinemets (2005)	V	
	1.3×10^{-4}		Mackay et al. (1993)	V	
	1.3×10^{-4}		Hine and Mookerjee (1975)	V	
	1.3×10^{-4}		Yaws (2003)	X	237
	1.8×10^{-3}		Duchowicz et al. (2020)	Q	
	4.1×10^{-4}		Wang et al. (2017)	Q	80, 238
	1.6×10^{-4}		Wang et al. (2017)	Q	80, 239
	1.9×10^{-4}		Wang et al. (2017)	Q	80, 240
	1.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	1.0×10^{-4}		Gharagheizi et al. (2010)	Q	246
	2.7×10^{-4}		Hilal et al. (2008)	Q	
	1.1×10^{-5}		Modarresi et al. (2005)	Q	247
	1.3×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	1.0×10^{-4}		Yao et al. (2002)	Q	229
	1.1×10^{-4}		Yao et al. (2002)	Q	229
	1.0×10^{-4}		English and Carroll (2001)	Q	230, 231
	1.4×10^{-4}		Suzuki et al. (1992)	Q	232
	6.7×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	1.1×10^{-4}		Yaws (1999)	?	21
	1.3×10^{-4}		Yaws (1999)	?	21
	1.3×10^{-4}		Yaws and Yang (1992)	?	21

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-pentadiene	1.1×10^{-4}		Yaws (2003)	X	237
C_5H_8	1.2×10^{-4}		Gharagheizi et al. (2012)	Q	
[591-95-7]	1.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
LVMTVPFRTKXRPH-UHFFFAOYSA-N	9.7×10^{-5}		Hilal et al. (2008)	Q	
	1.1×10^{-4}		Yaws (1999)	?	21
1,3-pentadiene	1.4×10^{-4}		HSDB (2015)	Q	99
C_5H_8					
[504-60-9]					
PMJHHCWVYXUKFD-UHFFFAOYSA-N					
trans-1,3-pentadiene	1.0×10^{-4}		Yaws (2003)	X	237
C_5H_8	8.2×10^{-5}		HSDB (2015)	Q	99
[2004-70-8]	2.2×10^{-4}		Gharagheizi et al. (2012)	Q	
PMJHHCWVYXUKFD-SNAWJCMRSA-N	1.0×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.1×10^{-4}		Yaws (1999)	?	21
cis-1,3-pentadiene	1.1×10^{-4}		Yaws (2003)	X	237
C_5H_8	2.4×10^{-4}		Gharagheizi et al. (2012)	Q	
[1574-41-0]	1.0×10^{-4}		Gharagheizi et al. (2010)	Q	246
PMJHHCWVYXUKFD-PLNGDYQASA-N	1.1×10^{-4}		Yaws (1999)	?	21
1,4-pentadiene	8.0×10^{-5}		Plyasunov and Shock (2000)	L	
C_5H_8	8.3×10^{-5}		Mackay and Shiu (1981)	L	
[591-93-5]	8.2×10^{-5}		Duchowicz et al. (2020)	V	186
QYZLKGVUSQXAMU-UHFFFAOYSA-N	8.4×10^{-5}		Mackay et al. (2006a)	V	
	8.4×10^{-5}		Mackay et al. (1993)	V	
	8.2×10^{-5}		Hine and Mookerjee (1975)	V	
	8.3×10^{-5}		Yaws (2003)	X	237
	5.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.1×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	8.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
	9.9×10^{-5}		Hilal et al. (2008)	Q	
	8.2×10^{-5}		Modarresi et al. (2007)	Q	67
	1.2×10^{-5}		Modarresi et al. (2005)	Q	247
	8.4×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	1.1×10^{-4}		Yao et al. (2002)	Q	229, 267
	9.9×10^{-5}		English and Carroll (2001)	Q	230, 260
	1.5×10^{-4}		Russell et al. (1992)	Q	279
	1.6×10^{-4}		Suzuki et al. (1992)	Q	232
	7.3×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	8.4×10^{-5}		Yaws (1999)	?	21
	8.3×10^{-5}		Yaws and Yang (1992)	?	21

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-pentadiene	1.1×10^{-4}		Yaws (2003)	X	237
C_5H_8	8.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[591-96-8]	9.6×10^{-5}		Gharagheizi et al. (2010)	Q	246
PODAMDNJNMAKAZ-UHFFFAOYSA-N	1.1×10^{-4}		Hilal et al. (2008)	Q	
	1.1×10^{-4}		Yaws (1999)	?	21
1,2-hexadiene	7.5×10^{-5}		Yaws (2003)	X	237
C_6H_{10}	1.2×10^{-4}		Gharagheizi et al. (2012)	Q	
[592-44-9]	9.8×10^{-5}		Gharagheizi et al. (2010)	Q	246
XIAJQOBRHVKGSP-UHFFFAOYSA-N					
cis-1,3-hexadiene	7.7×10^{-5}		Yaws (2003)	X	237
C_6H_{10}	2.1×10^{-4}		Gharagheizi et al. (2012)	Q	
[14596-92-0]	8.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
AHAREKHAZNPPMI-WAYWQWQTSA-N					
trans-1,3-hexadiene	7.7×10^{-5}		Yaws (2003)	X	237
C_6H_{10}	2.1×10^{-4}		Gharagheizi et al. (2012)	Q	
[20237-34-7]	8.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
AHAREKHAZNPPMI-AATRIKPKSA-N					
1,4-hexadiene	8.4×10^{-5}		HSDB (2015)	Q	99
C_6H_{10}					
[592-45-0]					
PRBHEGAFLDMLAL-UHFFFAOYSA-N					
cis-1,4-hexadiene	8.3×10^{-5}		Yaws (2003)	X	237
C_6H_{10}	1.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[7318-67-4]	8.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
PRBHEGAFLDMLAL-XQRVVYSFSA-N					
trans-1,4-hexadiene	8.3×10^{-5}		Yaws (2003)	X	237
C_6H_{10}	1.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[7319-00-8]	8.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
PRBHEGAFLDMLAL-GQCTYLIASA-N					
1,5-hexadiene	6.8×10^{-5}		Plyasunov and Shock (2000)	L	
C_6H_{10}	7.0×10^{-5}		Duchowicz et al. (2020)	V	186
[592-42-7]	6.9×10^{-5}		Mackay et al. (2006a)	V	
PYGSKMBEVAICCR-UHFFFAOYSA-N	6.7×10^{-5}		Hwang et al. (1992)	V	
	7.3×10^{-5}		Hine and Mookerjee (1975)	V	
	8.1×10^{-5}		Yaws (2003)	X	237
	5.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.0×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
	5.8×10^{-5}		Hilal et al. (2008)	Q	
	1.0×10^{-4}		Modarresi et al. (2007)	Q	67
	9.4×10^{-6}		Modarresi et al. (2005)	Q	247
	5.8×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	3.5×10^{-5}		Yao et al. (2002)	Q	229
	7.5×10^{-5}		English and Carroll (2001)	Q	230, 231

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-4}		Suzuki et al. (1992)	Q	232
	5.8×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	8.4×10^{-5}		Yaws (1999)	?	21
2,3-hexadiene C_6H_{10} [592-49-4] DPUXQWOMYBMHRN-UHFFFAOYSA-N	8.1×10^{-5}		Yaws (2003)	X	237
	6.7×10^{-5}		Gharagheizi et al. (2012)	Q	
	8.0×10^{-5}		Gharagheizi et al. (2010)	Q	246
cis-2,*cis*-4-hexadiene C_6H_{10} [6108-61-8] APPOKADJQUIAHP-GLIMQPGKSA-N	7.1×10^{-5}		Yaws (2003)	X	237
	1.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
cis-2,*trans*-4-hexadiene C_6H_{10} [5194-50-3] APPOKADJQUIAHP-CIIODKQPSA-N	6.8×10^{-5}		Yaws (2003)	X	237
	1.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
	7.0×10^{-5}		Yaws (1999)	?	21
trans-2,*trans*-4-hexadiene C_6H_{10} [5194-51-4] APPOKADJQUIAHP-GGWOSOGESA-N	7.0×10^{-5}		Yaws (2003)	X	237
	1.7×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
	7.2×10^{-5}		Yaws (1999)	?	21
2-methyl-1,4-pentadiene C_6H_{10} [763-30-4] DRWYRROCDFQZQF-UHFFFAOYSA-N	8.8×10^{-5}		Yaws (2003)	X	237
	1.1×10^{-4}		Gharagheizi et al. (2012)	Q	
	9.8×10^{-5}		Gharagheizi et al. (2010)	Q	246
2-methyl-1,*cis*-3-pentadiene C_6H_{10} [1501-60-6] RCJMVGJKROQDCB-PLNGDYQASA-N	7.3×10^{-5}		Yaws (2003)	X	237
	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
2-methyl-1,*trans*-3-pentadiene C_6H_{10} [926-54-5] RCJMVGJKROQDCB-SNAWJCMRSA-N	7.3×10^{-5}		Yaws (2003)	X	237
	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
2-methyl-2,3-pentadiene C_6H_{10} [3043-33-2] JWMDOGMKTRMFDS-UHFFFAOYSA-N	7.6×10^{-5}		Yaws (2003)	X	237
	5.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	8.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
3-methyl-1,2-pentadiene C_6H_{10} [7417-48-3] INFFCVIZNSUFGK-UHFFFAOYSA-N	7.8×10^{-5}		Yaws (2003)	X	237
	7.0×10^{-5}		Gharagheizi et al. (2012)	Q	
	7.9×10^{-5}		Gharagheizi et al. (2010)	Q	246

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-1,*cis*-3-pentadiene	7.2×10^{-5}		Yaws (2003)	X	237
C_6H_{10}	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[2787-45-3]	7.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
BOGRNZQRTNVZCZ-WAYWQWQTSA-N					
3-methyl-1,*trans*-3-pentadiene	7.2×10^{-5}		Yaws (2003)	X	237
C_6H_{10}	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[2787-43-1]	7.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
BOGRNZQRTNVZCZ-AATRIKPKSA-N					
3-methyl-1,4-pentadiene	8.6×10^{-5}		Yaws (2003)	X	237
C_6H_{10}	1.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[1115-08-8]	9.6×10^{-5}		Gharagheizi et al. (2010)	Q	246
IKQUUYYDRTYXAP-UHFFFAOYSA-N					
4-methyl-1,2-pentadiene	7.8×10^{-5}		Yaws (2003)	X	237
C_6H_{10}	9.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[13643-05-5]	9.2×10^{-5}		Gharagheizi et al. (2010)	Q	246
CAAAXQFHDYHTTC-UHFFFAOYSA-N					
4-methyl-1,3-pentadiene	7.3×10^{-5}		Yaws (2003)	X	237
C_6H_{10}	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[926-56-7]	7.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
CJSBUWDGPXGFGA-UHFFFAOYSA-N					
2-ethyl-1,3-butadiene	7.4×10^{-5}		Yaws (2003)	X	237
C_6H_{10}	2.2×10^{-4}		Gharagheizi et al. (2012)	Q	
[3404-63-5]	8.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
IGLWCQMNTGCUBB-UHFFFAOYSA-N					
2,3-dimethyl-1,3-butadiene	2.0×10^{-4}		Duchowicz et al. (2020)	V	186
C_6H_{10}	2.0×10^{-4}		Mackay et al. (2006a)	V	
[513-81-5]	2.0×10^{-4}		Mackay et al. (1993)	V	
SDJHPPZKZZWAKF-UHFFFAOYSA-N	2.0×10^{-4}		Meylan and Howard (1991)	V	
	2.1×10^{-4}		Hine and Mookerjee (1975)	V	
	7.7×10^{-5}		Yaws (2003)	X	237
	6.0×10^{-4}		Duchowicz et al. (2020)	Q	
	1.3×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-5}		Gharagheizi et al. (2010)	Q	246
	1.9×10^{-4}		Hilal et al. (2008)	Q	
	8.1×10^{-6}		Modarresi et al. (2005)	Q	247
	4.7×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	3.8×10^{-5}		Yao et al. (2002)	Q	229
	9.9×10^{-5}		Suzuki et al. (1992)	Q	232
	5.2×10^{-5}		Meylan and Howard (1991)	Q	
	4.7×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	8.0×10^{-5}		Yaws (1999)	?	21

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,6-heptadiene	5.6×10^{-5}		Plyasunov and Shock (2000)	L	
C_7H_{12}	4.6×10^{-5}		Hilal et al. (2008)	Q	
[3070-53-9]	1.5×10^{-4}		Yaffe et al. (2003)	Q	248, 249
GEAWFZNTIFJMHR-UHFFFAOYSA-N					
2,5-dimethyl-2,4-hexadiene	2.1×10^{-4}		Ebert et al. (2023)	?	316
C_8H_{14}					
[764-13-6]					
DZPCYXCBXGQBRN-UHFFFAOYSA-N					
1-methylcyclopropene	2.5×10^{-4}		HSDB (2015)	Q	99
C_4H_6					
[3100-04-7]					
SHDPRTQPPWIEJG-UHFFFAOYSA-N					
cyclopentene	2.0×10^{-4}	3300	Brockbank (2013)	L	1
C_5H_8	1.6×10^{-4}		Plyasunov and Shock (2000)	L	
[142-29-0]	2.3×10^{-4}	2200	Bakierowska and Trzeszczyński (2003)	M	
LPIQUOYDBNQMRZ-UHFFFAOYSA-N	1.5×10^{-4}		Duchowicz et al. (2020)	V	186
	1.5×10^{-4}		Mackay et al. (2006a)	V	
	1.5×10^{-4}		Mackay et al. (1993)	V	
	1.6×10^{-4}		Hwang et al. (1992)	V	
	1.6×10^{-4}		Hine and Mookerjee (1975)	V	
	1.5×10^{-4}		Yaws (2003)	X	237
	4.3×10^{-3}		Duchowicz et al. (2020)	Q	
	1.5×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
	3.1×10^{-4}		Hilal et al. (2008)	Q	
		3400	Kühne et al. (2005)	Q	
	1.5×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	2.8×10^{-4}		Yao et al. (2002)	Q	229
	4.5×10^{-4}		English and Carroll (2001)	Q	230, 231
	1.4×10^{-4}		Katritzky et al. (1998)	Q	
	1.7×10^{-4}		Suzuki et al. (1992)	Q	232
	1.6×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
		2200	Kühne et al. (2005)	?	
	1.6×10^{-4}		Yaws (1999)	?	21
	1.5×10^{-4}		Yaws and Yang (1992)	?	21

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyclohexene	2.9×10^{-4}	3600	Brockbank (2013)	L	1
C_6H_{10}	2.2×10^{-4}		Plyasunov and Shock (2000)	L	
[110-83-8]	3.3×10^{-4}	2000	Bakierowska and Trzeszczyński (2003)	M	
HGCIXCUEYOPUTN-UHFFFAOYSA-N	2.5×10^{-4}		Nielsen et al. (1994)	M	
	2.2×10^{-4}		Mackay et al. (2006a)	V	
	2.2×10^{-4}		Mackay et al. (1993)	V	
	2.2×10^{-4}		Hwang et al. (1992)	V	
	2.2×10^{-4}		Hine and Mookerjee (1975)	V	
	2.2×10^{-4}		Yaws (2003)	X	258
	2.2×10^{-4}		Yaws (2003)	X	237
	3.3×10^{-4}		Dupeux et al. (2022)	Q	259
	6.6×10^{-5}		Keshavarz et al. (2022)	Q	
	4.3×10^{-3}		Duchowicz et al. (2020)	Q	184
	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	9.9×10^{-5}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.5×10^{-4}		Gharagheizi et al. (2010)	Q	246
	2.5×10^{-4}		Hilal et al. (2008)	Q	
	1.4×10^{-4}		Modarresi et al. (2007)	Q	67
		3700	Kühne et al. (2005)	Q	
	2.2×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	2.5×10^{-4}		Yao et al. (2002)	Q	229
	3.3×10^{-4}		English and Carroll (2001)	Q	230, 231
	1.5×10^{-4}		Katritzky et al. (1998)	Q	
	2.0×10^{-4}		Russell et al. (1992)	Q	279
	1.3×10^{-4}		Suzuki et al. (1992)	Q	232
	1.3×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	2.2×10^{-4}		Duchowicz et al. (2020)	?	185, 21
		3600	Kühne et al. (2005)	?	
	2.2×10^{-4}		Yaws (1999)	?	21
	2.2×10^{-4}		Yaws and Yang (1992)	?	21
1-methylcyclopentene C_6H_{10} [693-89-0] ATQUFXWBVZUTKO-UHFFFAOYSA-N	2.4×10^{-4}		Hilal et al. (2008)	Q	
cycloheptene	2.0×10^{-4}		Brockbank (2013)	L	
C_7H_{12}	2.0×10^{-4}		Plyasunov and Shock (2000)	L	
[628-92-2]	2.6×10^{-4}		Mackay et al. (2006a)	V	
ZXIJMRYMVAMXQP-UHFFFAOYSA-N	2.0×10^{-4}		Mackay et al. (1993)	V	
	1.3×10^{-4}		Hilal et al. (2008)	Q	

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methylcyclohexene	1.4×10^{-4}		Plyasunov and Shock (2000)	L	
$C_6H_9CH_3$	1.3×10^{-4}		Duchowicz et al. (2020)	V	186
[591-49-1]	1.2×10^{-4}		Mackay et al. (2006a)	V	
CTMHWPIWNRWQEG-UHFFFAOYSA-N	1.3×10^{-4}		Hine and Mookerjee (1975)	V	
	1.4×10^{-3}		Duchowicz et al. (2020)	Q	
	1.9×10^{-4}		Hilal et al. (2008)	Q	
	1.2×10^{-4}		Modarresi et al. (2007)	Q	67
	1.3×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	2.4×10^{-4}		English and Carroll (2001)	Q	230, 231
	1.6×10^{-4}		Katritzky et al. (1998)	Q	
	9.2×10^{-5}		Suzuki et al. (1992)	Q	232
cyclooctene	2.1×10^{-4}	4300	Brockbank (2013)	L	1
C_8H_{14}	2.1×10^{-4}	4300	Dohányosová et al. (2004)	M	317
[931-88-4]	2.1×10^{-4}		Mackay et al. (2006a)	V	
URYYVOIYTNXXBN-UPHRSURJSA-N		4400	Kühne et al. (2005)	Q	
		4400	Kühne et al. (2005)	?	
1,1,2,3,3-pentamethyl-2,3,4,5,6,7-hexahydro-1H-indene	2.5×10^{-5}		Zhang et al. (2010)	Q	287, 288
$C_{14}H_{24}$	2.5×10^{-6}		Zhang et al. (2010)	Q	287, 289
[33704-59-5]	1.1×10^{-3}		Zhang et al. (2010)	Q	287, 290
CDEGOUYLXTUDAU-UHFFFAOYSA-N	7.3×10^{-5}		Zhang et al. (2010)	Q	287, 291
1,3-cyclopentadiene	1.8×10^{-4}		Plyasunov and Shock (2000)	L	
C_5H_6	4.7×10^{-4}		Duchowicz et al. (2020)	V	186
[542-92-7]	4.7×10^{-4}		HSDB (2015)	V	
ZSWFCLXCOIISFI-UHFFFAOYSA-N	5.1×10^{-3}		Duchowicz et al. (2020)	Q	
	1.2×10^{-3}		Hilal et al. (2008)	Q	
1,3-cyclohexadiene	6.7×10^{-4}		Yaws (2003)	X	237
C_6H_8	8.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[592-57-4]	4.4×10^{-4}		Gharagheizi et al. (2010)	Q	246
MGNZXYYWBUKAII-UHFFFAOYSA-N	1.1×10^{-3}		Hilal et al. (2008)	Q	
	6.7×10^{-4}		Yaws (1999)	?	21
1,4-cyclohexadiene	1.3×10^{-3}	4000	Brockbank (2013)	L	1
C_6H_8	1.0×10^{-3}	3800	Plyasunov and Shock (2000)	L	
(1,4-dihydrobenzene)	1.1×10^{-3}		Mackay et al. (2006a)	V	
[628-41-1]	9.7×10^{-4}		Mackay et al. (1993)	V	
UVJHQYIOXKWHFD-UHFFFAOYSA-N	1.0×10^{-3}		Hilal et al. (2008)	C	
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	8.0×10^{-4}		Hilal et al. (2008)	Q	
	5.4×10^{-4}		Modarresi et al. (2007)	Q	67

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Table A2.3: Aliphatic alkenes and cycloalkenes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3-cycloheptadiene C_7H_{10} [4054-38-0] GWYPDXLJACEENP-UHFFFAOYSA-N	6.2×10^{-4}		Hilal et al. (2008)	Q	
1,3,5-cycloheptatriene C_7H_8 [544-25-2] CHVJITGCYZJHLR-UHFFFAOYSA-N	2.2×10^{-3}	3900	Plyasunov and Shock (2000)	L	
	2.1×10^{-3}		Duchowicz et al. (2020)	V	186
			Mackay et al. (2006a)	V	292
	2.1×10^{-3}		Mackay et al. (1993)	V	
	2.1×10^{-3}		Cabani et al. (1981)	V	
	2.2×10^{-3}		Yaws (2003)	X	237
	6.0×10^{-3}		Duchowicz et al. (2020)	Q	
	4.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
	3.8×10^{-3}		Hilal et al. (2008)	Q	
	3.4×10^{-4}		Modarresi et al. (2007)	Q	67
	3.0×10^{-3}		English and Carroll (2001)	Q	230, 231
	8.4×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	2.1×10^{-3}		Yaws (1999)	?	21
	2.1×10^{-3}		Yaws and Yang (1992)	?	21
1,5-cyclooctadiene C_8H_{12} [111-78-4] VYXHVRARDIDEHS-QGTKBVGQSA-N	3.8×10^{-4}		Hilal et al. (2008)	Q	
1-ethenylcyclohexene C_8H_{12} [2622-21-1] SDRZFSPCVYEJTP-UHFFFAOYSA-N	7.7×10^{-4}		Hilal et al. (2008)	Q	
4-ethenylcyclohexene C_8H_{12} (4-vinylcyclohexene) [100-40-3] BBDKZWKEPDTENS-UHFFFAOYSA-N	2.2×10^{-4}		Plyasunov and Shock (2000)	L	
	2.2×10^{-4}		Duchowicz et al. (2020)	V	186
	2.2×10^{-4}		HSDB (2015)	V	
	5.9×10^{-3}		Duchowicz et al. (2020)	Q	
	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	1.8×10^{-4}		Hilal et al. (2008)	Q	
	2.7×10^{-4}		Modarresi et al. (2007)	Q	67
	2.2×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	2.7×10^{-4}		Katritzky et al. (1998)	Q	
	2.2×10^{-4}		Yaws (1999)	?	21
1,3,5,7-cyclooctatetraene C_8H_8 [629-20-9] KDUIUFJBNGTBMD-DLMDZQPMSA-N	3.6×10^{-2}		Hilal et al. (2008)	Q	

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Table A2.3: Aliphatic alkenes and cycloalkenes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
3a,4,7,7a-tetrahydro-4,7-methano-1H-indene $C_{10}H_{12}$ (dicyclopentadiene) [77-73-6] HECLRDQVFMWTQS-UHFFFAOYSA-N	1.6×10^{-4}		HSDB (2015)	Q	99
	2.8×10^{-5}		Hilal et al. (2008)	Q	
1,5,9-cyclododecatriene $C_{12}H_{18}$ [4904-61-4] ZOLLIQAKMYWTBR-UHFFFAOYSA-N	3.3×10^{-4}		HSDB (2015)	Q	99
(*E*,*E*,*Z*)-1,5,9-cyclododecatriene $C_{12}H_{18}$ [706-31-0] ZOLLIQAKMYWTBR-RYMQXAEESA-N	1.8×10^{-4}		Ebert et al. (2023)	?	318

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A2.4 Aliphatic alkynes

Table A2.4: Aliphatic alkynes

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethyne	4.1×10^{-4}	1800	Burkholder et al. (2019)	L	1
C_2H_2	4.1×10^{-4}	1800	Burkholder et al. (2015)	L	1
(acetylene)	4.1×10^{-4}	1700	Sander et al. (2011)	L	1
[74-86-2]	4.1×10^{-4}	1800	Sander et al. (2006)	L	1
HSFWRNGVRCDJHI-UHFFFAOYSA-N	4.1×10^{-4}	1700	Fogg et al. (2001)	L	
	4.1×10^{-4}	1800	Plyasunov and Shock (2000)	L	
	4.1×10^{-4}	1800	Wilhelm et al. (1977)	L	
	4.0×10^{-4}	2500	Jadkar and Chaudhari (1980)	M	
	2.5×10^{-4}		Maillard and Rosenthal (1952)	M	319
	3.3×10^{-4}		Grollman (1929)	M	58
	4.2×10^{-4}	1900	Gatterer (1926)	M	
	3.7×10^{-4}		Kremann and Hönel (1913)	M	
	4.1×10^{-4}	2000	Winkler (1906)	M	
	5.1×10^{-4}		Billitzer (1902)	M	80, 320
	4.5×10^{-4}		Duchowicz et al. (2020)	V	186
	4.5×10^{-4}		HSDB (2015)	V	
	3.9×10^{-4}		Hwang et al. (1992)	V	
	4.1×10^{-4}		Hine and Mookerjee (1975)	V	
	1.8×10^{-5}		Pierotti (1965)	T	
	3.9×10^{-4}		Yaws (2003)	X	237
	4.1×10^{-4}	1800	Schoen (1923)	X	321
	4.4×10^{-4}		Vítovec (1968)	X	321, 12
	4.1×10^{-4}		Deno and Berkheimer (1960)	C	
	4.2×10^{-4}		Hayer et al. (2022)	Q	20
	8.9×10^{-3}		Duchowicz et al. (2020)	Q	
	3.5×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.8×10^{-3}		Wang et al. (2017)	Q	80, 239
	2.9×10^{-3}		Wang et al. (2017)	Q	80, 240
	8.4×10^{-5}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.4×10^{-3}		Hilal et al. (2008)	Q	
		1800	Kühne et al. (2005)	Q	
	3.8×10^{-4}		Suzuki et al. (1992)	Q	232
	5.8×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	5.0×10^{-4}		Irmann (1965)	Q	
		1800	Kühne et al. (2005)	?	
	3.9×10^{-4}		Yaws (1999)	?	21
	4.1×10^{-4}	1800	Yaws et al. (1999)	?	21
	4.1×10^{-4}	1800	Dean and Lange (1999)	?	322, 23
	3.9×10^{-4}		Yaws and Yang (1992)	?	21
	4.1×10^{-4}		Abraham et al. (1990)	?	

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Table A2.4: Aliphatic alkynes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
propyne	7.5×10^{-4}	2400	Plyasunov and Shock (2000)	L	
CH_3CCH	9.0×10^{-4}		Mackay and Shiu (1981)	L	
[74-99-7]	9.2×10^{-4}		McAuliffe (1966)	M	
MWWATHDPGQKSAR-UHFFFAOYSA-N	7.7×10^{-4}	2500	Simpson and Lovell (1962)	M	
	6.2×10^{-4}	2000	Inga and McKetta (1961)	M	
	9.0×10^{-4}		Duchowicz et al. (2020)	V	186
	9.0×10^{-4}		HSDB (2015)	V	
	9.0×10^{-4}		Hine and Mookerjee (1975)	V	
	6.6×10^{-4}		Irmann (1965)	V	
	9.2×10^{-4}		Yaws (2003)	X	237
	7.6×10^{-4}		Hayer et al. (2022)	Q	20
	3.2×10^{-3}		Duchowicz et al. (2020)	Q	
	1.1×10^{-4}		Gharagheizi et al. (2012)	Q	
	9.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
	6.0×10^{-4}		Hilal et al. (2008)	Q	
	4.0×10^{-4}		Modarresi et al. (2007)	Q	67
		2100	Kühne et al. (2005)	Q	
	9.2×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	2.7×10^{-4}		Suzuki et al. (1992)	Q	232
	4.4×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	8.4×10^{-4}		Irmann (1965)	Q	
		2400	Kühne et al. (2005)	?	
	9.3×10^{-4}		Yaws (1999)	?	21
	9.2×10^{-4}		Yaws and Yang (1992)	?	21
	9.0×10^{-4}		Abraham et al. (1990)	?	
			Wilhelm et al. (1977)	W	86
1-butyne	5.6×10^{-3}		Burkholder et al. (2019)	L	
C_2H_5CCH	5.6×10^{-4}		Brockbank (2013)	L	
(ethylacetylene)	6.2×10^{-4}	1900	Plyasunov and Shock (2000)	L	
[107-00-6]	5.2×10^{-4}		Mackay and Shiu (1981)	L	
KDKYADYSIPSCCQ-UHFFFAOYSA-N	7.5×10^{-4}	1900	Wilhelm et al. (1977)	L	
	5.4×10^{-4}		McAuliffe (1966)	M	
	7.2×10^{-4}	1900	Simpson and Lovell (1962)	M	
	5.2×10^{-4}		Mackay et al. (2006a)	V	
	2.9×10^{-4}		Hwang et al. (1992)	V	
	5.3×10^{-4}		Hine and Mookerjee (1975)	V	
	5.4×10^{-4}		Yaws (2003)	X	237
	8.3×10^{-5}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Gharagheizi et al. (2010)	Q	246
	3.6×10^{-4}		Hilal et al. (2008)	Q	
	2.1×10^{-4}		Modarresi et al. (2007)	Q	67
		2500	Kühne et al. (2005)	Q	
	6.9×10^{-4}		English and Carroll (2001)	Q	230, 231
	2.1×10^{-4}		Suzuki et al. (1992)	Q	232
	3.7×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	6.4×10^{-4}		Irmann (1965)	Q	
		1900	Kühne et al. (2005)	?	

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Table A2.4: Aliphatic alkynes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.4×10^{-4}		Yaws (1999)	?	21
	5.4×10^{-4}		Yaws and Yang (1992)	?	21
	5.3×10^{-4}		Abraham et al. (1990)	?	
2-butyne	4.6×10^{-4}		Yaws (2003)	X	237
C_4H_6	1.1×10^{-4}		Gharagheizi et al. (2012)	Q	
(dimethylacetylene)	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
[503-17-3]	1.9×10^{-3}		Hilal et al. (2008)	Q	
XNMQEEKYCVKGBD-UHFFFAOYSA-N	4.7×10^{-4}		Yaws (1999)	?	21
1-pentyne	3.9×10^{-4}		Brockbank (2013)	L	
C_3H_7CCH	3.2×10^{-4}		Plyasunov and Shock (2000)	L	
[627-19-0]	4.0×10^{-4}		Mackay and Shiu (1981)	L	
IBXNCJKFFQIKKY-UHFFFAOYSA-N	4.0×10^{-4}		Duchowicz et al. (2020)	V	186
	4.0×10^{-4}		Mackay et al. (2006a)	V	
	4.0×10^{-4}		Mackay et al. (1993)	V	
	2.5×10^{-4}		Amoore and Buttery (1978)	V	
	3.9×10^{-4}		Hine and Mookerjee (1975)	V	
	4.0×10^{-4}		Yaws (2003)	X	237
	3.2×10^{-3}		Duchowicz et al. (2020)	Q	
	6.0×10^{-5}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
	2.4×10^{-4}		Hilal et al. (2008)	Q	
	1.5×10^{-4}		Modarresi et al. (2007)	Q	67
	1.3×10^{-5}		Modarresi et al. (2005)	Q	247
	4.6×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	7.5×10^{-5}		Yao et al. (2002)	Q	229
	2.3×10^{-4}		English and Carroll (2001)	Q	230, 260
	6.1×10^{-5}		Russell et al. (1992)	Q	279
	1.6×10^{-4}		Suzuki et al. (1992)	Q	232
	2.9×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	4.0×10^{-4}		Yaws (1999)	?	21
	2.0×10^{-4}		Yaws and Yang (1992)	?	21
	3.9×10^{-4}		Abraham et al. (1990)	?	
2-pentyne	5.6×10^{-4}		Yaws (2003)	X	237
C_5H_8	6.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[627-21-4]	7.0×10^{-4}		Gharagheizi et al. (2010)	Q	246
NKTDTMONXHODTI-UHFFFAOYSA-N	1.1×10^{-3}		Hilal et al. (2008)	Q	
	1.1×10^{-5}		Modarresi et al. (2005)	Q	247
	7.9×10^{-5}		Yao et al. (2002)	Q	229
	4.0×10^{-4}		Yaws (1999)	?	21
3-methyl-1-butyne	5.3×10^{-4}		Yaws (2003)	X	237
C_5H_8	4.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[598-23-2]	6.3×10^{-4}		Gharagheizi et al. (2010)	Q	246
USCSRAJGJYMJFZ-UHFFFAOYSA-N	3.7×10^{-4}		Yaws (1999)	?	21

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Table A2.4: Aliphatic alkynes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
1-hexyne	2.6×10^{-4}		Brockbank (2013)	L	
C_4H_9CCH	3.0×10^{-4}		Plyasunov and Shock (2000)	L	
[693-02-7]	2.5×10^{-4}		Duchowicz et al. (2020)	V	186
CGHIBGNXEGJPQZ-UHFFFAOYSA-N	2.5×10^{-4}		Duchowicz et al. (2020)	V	186
	2.4×10^{-4}		Mackay et al. (2006a)	V	
	2.4×10^{-4}		Mackay et al. (1993)	V	
	2.5×10^{-4}		Hine and Mookerjee (1975)	V	
	2.5×10^{-4}		Yaws (2003)	X	237
	3.2×10^{-3}		Duchowicz et al. (2020)	Q	
	3.2×10^{-3}		Duchowicz et al. (2020)	Q	
	4.8×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.7×10^{-4}		Hilal et al. (2008)	Q	
	1.5×10^{-4}		Modarresi et al. (2007)	Q	67
	1.1×10^{-5}		Modarresi et al. (2005)	Q	247
	2.4×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	2.7×10^{-5}		Yao et al. (2002)	Q	229
	1.8×10^{-4}		English and Carroll (2001)	Q	230, 274
	1.2×10^{-4}		Suzuki et al. (1992)	Q	232
	2.3×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	2.5×10^{-4}		Yaws (1999)	?	21
	4.6×10^{-4}		Yaws and Yang (1992)	?	21
	2.5×10^{-4}		Abraham et al. (1990)	?	
2-hexyne	3.5×10^{-4}		Yaws (2003)	X	237
C_6H_{10}	4.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[764-35-2]	3.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
MELUCTCJOARQQG-UHFFFAOYSA-N	5.8×10^{-4}		Hilal et al. (2008)	Q	
	1.0×10^{-5}		Modarresi et al. (2005)	Q	247
	3.1×10^{-5}		Yao et al. (2002)	Q	229
	2.5×10^{-4}		Yaws (1999)	?	21
3-hexyne	5.5×10^{-4}		Plyasunov and Shock (2000)	L	
C_6H_{10}	5.6×10^{-4}		Yaws (2003)	X	237
[928-49-4]	4.1×10^{-5}		Gharagheizi et al. (2012)	Q	
DQQNMIPXXNPGCV-UHFFFAOYSA-N	3.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
	6.0×10^{-4}		Hilal et al. (2008)	Q	
	1.0×10^{-5}		Modarresi et al. (2005)	Q	247
	3.2×10^{-5}		Yao et al. (2002)	Q	229, 267
	2.6×10^{-4}		Yaws (1999)	?	21
3-methyl-1-pentyne	4.6×10^{-4}		Yaws (2003)	X	237
C_6H_{10}	3.5×10^{-5}		Gharagheizi et al. (2012)	Q	
[922-59-8]	3.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
PLHJCCHSCFNKCC-UHFFFAOYSA-N					

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Table A2.4: Aliphatic alkynes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methyl-1-pentyne	4.5×10^{-4}		Yaws (2003)	X	237
C_6H_{10}	3.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[7154-75-8]	3.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
OXRWICUICBZVAE-UHFFFAOYSA-N					
4-methyl-2-pentyne	4.1×10^{-4}		Yaws (2003)	X	237
C_6H_{10}	3.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[21020-27-9]	4.6×10^{-4}		Gharagheizi et al. (2010)	Q	246
SLMFWJQZLPEDDU-UHFFFAOYSA-N					
3,3-dimethyl-1-butyne	4.6×10^{-4}		Yaws (2003)	X	237
C_6H_{10}	2.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[917-92-0]	4.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
PPWNCLVNXGCGAF-UHFFFAOYSA-N					
1-heptyne	1.8×10^{-4}		Brockbank (2013)	L	
$C_5H_{11}CCH$	1.8×10^{-4}		Plyasunov and Shock (2000)	L	
[628-71-7]	1.4×10^{-4}		Duchowicz et al. (2020)	V	186
YVXHZKKCZYLQOP-UHFFFAOYSA-N	1.3×10^{-4}		Mackay et al. (2006a)	V	
	2.2×10^{-4}		Mackay et al. (1993)	V	
	1.5×10^{-4}		Hine and Mookerjee (1975)	V	
	1.4×10^{-4}		Yaws (2003)	X	237
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	4.1×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.1×10^{-4}		Hilal et al. (2008)	Q	
	1.1×10^{-4}		Modarresi et al. (2007)	Q	67
	9.6×10^{-6}		Modarresi et al. (2005)	Q	247
	1.5×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	2.4×10^{-5}		Yao et al. (2002)	Q	229
	1.3×10^{-4}		English and Carroll (2001)	Q	230, 231
	9.5×10^{-5}		Suzuki et al. (1992)	Q	232
	1.8×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	1.4×10^{-4}		Yaws (1999)	?	21
	1.4×10^{-4}		Yaws and Yang (1992)	?	21
	1.5×10^{-4}		Abraham et al. (1990)	?	
2-heptyne	4.9×10^{-4}		Plyasunov and Shock (2000)	L	
C_7H_{12}	5.0×10^{-4}		Yaws (2003)	X	237
[1119-65-9]	4.1×10^{-5}		Gharagheizi et al. (2012)	Q	
AMSFEMSYKQQCHL-UHFFFAOYSA-N	2.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
3-heptyne	2.2×10^{-4}		Yaws (2003)	X	237
C_7H_{12}	3.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[2586-89-2]	2.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
KLYHSJRCIZOUHE-UHFFFAOYSA-N					

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Table A2.4: Aliphatic alkynes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-3-hexyne	2.2×10^{-4}		Plyasunov and Shock (2000)	L	
C_7H_{12}	2.6×10^{-4}		Yaws (2003)	X	237
[36566-80-0]	2.6×10^{-5}		Gharagheizi et al. (2012)	Q	
POBOUPFSQKXZFZ-UHFFFAOYSA-N	2.5×10^{-4}		Gharagheizi et al. (2010)	Q	246
3-methyl-1-hexyne	3.1×10^{-4}		Yaws (2003)	X	237
C_7H_{12}	2.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[40276-93-5]	2.5×10^{-4}		Gharagheizi et al. (2010)	Q	246
OPZULQHRFNTFFZ-UHFFFAOYSA-N					
4-methyl-1-hexyne	2.9×10^{-4}		Yaws (2003)	X	237
C_7H_{12}	3.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[52713-81-2]	2.5×10^{-4}		Gharagheizi et al. (2010)	Q	246
YFZSGTDENCTWGW-UHFFFAOYSA-N					
4-methyl-2-hexyne	2.5×10^{-4}		Yaws (2003)	X	237
C_7H_{12}	2.5×10^{-4}		Gharagheizi et al. (2010)	Q	246
[20198-49-6]					
ABEXZFRJQJSEBW-UHFFFAOYSA-N					
5-methyl-1-hexyne	2.8×10^{-4}		Yaws (2003)	X	237
C_7H_{12}	3.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[2203-80-7]	2.5×10^{-4}		Gharagheizi et al. (2010)	Q	246
HKNANEMUCJGPMS-UHFFFAOYSA-N					
5-methyl-2-hexyne	2.4×10^{-4}		Yaws (2003)	X	237
C_7H_{12}	3.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[53566-37-3]	2.5×10^{-4}		Gharagheizi et al. (2010)	Q	246
SVGAHRUSRQTQES-UHFFFAOYSA-N					
3,3-dimethyl-1-pentyne	3.6×10^{-4}		Yaws (2003)	X	237
C_7H_{12}	1.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[918-82-1]	3.0×10^{-4}		Gharagheizi et al. (2010)	Q	246
KQIIKSQUHGGYCU-UHFFFAOYSA-N					
3,4-dimethyl-1-pentyne	3.3×10^{-4}		Yaws (2003)	X	237
C_7H_{12}	2.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[61064-08-2]	3.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
JDQKSTIAVKXRSK-UHFFFAOYSA-N					
4,4-dimethyl-1-pentyne	3.3×10^{-4}		Yaws (2003)	X	237
C_7H_{12}	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[13361-63-2]	3.0×10^{-4}		Gharagheizi et al. (2010)	Q	246
KHBYKPSFBHWBJQ-UHFFFAOYSA-N					
4,4-dimethyl-2-pentyne	3.0×10^{-4}		Yaws (2003)	X	237
C_7H_{12}	1.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[999-78-0]	2.7×10^{-4}		Gharagheizi et al. (2010)	Q	246
FOALCTWKQSWRST-UHFFFAOYSA-N					

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Table A2.4: Aliphatic alkynes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-1-pentyne	3.2×10^{-4}		Yaws (2003)	X	237
C_7H_{12}	2.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[21020-26-8]	2.5×10^{-4}		Gharagheizi et al. (2010)	Q	246
WGWGXWSBPXLXTA-UHFFFAOYSA-N					
1-octyne	1.2×10^{-4}		Brockbank (2013)	L	
$C_6H_{13}CCH$	1.2×10^{-4}		Plyasunov and Shock (2000)	L	
[629-05-0]	1.2×10^{-4}		Duchowicz et al. (2020)	V	186
UMIPWJGWASORKV-UHFFFAOYSA-N	1.3×10^{-4}		Mackay et al. (2006a)	V	
	1.3×10^{-4}		Mackay et al. (1993)	V	
	1.2×10^{-4}		Hine and Mookerjee (1975)	V	
	1.3×10^{-4}		Yaws (2003)	X	237
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	3.1×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
	6.4×10^{-5}		Hilal et al. (2008)	Q	
	1.0×10^{-4}		Modarresi et al. (2007)	Q	67
	1.2×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	1.0×10^{-4}		English and Carroll (2001)	Q	230, 231
	7.2×10^{-5}		Suzuki et al. (1992)	Q	232
	1.5×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	1.2×10^{-4}		Yaws and Yang (1992)	?	21
	1.2×10^{-4}		Abraham et al. (1990)	?	
2-octyne	1.3×10^{-4}		Yaws (2003)	X	237
C_8H_{14}	3.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[2809-67-8]	1.3×10^{-4}		Gharagheizi et al. (2010)	Q	246
QCQALVMFTWRCFI-UHFFFAOYSA-N	2.2×10^{-4}		Hilal et al. (2008)	Q	
3-octyne	1.5×10^{-4}		Yaws (2003)	X	237
C_8H_{14}	2.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[15232-76-5]	1.3×10^{-4}		Gharagheizi et al. (2010)	Q	246
UDEISTCPVNLKRJ-UHFFFAOYSA-N					
2,2-dimethyl-3-hexyne	1.4×10^{-4}		Plyasunov and Shock (2000)	L	
C_8H_{14}					
[4911-60-8]					
XYBFBXTUWDPXLK-UHFFFAOYSA-N					
1-nonyne	8.5×10^{-5}		Brockbank (2013)	L	
$C_7H_{15}CCH$	9.7×10^{-5}		Plyasunov and Shock (2000)	L	
[3452-09-3]	6.9×10^{-5}		Duchowicz et al. (2020)	V	186
OSSQSXOTMIGBCF-UHFFFAOYSA-N	6.9×10^{-5}		Meylan and Howard (1991)	V	
	6.9×10^{-5}		Hine and Mookerjee (1975)	V	
	7.2×10^{-5}		Yaws (2003)	X	237
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	2.6×10^{-5}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-5}		Gharagheizi et al. (2010)	Q	246
	4.4×10^{-5}		Hilal et al. (2008)	Q	
	8.2×10^{-5}		Modarresi et al. (2007)	Q	67

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Table A2.4: Aliphatic alkynes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.9×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	7.9×10^{-5}		English and Carroll (2001)	Q	230, 231
	5.6×10^{-5}		Suzuki et al. (1992)	Q	232
	1.1×10^{-4}		Meylan and Howard (1991)	Q	
	1.2×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	6.9×10^{-5}		Yaws and Yang (1992)	?	21
	6.9×10^{-5}		Abraham et al. (1990)	?	
2-nonyne C_9H_{16} [19447-29-1] LXKRETAGISZJAD-UHFFFAOYSA-N	7.3×10^{-5}		Yaws (2003)	X	237
	2.5×10^{-5}		Gharagheizi et al. (2012)	Q	
	8.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
3-nonyne C_9H_{16} [20184-89-8] SRRDSRCWRHKEKU-UHFFFAOYSA-N	7.8×10^{-5}		Yaws (2003)	X	237
	2.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	8.3×10^{-5}		Gharagheizi et al. (2010)	Q	246
2,2,5-trimethyl-3-hexyne C_9H_{16} [17530-23-3] DKFPMSNUJIRAMR-UHFFFAOYSA-N	5.5×10^{-5}		Plyasunov and Shock (2000)	L	
2,2,5,5-tetramethyl-3-hexyne $C_{10}H_{18}$ [17530-24-4] FXVDWKZNFZMSOU-UHFFFAOYSA-N	3.4×10^{-5}		Plyasunov and Shock (2000)	L	
1-decyne $C_{10}H_{18}$ [764-93-2] ILLHQJIJCRNRCJ-UHFFFAOYSA-N	6.6×10^{-5}		Yaws (2003)	X	237
	3.0×10^{-5}		Gharagheizi et al. (2012)	Q	
	6.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
2-decyne $C_{10}H_{18}$ [2384-70-5] RWDDSTHSVISBEA-UHFFFAOYSA-N	5.2×10^{-5}		Yaws (2003)	X	237
	2.9×10^{-5}		Gharagheizi et al. (2012)	Q	
	5.9×10^{-5}		Gharagheizi et al. (2010)	Q	246
3-decyne $C_{10}H_{18}$ [2384-85-2] JUWXVJKQNKKRLD-UHFFFAOYSA-N	5.5×10^{-5}		Yaws (2003)	X	237
	2.5×10^{-5}		Gharagheizi et al. (2012)	Q	
	5.9×10^{-5}		Gharagheizi et al. (2010)	Q	246
1-undecyne $C_{11}H_{20}$ [2243-98-3] YVSFLVNWJIEJRV-UHFFFAOYSA-N	5.9×10^{-5}		Yaws (2003)	X	237
	5.3×10^{-5}		Gharagheizi et al. (2010)	Q	246

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Table A2.4: Aliphatic alkynes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-undecyne	4.5×10^{-5}		Yaws (2003)	X	237
$C_{11}H_{20}$	3.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[60212-29-5]	4.9×10^{-5}		Gharagheizi et al. (2010)	Q	246
XZSXEDPHMIFYOS-UHFFFAOYSA-N					
3-undecyne	4.6×10^{-5}		Yaws (2003)	X	237
$C_{11}H_{20}$	2.7×10^{-5}		Gharagheizi et al. (2012)	Q	
[60212-30-8]	4.9×10^{-5}		Gharagheizi et al. (2010)	Q	246
DPWGJNPCPLQVKQ-UHFFFAOYSA-N					
1-dodecyne	5.8×10^{-5}		Yaws (2003)	X	237
$C_{12}H_{22}$	3.8×10^{-5}		Gharagheizi et al. (2012)	Q	
[765-03-7]	5.4×10^{-5}		Gharagheizi et al. (2010)	Q	246
ZVDBUOGYYYNMQI-UHFFFAOYSA-N					
2-dodecyne	4.9×10^{-5}		Yaws (2003)	X	237
$C_{12}H_{22}$	3.6×10^{-5}		Gharagheizi et al. (2012)	Q	
[629-49-2]	4.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
NDIJGAGRSOPRNJ-UHFFFAOYSA-N					
3-dodecyne	4.5×10^{-5}		Yaws (2003)	X	237
$C_{12}H_{22}$	3.0×10^{-5}		Gharagheizi et al. (2012)	Q	
[6790-27-8]	4.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
ZFAGQZXKTQFQLE-UHFFFAOYSA-N					
1-tridecyne	7.4×10^{-5}		Yaws (2003)	X	237
$C_{13}H_{24}$	4.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[26186-02-7]	6.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
GZEDKDBFUBPZNG-UHFFFAOYSA-N					
2-tridecyne	6.7×10^{-5}		Yaws (2003)	X	237
$C_{13}H_{24}$	3.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[28467-75-6]	5.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
ZGKKGWBQPYIOBH-UHFFFAOYSA-N					
3-tridecyne	5.8×10^{-5}		Yaws (2003)	X	237
$C_{13}H_{24}$	3.2×10^{-5}		Gharagheizi et al. (2012)	Q	
[60186-78-9]	5.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
HDLJOUCNTFYRPD-UHFFFAOYSA-N					
1-tetradecyne	7.4×10^{-5}		Yaws (2003)	X	237
$C_{14}H_{26}$	4.4×10^{-5}		Gharagheizi et al. (2012)	Q	
[765-10-6]	9.9×10^{-5}		Gharagheizi et al. (2010)	Q	246
DZEFNRWGWQDGTR-UHFFFAOYSA-N					
3-tetradecyne	8.6×10^{-5}		Yaws (2003)	X	237
$C_{14}H_{26}$	3.3×10^{-5}		Gharagheizi et al. (2012)	Q	
[60212-32-0]	8.0×10^{-5}		Gharagheizi et al. (2010)	Q	246
DWWMJIDVLGUCDE-UHFFFAOYSA-N					

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Table A2.4: Aliphatic alkynes (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
1-pentadecyne $C_{15}H_{28}$ [765-13-9] DONJGKADZJEXRJ-UHFFFAOYSA-N	2.2×10^{-4} 4.5×10^{-5} 1.9×10^{-4}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2-pentadecyne $C_{15}H_{28}$ [52112-25-1] VWWAVTXUUYIIEE-UHFFFAOYSA-N	2.3×10^{-4} 4.4×10^{-5} 1.5×10^{-4}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
3-pentadecyne $C_{15}H_{28}$ [61886-61-1] RUHQUJVXUGQUNY-UHFFFAOYSA-N	1.5×10^{-4} 3.4×10^{-5} 1.5×10^{-4}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
1-hexadecyne $C_{16}H_{30}$ [629-74-3] UCIDYSLOTJMRAM-UHFFFAOYSA-N	8.3×10^{-4} 5.0×10^{-4}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
3-hexadecyne $C_{16}H_{30}$ [61886-62-2] HRFPRVYNMNOAQO-UHFFFAOYSA-N	3.3×10^{-4} 3.3×10^{-5} 3.8×10^{-4}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
3-buten-1-yne CH_2CHCCH (vinylacetylene) [689-97-4] WFYPICNXBKQZGB-UHFFFAOYSA-N	4.1×10^{-4} 3.7×10^{-4} 3.8×10^{-4} 3.4×10^{-4} 3.4×10^{-4} 1.1×10^{-2} 1.1×10^{-3} 3.5×10^{-4}	1700 1700 1800 2600 2100 	Plyasunov and Shock (2000) Wilhelm et al. (1977) Simpson and Lovell (1962) Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Hilal et al. (2008) Kühne et al. (2005) Kühne et al. (2005) Yaws (1999)	L L M V V Q Q Q ? ?	 323 186 21, 38
butadiyne C_4H_2 (biacetylene) [460-12-8] LLCSWKVOHICRDD-UHFFFAOYSA-N	2.0×10^{-3} 2.7×10^{-1} 8.6×10^{-3} 1.9×10^{-3} 1.9×10^{-3}		Irmann (1965) Hayer et al. (2022) Hilal et al. (2008) Yaws (1999) Yaws and Yang (1992)	C Q Q ? ?	 20 21 21
1,6-heptadiyne C_7H_8 [2396-63-6] RSPZSDWVQWRAEF-UHFFFAOYSA-N	4.6×10^{-3}		Plyasunov and Shock (2000)	L	
1,8-nonadiyne C_9H_{12} [2396-65-8] DMOVPHYFYSASTC-UHFFFAOYSA-N	3.0×10^{-3}		Plyasunov and Shock (2000)	L	

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Table A2.4: Aliphatic alkynes (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note

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A2.5 Mononuclear aromatics

Table A2.5: Mononuclear aromatics

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benzene	1.8×10^{-3}	3800	Schwardt et al. (2021)	L	1
C_6H_6	1.8×10^{-3}	3700	Brockbank (2013)	L	1
[71-43-2]	1.7×10^{-3}	4200	Staudinger and Roberts (2001)	L	
UHOVQNZJYSORNB-UHFFFAOYSA-N	1.8×10^{-3}	3800	Plyasunov and Shock (2000)	L	
	1.6×10^{-3}	4100	Staudinger and Roberts (1996)	L	
	1.8×10^{-3}		Mackay and Shiu (1981)	L	
	1.7×10^{-3}		Kim and Kim (2014)	M	
	1.8×10^{-3}	3800	Hiatt (2013)	M	
	2.7×10^{-3}	1400	Zhang et al. (2013)	M	324
	3.5×10^{-3}		Zhang et al. (2013)	M	325
	1.4×10^{-3}	2400	Lau et al. (2010)	M	11
	1.7×10^{-3}	4200	Sieg et al. (2009)	M	326
	1.8×10^{-3}		Li et al. (2008)	M	
	2.5×10^{-3}		Lodge and Danso (2007)	M	
	1.4×10^{-3}	2200	Lei et al. (2004)	M	327
			Cheng et al. (2003)	M	328
	1.8×10^{-3}		Karl et al. (2003)	M	87
	1.8×10^{-3}	4200	Bakierowska and Trzeszczyński (2003)	M	
	1.7×10^{-3}	3800	Görgényi et al. (2002)	M	329
	1.9×10^{-3}	3200	Bierwagen and Keller (2001)	M	
	2.1×10^{-3}		Kochetkov et al. (2001)	M	297, 330
	1.7×10^{-3}		Kochetkov et al. (2001)	M	297, 331
	1.8×10^{-3}		Miller and Stuart (2000)	M	72
	3.7×10^{-3}		Altschuh et al. (1999)	M	
	1.7×10^{-3}		Ryu and Park (1999)	M	
	1.8×10^{-3}		Dohnal and Hovorka (1999)	M	
	1.8×10^{-3}		Allen et al. (1998)	M	
	2.2×10^{-3}		Peng and Wan (1998)	M	
	1.4×10^{-3}	3300	Peng and Wan (1998)	M	70
	2.2×10^{-3}		de Wolf and Lieder (1998)	M	87
	1.6×10^{-3}		Welke et al. (1998)	M	
	1.9×10^{-3}	3200	Peng and Wan (1997)	M	
	1.8×10^{-3}	2700	Kondoh and Nakajima (1997)	M	
	1.4×10^{-3}	3300	Park et al. (1997)	M	
	1.8×10^{-3}	4200	Alaee et al. (1996)	M	
	1.6×10^{-3}	4300	Turner et al. (1996)	M	
	2.1×10^{-3}	3900	Dewulf et al. (1995)	M	
	2.0×10^{-3}		Nielsen et al. (1994)	M	
	1.7×10^{-3}	4100	Khalfaoui and Newsham (1994b)	M	332
	1.8×10^{-3}	3400	Robbins et al. (1993)	M	333
	1.7×10^{-3}		Hoff et al. (1993)	M	
	1.8×10^{-3}	2300	Ettre et al. (1993)	M	11
	1.5×10^{-3}		Hansen et al. (1993)	M	334
	1.7×10^{-3}	4000	Perlinger et al. (1993)	M	

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	1.7×10^{-3}		Li and Carr (1993)	M	
	1.8×10^{-3}		Li et al. (1993)	M	
	1.5×10^{-3}		Zhang and Pawliszyn (1993)	M	
	1.7×10^{-3}	4300	Cooling et al. (1992)	M	335
	1.8×10^{-3}		Anderson (1992)	M	72
	1.9×10^{-3}		Yu (1992)	M	12
	1.6×10^{-3}	4300	Bissonette et al. (1990)	M	
	2.0×10^{-3}		Guitart et al. (1989)	M	14
	1.8×10^{-3}	3200	Ashworth et al. (1988)	M	278
	1.7×10^{-3}		Keeley et al. (1988)	M	
	2.0×10^{-3}		Hellmann (1987)	M	87
	1.3×10^{-3}		Yurteri et al. (1987)	M	12
	1.8×10^{-3}	3600	Tsonopoulos and Wilson (1983)	M	1
	1.7×10^{-3}	3900	Sanemasa et al. (1982)	M	
	1.8×10^{-3}	4000	Leighton and Calo (1981)	M	
	1.7×10^{-3}	3500	Sanemasa et al. (1981)	M	
	1.2×10^{-3}	5300	Ervin et al. (1980)	M	
	1.8×10^{-3}		Warner et al. (1980)	M	
	1.8×10^{-3}		Mackay et al. (1979)	M	
	1.1×10^{-3}		Sato and Nakajima (1979a)	M	14
	1.6×10^{-3}	3800	Tsibul'skii et al. (1979)	M	
	1.8×10^{-3}	4200	Green and Frank (1979)	M	
	1.8×10^{-3}		Vitenberg et al. (1975)	M	
	1.2×10^{-3}		Vitenberg et al. (1974)	M	12
	1.7×10^{-3}	4400	Brown and Wasik (1974)	M	
	2.1×10^{-3}	4500	Hartkopf and Karger (1973)	M	
	1.6×10^{-3}	4500	Wasik and Tsang (1970)	M	
	1.5×10^{-3}		Saylor et al. (1938)	M	38
	3.5×10^{-4}		Abraham and Acree (2007)	V	
	1.8×10^{-3}		Mackay et al. (2006a)	V	
	1.8×10^{-3}		Kochetkov et al. (2001)	V	
	1.8×10^{-3}		Shiu and Ma (2000)	V	
	1.8×10^{-3}		Shiu and Mackay (1997)	V	
	1.8×10^{-3}		Park et al. (1997)	V	
	1.8×10^{-3}		Mackay et al. (1992a)	V	
	1.8×10^{-3}		Hwang et al. (1992)	V	
	1.8×10^{-3}		Eastcott et al. (1988)	V	
	1.8×10^{-3}	3800	Abraham (1984)	V	
	1.8×10^{-3}	3600	Ben-Naim and Wilf (1980)	V	1
	1.8×10^{-3}		Warner et al. (1980)	V	
	1.8×10^{-3}		Hine and Mookerjee (1975)	V	
	1.8×10^{-3}	4100	Mackay and Leinonen (1975)	V	
	1.7×10^{-3}	3800	Wauchope and Haque (1972)	V	
	1.7×10^{-3}	3800	Wauchope and Haque (1972)	V	
	2.0×10^{-3}		McAuliffe (1966)	V	24
	1.8×10^{-3}	3800	Andon et al. (1954)	V	336
	1.8×10^{-3}		Bohon and Claussen (1951)	V	

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Table A2.5: Mononuclear aromatics (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.8×10^{-3}	3800	Plyasunov et al. (2001)	T	
	1.8×10^{-3}		Mackay et al. (1979)	T	
		3800	Gill et al. (1976)	T	
	2.7×10^{-3}		Pierotti (1965)	T	
	1.8×10^{-3}		Yaws (2003)	X	258
	1.8×10^{-3}		Yaws (2003)	X	237
	1.8×10^{-3}	2200	Goldstein (1982)	X	298
	1.8×10^{-3}		Sieg et al. (2008)	C	
	1.8×10^{-3}		Schüürmann (2000)	C	21
	1.8×10^{-3}		Smith et al. (1993)	C	12
	1.8×10^{-3}		Ryan et al. (1988)	C	
	1.8×10^{-3}		Shen (1982)	C	
	1.8×10^{-3}		Dupeux et al. (2022)	Q	259
	1.4×10^{-3}		Hayer et al. (2022)	Q	20
	7.2×10^{-4}		Keshavarz et al. (2022)	Q	
	6.0×10^{-3}		Duchowicz et al. (2020)	Q	299
	6.5×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.3×10^{-3}		Wang et al. (2017)	Q	80, 239
	3.2×10^{-3}		Wang et al. (2017)	Q	80, 240
	1.8×10^{-3}		Li et al. (2014)	Q	241
	4.4×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.7×10^{-3}		Hilal et al. (2008)	Q	
	2.2×10^{-3}		Modarresi et al. (2007)	Q	67
		4000	Kühne et al. (2005)	Q	
	1.8×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	7.4×10^{-4}		Yao et al. (2002)	Q	229
	2.2×10^{-3}		English and Carroll (2001)	Q	230, 231
	7.7×10^{-5}		Katritzky et al. (1998)	Q	
	2.1×10^{-3}		Suzuki et al. (1992)	Q	232
	2.2×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.8×10^{-3}		Arbuckle (1983)	Q	
	1.8×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		3700	Kühne et al. (2005)	?	
	1.8×10^{-3}		Yaws (1999)	?	21
	1.1×10^{-3}		Abraham and Weathersby (1994)	?	21
	1.8×10^{-3}		Yaws and Yang (1992)	?	21
	1.8×10^{-3}		Abraham et al. (1990)	?	
	2.2×10^{-3}		Mackay and Yeun (1983)	?	
benzene-d6 C_6D_6 [1076-43-3] UHOVQNZJYSORNB-MZWXYZOWSA-N	1.8×10^{-3}	4000	Hiatt (2013)	M	
	1.6×10^{-3}	4500	Wasik and Tsang (1970)	M	
		3800	Gill et al. (1976)	T	

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methylbenzene	1.6×10^{-3}	4100	Schwardt et al. (2021)	L	1
$C_6H_5CH_3$	1.9×10^{-3}	4000	Brockbank (2013)	L	1, 337
(toluene)	1.5×10^{-3}	4300	Staudinger and Roberts (2001)	L	
[108-88-3]	1.6×10^{-3}	4400	Plyasunov and Shock (2000)	L	
YXFVVABEGXRONW-UHFFFAOYSA-N	1.5×10^{-3}	4000	Staudinger and Roberts (1996)	L	
	1.5×10^{-3}		Mackay and Shiu (1981)	L	
	1.5×10^{-3}	4600	Kutsuna and Kaneyasu (2021)	M	
	1.5×10^{-3}		Kim and Kim (2014)	M	
	2.1×10^{-3}	4400	Hiatt (2013)	M	
	2.8×10^{-3}		Zhang et al. (2013)	M	325
	1.7×10^{-3}	4200	Lee et al. (2013)	M	
	1.5×10^{-3}		Kish et al. (2013)	M	
	1.3×10^{-3}	2700	Lau et al. (2010)	M	11
	1.5×10^{-3}	4300	Sieg et al. (2009)	M	326
	1.4×10^{-3}		Helburn et al. (2008)	M	
	1.5×10^{-3}		Li et al. (2008)	M	
	1.3×10^{-3}	2100	Falabella and Teja (2008)	M	11, 338
	1.4×10^{-3}		Lodge and Danso (2007)	M	
	1.5×10^{-3}	3900	Lin and Chou (2006)	M	
			Cheng et al. (2004)	M	328
	1.4×10^{-3}	2200	Lei et al. (2004)	M	327
			Cheng et al. (2003)	M	328
	1.4×10^{-3}		Karl et al. (2003)	M	87
	2.1×10^{-3}		Bobadilla et al. (2003)	M	
	1.7×10^{-3}	4300	Bakierowska and Trzeszczyński (2003)	M	
	2.0×10^{-3}		Destaillats and Charles (2002)	M	
	1.5×10^{-3}	4200	Görgényi et al. (2002)	M	339
	1.7×10^{-3}	3600	Bierwagen and Keller (2001)	M	
	1.0×10^{-3}		Ayuttaya et al. (2001)	M	340
	1.7×10^{-4}		Ayuttaya et al. (2001)	M	341
	7.8×10^{-4}		Ayuttaya et al. (2001)	M	342
	2.3×10^{-3}		Ayuttaya et al. (2001)	M	343
	1.5×10^{-3}		David et al. (2000)	M	72
	1.6×10^{-3}		Miller and Stuart (2000)	M	72
	1.9×10^{-3}	4000	Vane and Giroux (2000)	M	
	8.5×10^{-4}		McIntosh and Heffron (2000)	M	14
	1.5×10^{-3}	4700	Dewulf et al. (1999)	M	
	1.7×10^{-3}		Altschuh et al. (1999)	M	
	1.5×10^{-3}		Ryu and Park (1999)	M	
	1.6×10^{-3}		Dohnal and Hovorka (1999)	M	
	1.5×10^{-3}		Allen et al. (1998)	M	
	2.1×10^{-3}		Peng and Wan (1998)	M	
	1.2×10^{-3}	3600	Peng and Wan (1998)	M	70
	2.0×10^{-3}		de Wolf and Lieder (1998)	M	87
	1.4×10^{-3}		Welke et al. (1998)	M	
	1.7×10^{-3}	3700	Peng and Wan (1997)	M	

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.7×10^{-3}	2800	Kondoh and Nakajima (1997)	M	
	1.3×10^{-3}	3900	Park et al. (1997)	M	
	1.4×10^{-3}	4100	Turner et al. (1996)	M	
	1.5×10^{-3}		Ramachandran et al. (1996)	M	
	1.8×10^{-3}	4400	Dewulf et al. (1995)	M	
	1.6×10^{-3}		Nielsen et al. (1994)	M	
	1.5×10^{-3}	4400	Robbins et al. (1993)	M	344
	1.3×10^{-3}		Hoff et al. (1993)	M	
	1.5×10^{-3}	2500	Ettre et al. (1993)	M	11
	1.4×10^{-3}		Hansen et al. (1993)	M	334
	1.5×10^{-3}	4500	Perlinger et al. (1993)	M	
	1.6×10^{-3}		Li and Carr (1993)	M	
	1.6×10^{-3}		Li et al. (1993)	M	
	1.5×10^{-3}		Zhang and Pawliszyn (1993)	M	
	1.6×10^{-3}	2500	Kolb et al. (1992)	M	277
	1.5×10^{-3}		Anderson (1992)	M	72
	3.7×10^{-3}		Yu (1992)	M	12
	1.4×10^{-3}	5000	Bissonette et al. (1990)	M	
	1.5×10^{-3}	6500	Lamarche and Droste (1989)	M	345
	1.5×10^{-3}	3000	Ashworth et al. (1988)	M	278
	1.6×10^{-3}		Keeley et al. (1988)	M	
	1.7×10^{-3}		Yurteri et al. (1987)	M	12
	1.2×10^{-3}	5400	Schoene and Steinhanses (1985)	M	
	1.5×10^{-3}		Garbarini and Lion (1985)	M	
	1.5×10^{-3}	4200	Sanemasa et al. (1982)	M	
	1.5×10^{-3}	3800	Leighton and Calo (1981)	M	
	1.6×10^{-3}	4100	Sanemasa et al. (1981)	M	
	1.5×10^{-3}	4900	Ervin et al. (1980)	M	
	1.7×10^{-3}		Warner et al. (1980)	M	
	1.5×10^{-3}		Mackay et al. (1979)	M	
	8.6×10^{-4}		Sato and Nakajima (1979a)	M	14
	1.5×10^{-3}	4700	Tsibul'skii et al. (1979)	M	
	1.9×10^{-3}		Vitenberg et al. (1975)	M	
	1.6×10^{-3}	5000	Brown and Wasik (1974)	M	
	2.0×10^{-3}	4900	Hartkopf and Karger (1973)	M	
	1.7×10^{-3}	5900	Wasik and Tsang (1970)	M	
	1.6×10^{-3}		Martins et al. (2017)	V	315
	1.5×10^{-3}		Mackay et al. (2006a)	V	
	1.9×10^{-3}	4300	Fogg and Sangster (2003)	V	346
	1.5×10^{-3}		Shiu and Ma (2000)	V	
	1.5×10^{-3}		Park et al. (1997)	V	
	1.5×10^{-3}		Mackay et al. (1992a)	V	
	1.3×10^{-3}		Hwang et al. (1992)	V	
	1.7×10^{-3}		Eastcott et al. (1988)	V	
	1.5×10^{-3}	4400	Abraham (1984)	V	
	1.9×10^{-3}	4200	Ben-Naim and Wilf (1980)	V	1
	1.5×10^{-3}		Warner et al. (1980)	V	

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	1.5×10^{-3}		Hine and Mookerjee (1975)	V	
	1.5×10^{-3}		Mackay and Leinonen (1975)	V	
	1.8×10^{-3}	4400	Wauchope and Haque (1972)	V	
	1.7×10^{-3}		McAuliffe (1966)	V	24
	1.8×10^{-3}	4300	Andon et al. (1954)	V	336
	1.8×10^{-3}		Bohon and Claussen (1951)	V	
	1.6×10^{-3}	4400	Plyasunov et al. (2001)	T	
	1.5×10^{-3}		Mackay et al. (1979)	T	
		4400	Gill et al. (1976)	T	
	1.6×10^{-3}		Yaws (2003)	X	258
	1.5×10^{-3}		Yaws (2003)	X	237
	1.5×10^{-3}	1900	Goldstein (1982)	X	298
	1.5×10^{-3}		McAuliffe (1971)	X	347
	1.5×10^{-3}		Sieg et al. (2008)	C	
	1.5×10^{-3}		Schüürmann (2000)	C	21
	1.7×10^{-3}		Smith et al. (1993)	C	12
	1.4×10^{-3}		Ryan et al. (1988)	C	
	1.7×10^{-3}		Shen (1982)	C	
	1.5×10^{-3}		Dupeux et al. (2022)	Q	259
	1.2×10^{-3}		Hayer et al. (2022)	Q	20
	9.7×10^{-4}		Keshavarz et al. (2022)	Q	
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	299
	3.8×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.1×10^{-3}		Wang et al. (2017)	Q	80, 239
	3.0×10^{-3}		Wang et al. (2017)	Q	80, 240
	1.5×10^{-3}		Li et al. (2014)	Q	241
	2.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.5×10^{-3}		Hilal et al. (2008)	Q	
	1.2×10^{-3}		Modarresi et al. (2007)	Q	67
		4300	Kühne et al. (2005)	Q	
	1.6×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	7.2×10^{-4}		Yao et al. (2002)	Q	229
	1.6×10^{-3}		English and Carroll (2001)	Q	230, 231
	2.7×10^{-4}		Katritzky et al. (1998)	Q	
	1.5×10^{-3}		Suzuki et al. (1992)	Q	232
	1.6×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.2×10^{-3}		Arbuckle (1983)	Q	
	1.5×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4200	Kühne et al. (2005)	?	
	1.6×10^{-3}		Yaws (1999)	?	21
	9.0×10^{-4}		Abraham and Weathersby (1994)	?	21
	1.5×10^{-3}		Yaws and Yang (1992)	?	21
	1.5×10^{-3}		Abraham et al. (1990)	?	

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Table A2.5: Mononuclear aromatics (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	1.9×10^{-3}		Mackay and Yeun (1983)	?	
methylbenzene-d8 $C_6D_5CD_3$ (toluene-d8) [2037-26-5] YXFVVABEGXRONW-JGUCLWPXSA-N	2.0×10^{-3}	4300	Hiatt (2013)	M	
1,2-dimethylbenzene $C_6H_4(CH_3)_2$ (*o*-xylene) [95-47-6] CTQNGGLPUBDAKN-UHFFFAOYSA-N	2.0×10^{-3}	4600	Schwardt et al. (2021)	L	1
	2.0×10^{-3}	4700	Brockbank (2013)	L	1
	2.4×10^{-3}	4200	Fogg and Sangster (2003)	L	
	2.0×10^{-3}	4300	Staudinger and Roberts (2001)	L	
	2.0×10^{-3}	4400	Plyasunov and Shock (2000)	L	
	1.9×10^{-3}	4000	Staudinger and Roberts (1996)	L	
	2.0×10^{-3}		Mackay and Shiu (1981)	L	
	1.9×10^{-3}		Kim and Kim (2014)	M	
	3.2×10^{-3}	4500	Hiatt (2013)	M	
	2.7×10^{-3}	8500	Zhang et al. (2013)	M	324
	2.2×10^{-3}		Zhang et al. (2013)	M	325
	2.0×10^{-3}	4300	Sieg et al. (2009)	M	326
	2.3×10^{-3}		Li et al. (2008)	M	
	1.7×10^{-3}	2500	Falabella and Teja (2008)	M	11, 338
	9.6×10^{-4}		McIntosh and Heffron (2000)	M	14
	2.1×10^{-3}		Dohnal and Hovorka (1999)	M	
	2.2×10^{-3}		Welke et al. (1998)	M	
	1.9×10^{-3}	3400	Kondoh and Nakajima (1997)	M	
	1.4×10^{-3}		Turner et al. (1996)	M	
	2.4×10^{-3}	4500	Dewulf et al. (1995)	M	
	2.0×10^{-3}	5800	Robbins et al. (1993)	M	348
	1.9×10^{-3}		Li and Carr (1993)	M	
	2.1×10^{-3}		Li et al. (1993)	M	
	2.7×10^{-3}		Zhang and Pawliszyn (1993)	M	
	1.4×10^{-3}	3000	Kolb et al. (1992)	M	277
	1.7×10^{-3}		Anderson (1992)	M	72
	2.1×10^{-3}	5600	Bissonette et al. (1990)	M	
	1.9×10^{-3}	3200	Ashworth et al. (1988)	M	278
	2.3×10^{-3}		Yurteri et al. (1987)	M	12
	1.9×10^{-3}	4500	Sanemasa et al. (1982)	M	
	1.0×10^{-3}		Sato and Nakajima (1979a)	M	14
	2.9×10^{-3}	5400	Wasik and Tsang (1970)	M	
	1.8×10^{-3}		Mackay et al. (2006a)	V	
	1.8×10^{-3}		Shiu and Ma (2000)	V	
	1.8×10^{-3}		Mackay et al. (1992a)	V	
	2.3×10^{-3}		Eastcott et al. (1988)	V	
	1.8×10^{-3}		Hine and Mookerjee (1975)	V	
	1.9×10^{-3}		Mackay and Leinonen (1975)	V	
	1.9×10^{-3}		McAuliffe (1966)	V	24
	2.3×10^{-3}		Yaws (2003)	X	237

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.9×10^{-3}		Sieg et al. (2008)	C	
	1.3×10^{-3}		Keshavarz et al. (2022)	Q	
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.3×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.6×10^{-3}		Wang et al. (2017)	Q	80, 239
	3.2×10^{-3}		Wang et al. (2017)	Q	80, 240
	1.3×10^{-3}		Gharagheizi et al. (2012)	Q	
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.0×10^{-3}		Hilal et al. (2008)	Q	
	1.1×10^{-3}		Modarresi et al. (2007)	Q	67
		4100	Kühne et al. (2005)	Q	
	1.9×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.7×10^{-3}		English and Carroll (2001)	Q	230, 274
	3.8×10^{-4}		Katritzky et al. (1998)	Q	
	1.0×10^{-3}		Suzuki et al. (1992)	Q	232
	1.1×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.9×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4100	Kühne et al. (2005)	?	
	2.4×10^{-3}		Yaws (1999)	?	21
	1.1×10^{-3}		Abraham and Weathersby (1994)	?	21
	2.3×10^{-3}		Yaws and Yang (1992)	?	21
	1.9×10^{-3}		Abraham et al. (1990)	?	
1,2-dimethylbenzene-d10 $C_6D_4(CD_3)_2$ (*o*-xylene-d10) [56004-61-6] CTQNGGLPUBDAKN-ZGYYUIRESA-N	3.0×10^{-3}	4700	Hiatt (2013)	M	
1,3-dimethylbenzene $C_6H_4(CH_3)_2$ (*m*-xylene) [108-38-3] IVSZLXZYQVIEFR-UHFFFAOYSA-N	1.4×10^{-3}	4100	Schwardt et al. (2021)	L	1
	1.5×10^{-3}	4300	Brockbank (2013)	L	1
	1.4×10^{-3}	4200	Staudinger and Roberts (2001)	L	
	1.4×10^{-3}	4600	Plyasunov and Shock (2000)	L	
	1.3×10^{-3}	4200	Staudinger and Roberts (1996)	L	
	1.4×10^{-3}		Mackay and Shiu (1981)	L	
	1.3×10^{-3}		Kim and Kim (2014)	M	
	1.4×10^{-3}		Li et al. (2008)	M	
	1.3×10^{-3}		Karl et al. (2003)	M	87
	6.6×10^{-4}		McIntosh and Heffron (2000)	M	14
	1.5×10^{-3}		Dohnal and Hovorka (1999)	M	
	1.5×10^{-3}	2900	Kondoh and Nakajima (1997)	M	
	1.6×10^{-3}	4300	Dewulf et al. (1995)	M	
	1.3×10^{-3}		Li and Carr (1993)	M	
	1.5×10^{-3}		Li et al. (1993)	M	
	1.4×10^{-3}	6000	Bissonette et al. (1990)	M	

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Table A2.5: Mononuclear aromatics (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	1.3×10^{-3}	3300	Ashworth et al. (1988)	M	278
	1.4×10^{-3}	4700	Sanemasa et al. (1982)	M	
	6.4×10^{-4}		Sato and Nakajima (1979a)	M	14
	1.8×10^{-3}	4500	Tsibul'skii et al. (1979)	M	
	1.4×10^{-3}		Mackay et al. (2006a)	V	
	1.7×10^{-3}	4300	Fogg and Sangster (2003)	V	
	1.4×10^{-3}		Shiu and Ma (2000)	V	
	1.4×10^{-3}		Mackay et al. (1992a)	V	
	1.4×10^{-3}		Eastcott et al. (1988)	V	
	1.6×10^{-3}		Hine and Mookerjee (1975)	V	
	1.6×10^{-3}	4800	Wauchope and Haque (1972)	V	
	1.7×10^{-3}	5000	Andon et al. (1954)	V	336
	1.7×10^{-3}		Bohon and Claussen (1951)	V	
	1.5×10^{-3}		Yaws (2003)	X	237
	1.4×10^{-3}		Sieg et al. (2008)	C	
	1.3×10^{-3}		Keshavarz et al. (2022)	Q	
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	2.3×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.2×10^{-3}		Wang et al. (2017)	Q	80, 239
	2.8×10^{-3}		Wang et al. (2017)	Q	80, 240
	1.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.5×10^{-3}		Hilal et al. (2008)	Q	
	7.5×10^{-4}		Modarresi et al. (2007)	Q	67
		4700	Kühne et al. (2005)	Q	
	1.4×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	4.4×10^{-4}		Yao et al. (2002)	Q	229
	1.7×10^{-3}		English and Carroll (2001)	Q	230, 231
	3.8×10^{-4}		Katritzky et al. (1998)	Q	
	1.4×10^{-3}		Russell et al. (1992)	Q	279
	1.0×10^{-3}		Suzuki et al. (1992)	Q	232
	1.1×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.4×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4900	Kühne et al. (2005)	?	
	1.5×10^{-3}		Yaws (1999)	?	21
	6.7×10^{-4}		Abraham and Weathersby (1994)	?	21
	1.5×10^{-3}		Yaws and Yang (1992)	?	21
	1.3×10^{-3}		Abraham et al. (1990)	?	

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,4-dimethylbenzene	1.5×10^{-3}	5000	Schwardt et al. (2021)	L	1
$C_6H_4(CH_3)_2$	1.4×10^{-3}	5000	Brockbank (2013)	L	1
(p-xylene)	1.9×10^{-3}	4200	Fogg and Sangster (2003)	L	
[106-42-3]	1.3×10^{-3}	4000	Staudinger and Roberts (2001)	L	
URLKBWYHVLBVBO-UHFFFAOYSA-N	1.4×10^{-3}	4600	Plyasunov and Shock (2000)	L	
	1.3×10^{-3}	3800	Staudinger and Roberts (1996)	L	
	1.4×10^{-3}		Mackay and Shiu (1981)	L	
	1.0×10^{-3}	2600	Schwardt et al. (2021)	M	349, 11
	1.3×10^{-3}		Kim and Kim (2014)	M	
	1.4×10^{-3}		Li et al. (2008)	M	
	1.6×10^{-3}	4800	Lin and Chou (2006)	M	
	2.0×10^{-3}		Bobadilla et al. (2003)	M	
	6.7×10^{-4}		McIntosh and Heffron (2000)	M	14
	1.4×10^{-3}		Ryu and Park (1999)	M	
	1.5×10^{-3}		Dohnal and Hovorka (1999)	M	
	1.5×10^{-3}	2900	Kondoh and Nakajima (1997)	M	
	9.8×10^{-4}	3200	Park et al. (1997)	M	
	1.7×10^{-3}	4800	Dewulf et al. (1995)	M	
	1.2×10^{-3}	3100	Hansen et al. (1993)	M	281
	1.3×10^{-3}		Li and Carr (1993)	M	
	1.4×10^{-3}		Li et al. (1993)	M	
	1.7×10^{-3}		Zhang and Pawliszyn (1993)	M	
	1.2×10^{-3}	5300	Bissonette et al. (1990)	M	
	1.3×10^{-3}	3500	Ashworth et al. (1988)	M	278
	1.3×10^{-3}	4800	Sanemasa et al. (1982)	M	
	6.1×10^{-4}		Sato and Nakajima (1979a)	M	14
	2.3×10^{-3}	5400	Wasik and Tsang (1970)	M	
	1.2×10^{-3}		Martins et al. (2017)	V	315
	1.8×10^{-4}		Abraham and Acree (2007)	V	
	1.7×10^{-3}		Mackay et al. (2006a)	V	
	1.4×10^{-3}		Shiu and Ma (2000)	V	
	1.5×10^{-3}		Park et al. (1997)	V	
	1.7×10^{-3}		Mackay et al. (1992a)	V	
	1.5×10^{-3}		Hwang et al. (1992)	V	
	1.8×10^{-3}		Eastcott et al. (1988)	V	
	1.6×10^{-3}		Hine and Mookerjee (1975)	V	
	1.6×10^{-3}	4800	Wauchope and Haque (1972)	V	
	1.6×10^{-3}	4900	Andon et al. (1954)	V	336
	1.6×10^{-3}		Bohon and Claussen (1951)	V	
	1.4×10^{-3}		Foster et al. (1994)	X	350
	1.6×10^{-3}		Yaws (2003)	X	237
	1.4×10^{-3}		Sieg et al. (2008)	C	
	1.3×10^{-3}		Schüürmann (2000)	C	21
	1.3×10^{-3}		Keshavarz et al. (2022)	Q	
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	184
	2.3×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.4×10^{-3}		Wang et al. (2017)	Q	80, 239

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	2.6×10^{-3}		Wang et al. (2017)	Q	80, 240
	9.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.5×10^{-3}		Hilal et al. (2008)	Q	
	1.1×10^{-3}		Modarresi et al. (2007)	Q	67
		4700	Kühne et al. (2005)	Q	
	1.5×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	8.1×10^{-4}		Yao et al. (2002)	Q	229
	1.7×10^{-3}		English and Carroll (2001)	Q	230, 231
	3.9×10^{-4}		Katritzky et al. (1998)	Q	
	1.0×10^{-3}		Suzuki et al. (1992)	Q	232
	1.1×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.4×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4500	Kühne et al. (2005)	?	
	1.6×10^{-3}		Yaws (1999)	?	21
	6.4×10^{-4}		Abraham and Weathersby (1994)	?	21
	1.6×10^{-3}		Yaws and Yang (1992)	?	21
	1.4×10^{-3}		Abraham et al. (1990)	?	
1,2,3-trimethylbenzene $C_6H_3(CH_3)_3$ [526-73-8] FYGHSUNMUKGBRK-UHFFFAOYSA-N	2.4×10^{-3}	4600	Brockbank (2013)	L	1
	2.7×10^{-3}	4800	Fogg and Sangster (2003)	L	
	2.6×10^{-3}	4500	Plyasunov and Shock (2000)	L	
	3.1×10^{-3}		Mackay and Shiu (1981)	L	
	1.1×10^{-3}		Järnberg and Johanson (1995)	M	14
	2.4×10^{-3}	4500	Sanemasa et al. (1982)	M	
	2.9×10^{-3}		Mackay et al. (2006a)	V	
	2.9×10^{-3}		Shiu and Ma (2000)	V	
	3.1×10^{-3}		Abraham et al. (1994a)	V	
	2.9×10^{-3}		Mackay et al. (1992a)	V	
	2.7×10^{-3}		Eastcott et al. (1988)	V	
	1.3×10^{-3}		Yaws (2003)	X	237
	1.8×10^{-3}		Keshavarz et al. (2022)	Q	
	7.9×10^{-4}		Duchowicz et al. (2020)	Q	299
	1.4×10^{-3}		Wang et al. (2017)	Q	80, 238
	2.2×10^{-3}		Wang et al. (2017)	Q	80, 239
	3.5×10^{-3}		Wang et al. (2017)	Q	80, 240
	8.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-3}		Gharagheizi et al. (2010)	Q	246
	3.1×10^{-3}		Hilal et al. (2008)	Q	
	8.2×10^{-4}		Modarresi et al. (2007)	Q	67
		3900	Kühne et al. (2005)	Q	
	3.1×10^{-3}		Yaffe et al. (2003)	Q	248, 249

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	2.0×10^{-3}		English and Carroll (2001)	Q	230, 274
	4.6×10^{-4}		Katritzky et al. (1998)	Q	
	8.2×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	2.3×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4400	Kühne et al. (2005)	?	
	1.3×10^{-3}		Yaws (1999)	?	21
	2.7×10^{-3}		Yaws and Yang (1992)	?	21
	2.1×10^{-3}		Abraham et al. (1990)	?	
1,2,4-trimethylbenzene	1.6×10^{-3}	4700	Brockbank (2013)	L	1
$C_6H_3(CH_3)_3$	1.7×10^{-3}	3100	Fogg and Sangster (2003)	L	
[95-63-6]	1.6×10^{-3}	4800	Plyasunov and Shock (2000)	L	
GWHJZXXIDMPWGX-UHFFFAOYSA-N	1.7×10^{-3}		Mackay and Shiu (1981)	L	
	3.2×10^{-3}	5200	Hiatt (2013)	M	
	1.7×10^{-3}		Li et al. (2008)	M	
	2.3×10^{-3}	3600	Kondoh and Nakajima (1997)	M	
	6.2×10^{-4}		Järnberg and Johanson (1995)	M	14
	1.5×10^{-3}	4300	Hansen et al. (1993)	M	281
	2.1×10^{-3}		Yurteri et al. (1987)	M	12
	1.6×10^{-3}	4800	Sanemasa et al. (1982)	M	
	1.8×10^{-3}		Mackay et al. (2006a)	V	
	1.8×10^{-3}		Shiu and Ma (2000)	V	
	1.7×10^{-3}		Abraham et al. (1994a)	V	
	1.8×10^{-3}		Mackay et al. (1992a)	V	
	1.6×10^{-3}		Eastcott et al. (1988)	V	
	1.7×10^{-3}		Hine and Mookerjee (1975)	V	
	1.4×10^{-3}		Yaws (2003)	X	237
	1.8×10^{-3}		Keshavarz et al. (2022)	Q	
	7.9×10^{-4}		Duchowicz et al. (2020)	Q	299
	1.4×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.9×10^{-3}		Wang et al. (2017)	Q	80, 239
	2.8×10^{-3}		Wang et al. (2017)	Q	80, 240
	6.3×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.1×10^{-3}		Hilal et al. (2008)	Q	
	7.5×10^{-4}		Modarresi et al. (2007)	Q	67
		4500	Kühne et al. (2005)	Q	
	1.8×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	2.0×10^{-3}		English and Carroll (2001)	Q	230, 231
	4.7×10^{-4}		Katritzky et al. (1998)	Q	
	7.3×10^{-4}		Suzuki et al. (1992)	Q	232
	8.0×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	8.2×10^{-4}		Arbuckle (1983)	Q	
	1.6×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4700	Kühne et al. (2005)	?	

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	1.5×10^{-3}		Yaws (1999)	?	21
	1.7×10^{-3}		Yaws and Yang (1992)	?	21
	1.6×10^{-3}		Abraham et al. (1990)	?	
1,3,5-trimethylbenzene $C_6H_3(CH_3)_3$ (mesitylene) [108-67-8] AUHZEENZYGFFBQ-UHFFFAOYSA-N	1.2×10^{-3}	4400	Brockbank (2013)	L	1
	1.3×10^{-3}	4900	Plyasunov and Shock (2000)	L	
	1.7×10^{-3}		Mackay and Shiu (1981)	L	
	2.3×10^{-3}	5100	Hiatt (2013)	M	
	2.0×10^{-3}		Karl et al. (2003)	M	87
	1.5×10^{-3}	3000	Kondoh and Nakajima (1997)	M	
	4.8×10^{-4}		Järnberg and Johanson (1995)	M	14
	1.3×10^{-3}		Li and Carr (1993)	M	
	1.4×10^{-3}		Li et al. (1993)	M	
	1.4×10^{-3}	3600	Ashworth et al. (1988)	M	278
	1.1×10^{-3}	4700	Sanemasa et al. (1982)	M	
	1.1×10^{-3}	4600	Sanemasa et al. (1981)	M	
	1.4×10^{-4}		Abraham and Acree (2007)	V	
	1.3×10^{-3}		Mackay et al. (2006a)	V	
	1.3×10^{-3}		Shiu and Ma (2000)	V	
	1.8×10^{-3}		Abraham et al. (1994a)	V	
	1.3×10^{-3}		Mackay et al. (1992a)	V	
	1.2×10^{-3}		Eastcott et al. (1988)	V	
	1.2×10^{-3}		Yaws (2003)	X	237
	9.1×10^{-4}		Hayer et al. (2022)	Q	20
	1.8×10^{-3}		Keshavarz et al. (2022)	Q	
	7.9×10^{-4}		Duchowicz et al. (2020)	Q	299
	1.4×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.1×10^{-3}		Wang et al. (2017)	Q	80, 239
	2.5×10^{-3}		Wang et al. (2017)	Q	80, 240
	5.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.4×10^{-3}		Hilal et al. (2008)	Q	
	9.0×10^{-4}		Modarresi et al. (2007)	Q	67
		5000	Kühne et al. (2005)	Q	
	1.8×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	4.6×10^{-4}		Katritzky et al. (1998)	Q	
	8.0×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	1.1×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4400	Kühne et al. (2005)	?	
	1.2×10^{-3}		Yaws (1999)	?	21
	1.2×10^{-3}		Yaws and Yang (1992)	?	21
	1.3×10^{-3}		Abraham et al. (1990)	?	
1,2,3,4-tetramethylbenzene $C_{10}H_{14}$ [488-23-3] UOHMMEJUHBCKEE-UHFFFAOYSA-N	2.9×10^{-3}	5900	Brockbank (2013)	L	1

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,5-tetramethylbenzene	1.2×10^{-3}		Zhang et al. (2010)	Q	287, 288
$C_{10}H_{14}$	2.2×10^{-3}		Zhang et al. (2010)	Q	287, 289
[527-53-7]	2.2×10^{-3}		Zhang et al. (2010)	Q	287, 290
BFIMMTCNYPIMRN-UHFFFAOYSA-N	4.1×10^{-4}		Zhang et al. (2010)	Q	287, 291
	1.2×10^{-3}		Yaws (1999)	?	21
1,2,4,5-tetramethylbenzene	1.4×10^{-3}		Brockbank (2013)	L	
$C_{10}H_{14}$	1.3×10^{-3}		Plyasunov and Shock (2000)	L	
[95-93-2]	3.9×10^{-4}		Mackay and Shiu (1981)	L	
SQNZJJAZBFDUTD-UHFFFAOYSA-N	3.9×10^{-4}		Mackay et al. (2006a)	V	
	3.9×10^{-4}		Mackay et al. (1992a)	V	
	3.9×10^{-4}		Eastcott et al. (1988)	V	
	3.5×10^{-4}		Yaws (2003)	X	237
	1.4×10^{-3}		Abraham et al. (2019)	Q	
	3.7×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-3}		Zhang et al. (2010)	Q	287, 288
	2.5×10^{-3}		Zhang et al. (2010)	Q	287, 289
	1.9×10^{-3}		Zhang et al. (2010)	Q	287, 290
	4.1×10^{-4}		Zhang et al. (2010)	Q	287, 291
	3.7×10^{-4}		Gharagheizi et al. (2010)	Q	246
	2.9×10^{-3}		Hilal et al. (2008)	Q	
	8.2×10^{-4}		Modarresi et al. (2007)	Q	67
	3.9×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	3.9×10^{-4}		Yaws and Yang (1992)	?	21
ethylbenzene	1.4×10^{-3}	4500	Schwardt et al. (2021)	L	1, 351
$C_6H_5C_2H_5$	1.3×10^{-3}	5000	Brockbank (2013)	L	1
[100-41-4]	1.4×10^{-3}	4800	Fogg and Sangster (2003)	L	
YNQLUTRBYVCPMQ-UHFFFAOYSA-N	1.3×10^{-3}	5100	Staudinger and Roberts (2001)	L	
	1.3×10^{-3}	4800	Plyasunov and Shock (2000)	L	
	1.2×10^{-3}	5100	Staudinger and Roberts (1996)	L	
	1.3×10^{-3}		Mackay and Shiu (1981)	L	
	1.3×10^{-3}	4400	Schwardt et al. (2021)	M	352
	2.0×10^{-3}	4100	Hiatt (2013)	M	
	1.9×10^{-3}	4200	Zhang et al. (2013)	M	324
	1.4×10^{-3}		Zhang et al. (2013)	M	325
	1.3×10^{-3}	5100	Sieg et al. (2009)	M	326
	1.4×10^{-3}		Li et al. (2008)	M	
	1.2×10^{-3}	2700	Falabella and Teja (2008)	M	11, 338
	1.1×10^{-3}		Lodge and Danso (2007)	M	
			Cheng et al. (2003)	M	328
	1.6×10^{-3}		Miller and Stuart (2000)	M	72
	1.1×10^{-3}		Ryu and Park (1999)	M	353
	1.3×10^{-3}		Allen et al. (1998)	M	
	1.4×10^{-3}	2800	Kondoh and Nakajima (1997)	M	
	1.1×10^{-3}		Turner et al. (1996)	M	
	1.5×10^{-3}	4900	Dewulf et al. (1995)	M	
	1.3×10^{-3}	5000	Robbins et al. (1993)	M	354

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Table A2.5: Mononuclear aromatics (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.3×10^{-3}	5300	Perlinger et al. (1993)	M	
	1.3×10^{-3}		Li and Carr (1993)	M	
	1.3×10^{-3}		Li et al. (1993)	M	
	2.5×10^{-3}		Zhang and Pawliszyn (1993)	M	
	1.1×10^{-3}	5500	Bissonette et al. (1990)	M	
	1.2×10^{-3}	5000	Ashworth et al. (1988)	M	278
	1.3×10^{-3}	4400	Heidman et al. (1985)	M	1
	1.3×10^{-3}	4600	Sanemasa et al. (1982)	M	
	1.4×10^{-3}	4500	Sanemasa et al. (1981)	M	
	1.4×10^{-3}	5500	Ervin et al. (1980)	M	
	1.5×10^{-3}		Warner et al. (1980)	M	
	1.2×10^{-3}		Mackay et al. (1979)	M	
	6.6×10^{-4}		Sato and Nakajima (1979a)	M	14
	1.3×10^{-3}	5600	Brown and Wasik (1974)	M	
	1.6×10^{-3}	6400	Hartkopf and Karger (1973)	M	
	1.6×10^{-4}		Abraham and Acree (2007)	V	
	1.1×10^{-3}		Mackay et al. (2006a)	V	
	1.2×10^{-3}		Shiu and Ma (2000)	V	
	1.2×10^{-3}		Lide and Frederikse (1995)	V	
	1.1×10^{-3}		Mackay et al. (1992a)	V	
	1.2×10^{-3}		Hwang et al. (1992)	V	
	1.0×10^{-3}		Eastcott et al. (1988)	V	
	1.2×10^{-3}	4800	Abraham (1984)	V	
	1.6×10^{-3}	4900	Ben-Naim and Wilf (1980)	V	1
	1.5×10^{-3}		Warner et al. (1980)	V	
	1.1×10^{-3}		Hine and Mookerjee (1975)	V	
	1.5×10^{-3}	4800	Wauchope and Haque (1972)	V	
	1.3×10^{-3}		McAuliffe (1966)	V	24
	1.5×10^{-3}	4900	Andon et al. (1954)	V	336
	1.5×10^{-3}		Bohon and Claussen (1951)	V	
	1.4×10^{-3}	4900	Owens et al. (1986)	T	
	1.1×10^{-3}		Mackay et al. (1979)	T	
		4800	Gill et al. (1976)	T	
	1.2×10^{-3}		Yaws (2003)	X	237
	1.6×10^{-3}	1700	Goldstein (1982)	X	298
	1.3×10^{-3}		Sieg et al. (2008)	C	
	1.6×10^{-3}		Ryan et al. (1988)	C	
	1.5×10^{-3}		Shen (1982)	C	
	9.7×10^{-4}		Hayer et al. (2022)	Q	20
	1.3×10^{-3}		Keshavarz et al. (2022)	Q	
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	3.1×10^{-3}		Wang et al. (2017)	Q	80, 238
	9.3×10^{-4}		Wang et al. (2017)	Q	80, 239
	2.8×10^{-3}		Wang et al. (2017)	Q	80, 240
	1.4×10^{-3}		Gharagheizi et al. (2012)	Q	
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	244

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.4×10^{-3}		Hilal et al. (2008)	Q	
	9.6×10^{-4}		Modarresi et al. (2007)	Q	67
		4700	Kühne et al. (2005)	Q	
	1.2×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	5.8×10^{-4}		Yao et al. (2002)	Q	229
	1.4×10^{-3}		English and Carroll (2001)	Q	230, 260
	4.1×10^{-4}		Katritzky et al. (1998)	Q	
	1.6×10^{-3}		Russell et al. (1992)	Q	279
	1.1×10^{-3}		Suzuki et al. (1992)	Q	232
	1.3×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.3×10^{-3}		Arbuckle (1983)	Q	
	1.3×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		5000	Kühne et al. (2005)	?	
	1.2×10^{-3}		Yaws (1999)	?	21
	6.9×10^{-4}		Abraham and Weathersby (1994)	?	21
	1.1×10^{-3}		Hoff et al. (1993)	?	21
	1.2×10^{-3}		Yaws and Yang (1992)	?	21
	1.2×10^{-3}		Abraham et al. (1990)	?	
ethylbenzene-d10 $C_6D_5C_2D_5$ [25837-05-2] YNQLUTRBYVCPMQ-CFTAVCBPSA-N	2.0×10^{-3}	4200	Hiatt (2013)	M	
1,2-diethylbenzene $C_{10}H_{14}$ (*o*-diethylbenzene) [135-01-3] KVNYFPKFSJIPBJ-UHFFFAOYSA-N	3.8×10^{-3}		Duchowicz et al. (2020)	V	186
	3.8×10^{-3}		HSDB (2015)	V	
	1.3×10^{-3}		Yaws (2003)	X	237
	1.2×10^{-3}		Hilal et al. (2008)	C	
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	5.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.3×10^{-3}		Hilal et al. (2008)	Q	
	1.2×10^{-3}		Modarresi et al. (2007)	Q	67
		4800	Kühne et al. (2005)	Q	
	3.8×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	5.6×10^{-4}		Katritzky et al. (1998)	Q	
		5100	Kühne et al. (2005)	?	
	1.3×10^{-3}		Yaws (1999)	?	21

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3-diethylbenzene	1.2×10^{-3}		Duchowicz et al. (2020)	V	186
$C_{10}H_{14}$	1.1×10^{-3}		HSDB (2015)	V	
(m-diethylbenzene)	1.3×10^{-3}		Yaws (2003)	X	237
[141-93-5]	3.8×10^{-3}		Hilal et al. (2008)	C	
AFZZYIJIWUTJFO-UHFFFAOYSA-N	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	4.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
	9.7×10^{-4}		Hilal et al. (2008)	Q	
	4.7×10^{-4}		Modarresi et al. (2007)	Q	67
		5300	Kühne et al. (2005)	Q	
	5.6×10^{-4}		Katritzky et al. (1998)	Q	
		5300	Kühne et al. (2005)	?	
	1.3×10^{-3}		Yaws (1999)	?	21
1,4-diethylbenzene	1.3×10^{-3}		Duchowicz et al. (2020)	V	186
$C_{10}H_{14}$	1.4×10^{-3}		HSDB (2015)	V	
(p-diethylbenzene)	1.2×10^{-3}		Yaws (2003)	X	237
[105-05-5]	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
DSNHSQKRULAAEI-UHFFFAOYSA-N	5.0×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.1×10^{-3}		Hilal et al. (2008)	Q	
	7.6×10^{-4}		Modarresi et al. (2007)	Q	67
		5300	Kühne et al. (2005)	Q	
	1.4×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	5.7×10^{-4}		Katritzky et al. (1998)	Q	
	7.9×10^{-4}		Nirmalakhandan et al. (1997)	Q	
		5900	Kühne et al. (2005)	?	
	1.2×10^{-3}		Yaws (1999)	?	21
			Brockbank (2013)	W	355
propylbenzene	9.0×10^{-4}	3800	Schwardt et al. (2021)	L	1
$C_6H_5C_3H_7$	9.1×10^{-4}	4700	Brockbank (2013)	L	1
[103-65-1]	9.1×10^{-4}	5300	Plyasunov and Shock (2000)	L	
ODLMAHJVESYWTB-UHFFFAOYSA-N	1.4×10^{-3}		Mackay and Shiu (1981)	L	
	1.9×10^{-3}	4500	Hiatt (2013)	M	
	1.5×10^{-3}		Karl et al. (2003)	M	87
	1.1×10^{-3}	2600	Kondoh and Nakajima (1997)	M	
	8.6×10^{-4}	5400	Perlinger et al. (1993)	M	
	9.3×10^{-4}		Li and Carr (1993)	M	
	9.1×10^{-4}		Li et al. (1993)	M	
	9.0×10^{-4}	3700	Ashworth et al. (1988)	M	278
	9.5×10^{-4}	4700	Sanemasa et al. (1982)	M	
	5.0×10^{-4}		Sato and Nakajima (1979a)	M	14
	9.6×10^{-4}		Mackay et al. (2006a)	V	
	9.6×10^{-4}		Shiu and Ma (2000)	V	
	9.6×10^{-4}		Mackay et al. (1992a)	V	
	9.7×10^{-4}		Eastcott et al. (1988)	V	
	9.7×10^{-4}	5300	Abraham (1984)	V	

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.5×10^{-3}	5500	Ben-Naim and Wilf (1980)	V	1
	9.9×10^{-4}		Hine and Mookerjee (1975)	V	
	9.6×10^{-4}	5100	Owens et al. (1986)	T	
		5300	Gill et al. (1976)	T	
	7.4×10^{-4}		Yaws (2003)	X	237
	1.8×10^{-3}		Keshavarz et al. (2022)	Q	
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	2.5×10^{-3}		Wang et al. (2017)	Q	80, 238
	6.6×10^{-4}		Wang et al. (2017)	Q	80, 239
	2.6×10^{-3}		Wang et al. (2017)	Q	80, 240
	9.9×10^{-4}		Li et al. (2014)	Q	241
	1.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	8.6×10^{-4}		Gharagheizi et al. (2010)	Q	246
	9.9×10^{-4}		Hilal et al. (2008)	Q	
	8.6×10^{-4}		Modarresi et al. (2007)	Q	67
		5000	Kühne et al. (2005)	Q	
	1.0×10^{-3}		Yaffe et al. (2003)	Q	248, 272
	1.1×10^{-3}		English and Carroll (2001)	Q	230, 231
	5.1×10^{-4}		Katritzky et al. (1998)	Q	
	1.3×10^{-3}		Russell et al. (1992)	Q	279
	8.8×10^{-4}		Suzuki et al. (1992)	Q	232
	1.1×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	9.4×10^{-4}		Duchowicz et al. (2020)	?	185, 21
		4700	Kühne et al. (2005)	?	
	1.7×10^{-3}		Yaws (1999)	?	21
	5.2×10^{-4}		Abraham and Weathersby (1994)	?	21
	9.6×10^{-4}		Yaws and Yang (1992)	?	21
	9.7×10^{-4}		Abraham et al. (1990)	?	
(2-propyl)-benzene	9.0×10^{-4}	4800	Brockbank (2013)	L	1
$C_6H_5C_3H_7$	1.2×10^{-3}	3200	Staudinger and Roberts (2001)	L	
(isopropylbenzene; cumene)	8.4×10^{-4}	4800	Plyasunov and Shock (2000)	L	
[98-82-8]	7.7×10^{-3}		Mackay and Shiu (1981)	L	
RWGFKTVRMDUZSP-UHFFFAOYSA-N	1.4×10^{-3}	4900	Hiatt (2013)	M	
	1.0×10^{-3}	2500	Kondoh and Nakajima (1997)	M	
	8.7×10^{-4}	3300	Hansen et al. (1993)	M	281
	9.1×10^{-4}		Li and Carr (1993)	M	
	8.9×10^{-4}		Li et al. (1993)	M	
	1.6×10^{-3}	3200	Ashworth et al. (1988)	M	278
	8.9×10^{-4}	4700	Sanemasa et al. (1982)	M	
	5.6×10^{-4}		Sato and Nakajima (1979a)	M	14
	6.8×10^{-4}		Mackay et al. (2006a)	V	
	6.8×10^{-4}		Shiu and Ma (2000)	V	
	6.8×10^{-4}		Mackay et al. (1992a)	V	
	6.8×10^{-4}		Hwang et al. (1992)	V	

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	6.6×10^{-4}		Eastcott et al. (1988)	V	
	6.7×10^{-4}		Hine and Mookerjee (1975)	V	
	6.8×10^{-4}		Mackay and Leinonen (1975)	V	
	1.1×10^{-3}	5000	Wauchope and Haque (1972)	V	
	1.1×10^{-3}		McAuliffe (1966)	V	24
	6.8×10^{-4}		Yaws (2003)	X	237
	1.8×10^{-3}		Keshavarz et al. (2022)	Q	
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	299
	2.9×10^{-3}		Wang et al. (2017)	Q	80, 238
	5.3×10^{-4}		Wang et al. (2017)	Q	80, 239
	2.8×10^{-3}		Wang et al. (2017)	Q	80, 240
	9.4×10^{-4}		Savary et al. (2014)	Q	
	8.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	8.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
	8.6×10^{-4}		Hilal et al. (2008)	Q	
	7.7×10^{-4}		Modarresi et al. (2007)	Q	67
		5000	Kühne et al. (2005)	Q	
			Yaffe et al. (2003)	Q	356
	3.6×10^{-4}		Yao et al. (2002)	Q	229
	1.2×10^{-3}		English and Carroll (2001)	Q	230, 231
	4.7×10^{-4}		Katritzky et al. (1998)	Q	
	9.2×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	8.0×10^{-4}		Suzuki et al. (1992)	Q	232
	9.2×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	8.6×10^{-4}		Duchowicz et al. (2020)	?	185, 21
		4400	Kühne et al. (2005)	?	
	6.9×10^{-4}		Yaws (1999)	?	21
	5.8×10^{-4}		Abraham and Weathersby (1994)	?	21
	6.8×10^{-4}		Hoff et al. (1993)	?	21
	6.8×10^{-4}		Yaws and Yang (1992)	?	21
	8.8×10^{-4}		Abraham et al. (1990)	?	
			Fogg and Sangster (2003)	W	357
1-ethyl-2-methylbenzene $C_6H_4CH_3C_2H_5$ (*o*-ethyltoluene) [611-14-3] HYFLWBNQFMXCPA-UHFFFAOYSA-N	1.8×10^{-3}		Plyasunov and Shock (2000)	L	
	2.3×10^{-3}		Mackay and Shiu (1981)	L	
	1.8×10^{-3}		Duchowicz et al. (2020)	V	186
	1.9×10^{-3}		Mackay et al. (2006a)	V	
	1.9×10^{-3}		Mackay et al. (1992a)	V	
	1.9×10^{-3}		Eastcott et al. (1988)	V	
	2.2×10^{-3}		Yaws (2003)	X	237
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.8×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.2×10^{-3}		Wang et al. (2017)	Q	80, 239
	3.0×10^{-3}		Wang et al. (2017)	Q	80, 240
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.8×10^{-3}		Hilal et al. (2008)	Q	
	8.9×10^{-4}		Modarresi et al. (2007)	Q	67
		4500	Kühne et al. (2005)	Q	
	2.4×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	5.1×10^{-4}		Katritzky et al. (1998)	Q	
	9.5×10^{-4}		Nirmalakhandan et al. (1997)	Q	
		3200	Kühne et al. (2005)	?	
	2.2×10^{-3}		Yaws (1999)	?	21
	2.3×10^{-3}		Yaws and Yang (1992)	?	21
1-ethyl-3-methylbenzene	1.7×10^{-3}		Yaws (2003)	X	237
$C_6H_4CH_3C_2H_5$	1.8×10^{-3}		Wang et al. (2017)	Q	80, 238
(m-ethyltoluene)	9.8×10^{-4}		Wang et al. (2017)	Q	80, 239
[620-14-4]	2.6×10^{-3}		Wang et al. (2017)	Q	80, 240
ZLCSFXXPPANWQY-UHFFFAOYSA-N	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.3×10^{-3}		Hilal et al. (2008)	Q	
	1.7×10^{-3}		Yaws (1999)	?	21
1-ethyl-4-methylbenzene	2.0×10^{-3}		Mackay and Shiu (1981)	L	
$C_6H_4CH_3C_2H_5$	2.0×10^{-3}		Duchowicz et al. (2020)	V	186
(p-ethyltoluene)	1.6×10^{-3}		Duchowicz et al. (2020)	V	186
[622-96-8]	2.0×10^{-3}		Mackay et al. (2006a)	V	
JRLPEMVDPFPYPJ-UHFFFAOYSA-N	2.0×10^{-3}		Mackay et al. (1992a)	V	
	2.0×10^{-3}		Eastcott et al. (1988)	V	
	2.0×10^{-3}		Yaws (2003)	X	237
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.8×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.1×10^{-3}		Wang et al. (2017)	Q	80, 239
	2.5×10^{-3}		Wang et al. (2017)	Q	80, 240
	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.4×10^{-3}		Hilal et al. (2008)	Q	
	7.1×10^{-4}		Modarresi et al. (2007)	Q	67
	2.1×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.7×10^{-3}		English and Carroll (2001)	Q	230, 260
	5.1×10^{-4}		Katritzky et al. (1998)	Q	
	9.5×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	2.0×10^{-3}		Yaws (1999)	?	21
	2.0×10^{-3}		Yaws and Yang (1992)	?	21

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
butylbenzene	7.1×10^{-4}	5100	Brockbank (2013)	L	1
$C_6H_5C_4H_9$	7.1×10^{-4}	5500	Plyasunov and Shock (2000)	L	
[104-51-8]	7.7×10^{-4}		Mackay and Shiu (1981)	L	
OCKPCBLVNKHBMX-UHFFFAOYSA-N	2.0×10^{-3}	4500	Hiatt (2013)	M	
	7.4×10^{-4}		Ryu and Park (1999)	M	
	9.1×10^{-4}	2700	Kondoh and Nakajima (1997)	M	
	6.2×10^{-4}	6000	Perlinger et al. (1993)	M	
	7.1×10^{-4}		Li and Carr (1993)	M	
	6.7×10^{-4}		Li et al. (1993)	M	
	6.2×10^{-4}		Duchowicz et al. (2020)	V	186
	6.2×10^{-4}		HSDB (2015)	V	
	9.9×10^{-5}		Abraham and Acree (2007)	V	
	7.5×10^{-4}		Mackay et al. (2006a)	V	
	7.5×10^{-4}		Shiu and Ma (2000)	V	
	7.5×10^{-4}		Mackay et al. (1992a)	V	
	7.6×10^{-4}		Meylan and Howard (1991)	V	
	7.5×10^{-4}		Eastcott et al. (1988)	V	
	7.4×10^{-4}		Abraham (1984)	V	
	1.7×10^{-3}	6500	Ben-Naim and Wilf (1980)	V	1
	7.9×10^{-4}		Hine and Mookerjee (1975)	V	
	7.2×10^{-4}	5300	Owens et al. (1986)	T	
	7.5×10^{-4}		Yaws (2003)	X	237
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	7.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	7.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
	7.7×10^{-4}		Hilal et al. (2008)	Q	
	4.9×10^{-4}		Modarresi et al. (2007)	Q	67
		5300	Kühne et al. (2005)	Q	
	7.2×10^{-4}		Yaffe et al. (2003)	Q	248, 272
	6.4×10^{-4}		Yao et al. (2002)	Q	229
	7.9×10^{-4}		English and Carroll (2001)	Q	230, 231
	5.7×10^{-4}		Katritzky et al. (1998)	Q	
	6.9×10^{-4}		Russell et al. (1992)	Q	358
	6.9×10^{-4}		Suzuki et al. (1992)	Q	232
	7.1×10^{-4}		Meylan and Howard (1991)	Q	
	8.4×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
		4900	Kühne et al. (2005)	?	
	7.6×10^{-4}		Yaws (1999)	?	21
	7.5×10^{-4}		Yaws and Yang (1992)	?	21
	7.5×10^{-4}		Abraham et al. (1990)	?	

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(1-methylpropyl)-benzene	5.3×10^{-4}		Plyasunov and Shock (2000)	L	
$C_6H_5C_4H_9$	7.1×10^{-4}		Mackay and Shiu (1981)	L	
(*sec*-butylbenzene)	1.3×10^{-3}	4600	Hiatt (2013)	M	
[135-98-8]	7.5×10^{-4}	2300	Kondoh and Nakajima (1997)	M	
ZJMWRROPUADPEA-UHFFFAOYSA-N	5.6×10^{-4}		Duchowicz et al. (2020)	V	186
	5.5×10^{-4}		HSDB (2015)	V	
	5.3×10^{-4}		Mackay et al. (2006a)	V	
	5.3×10^{-4}		Mackay et al. (1992a)	V	
	5.4×10^{-4}		Eastcott et al. (1988)	V	
	8.6×10^{-4}		Hine and Mookerjee (1975)	V	
	5.9×10^{-4}		Yaws (2003)	X	237
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	5.9×10^{-4}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	6.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
	8.6×10^{-4}		Hilal et al. (2008)	Q	
	6.9×10^{-4}		Modarresi et al. (2007)	Q	67
	7.2×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	9.0×10^{-4}		English and Carroll (2001)	Q	230, 231
	9.9×10^{-5}		Nirmalakhandan et al. (1997)	Q	
	6.1×10^{-4}		Suzuki et al. (1992)	Q	232
	7.2×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	1.3×10^{-3}		Yaws (1999)	?	21
(2-methylpropyl)-benzene	2.9×10^{-4}		Plyasunov and Shock (2000)	L	
$C_6H_5C_4H_9$	3.0×10^{-4}		Mackay and Shiu (1981)	L	
(isobutylbenzene)	2.9×10^{-4}		Duchowicz et al. (2020)	V	186
[538-93-2]	3.0×10^{-4}		Mackay et al. (2006a)	V	
KXUHSQYYJYAXGZ-UHFFFAOYSA-N	3.0×10^{-4}		Mackay et al. (1992a)	V	
	3.0×10^{-4}		Eastcott et al. (1988)	V	
	5.5×10^{-4}		Yaws (2003)	X	237
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	6.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	6.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
	7.0×10^{-4}		Hilal et al. (2008)	Q	
	5.2×10^{-4}		Modarresi et al. (2007)	Q	67
	3.1×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	4.3×10^{-4}		Yao et al. (2002)	Q	229
	7.7×10^{-4}		English and Carroll (2001)	Q	230, 231
	5.4×10^{-4}		Katritzky et al. (1998)	Q	
	7.0×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	1.3×10^{-3}		Yaws (1999)	?	21

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(1,1-dimethylethyl)-benzene	7.9×10^{-4}		Plyasunov and Shock (2000)	L	
$C_6H_5C_4H_9$	8.3×10^{-4}		Mackay and Shiu (1981)	L	
(*tert*-butylbenzene)	1.6×10^{-3}	4700	Hiatt (2013)	M	
[98-06-6]	9.4×10^{-4}	2400	Kondoh and Nakajima (1997)	M	
YTZKOQUCBOVLHL-UHFFFAOYSA-N	7.5×10^{-4}		Duchowicz et al. (2020)	V	186
	7.5×10^{-4}		HSDB (2015)	V	
	7.8×10^{-4}		Mackay et al. (2006a)	V	
	7.8×10^{-4}		Mackay et al. (1992a)	V	
	7.7×10^{-4}		Eastcott et al. (1988)	V	
	8.4×10^{-4}		Hine and Mookerjee (1975)	V	
	6.1×10^{-4}		Yaws (2003)	X	237
	5.3×10^{-4}		Duchowicz et al. (2020)	Q	
	5.3×10^{-4}		Gharagheizi et al. (2012)	Q	
	5.6×10^{-4}		Gharagheizi et al. (2010)	Q	246
	7.7×10^{-4}		Hilal et al. (2008)	Q	
	6.6×10^{-4}		Modarresi et al. (2007)	Q	67
	8.6×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	9.0×10^{-4}		English and Carroll (2001)	Q	230, 231
	4.8×10^{-4}		Katritzky et al. (1998)	Q	
	5.3×10^{-4}		Suzuki et al. (1992)	Q	232
	6.0×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	1.4×10^{-3}		Yaws (1999)	?	21
1-methyl-2-propylbenzene	7.2×10^{-4}		Yaws (2003)	X	237
$C_{10}H_{14}$	5.3×10^{-4}		Gharagheizi et al. (2012)	Q	
[1074-17-5]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
YQZBFMJOASEONC-UHFFFAOYSA-N					
1-methyl-3-propylbenzene	7.7×10^{-4}		Yaws (2003)	X	237
$C_{10}H_{14}$	4.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[1074-43-7]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
QUEBYVKXYIKVSO-UHFFFAOYSA-N					
1-methyl-4-propylbenzene	9.6×10^{-4}		Yaws (2003)	X	237
$C_{10}H_{14}$	4.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[1074-55-1]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
JXFVMNFKABWTHD-UHFFFAOYSA-N					
2-ethyl-*m*-xylene	1.3×10^{-3}		Yaws (2003)	X	237
$C_{10}H_{14}$	4.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[2870-04-4]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
CHIKRULMSSADAF-UHFFFAOYSA-N	1.3×10^{-3}		Yaws (1999)	?	21
2-ethyl-*p*-xylene	1.2×10^{-3}		Yaws (2003)	X	237
$C_{10}H_{14}$	3.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[1758-88-9]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
AXIUBBVSOWPLDA-UHFFFAOYSA-N	1.2×10^{-3}		Yaws (1999)	?	21

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-*o*-xylene	1.2×10^{-3}		Yaws (2003)	X	237
$C_{10}H_{14}$	4.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[933-98-2]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
QUBBAXISAHIDNM-UHFFFAOYSA-N	1.2×10^{-3}		Yaws (1999)	?	21
4-ethyl-*o*-xylene	1.3×10^{-3}		Yaws (2003)	X	237
$C_{10}H_{14}$	4.2×10^{-4}		Gharagheizi et al. (2012)	Q	
[934-80-5]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
SBUYFICWQNHBCM-UHFFFAOYSA-N	4.5×10^{-4}		Yao et al. (2002)	Q	229
	1.3×10^{-3}		Yaws (1999)	?	21
4-ethyl-*m*-xylene	1.1×10^{-3}		Yaws (2003)	X	237
$C_{10}H_{14}$	4.0×10^{-4}		Gharagheizi et al. (2012)	Q	
[874-41-9]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
MEMBJMDZWKVOTB-UHFFFAOYSA-N	3.0×10^{-4}		Yao et al. (2002)	Q	229
	1.1×10^{-3}		Yaws (1999)	?	21
5-ethyl-*m*-xylene	1.3×10^{-3}		Yaws (2003)	X	237
$C_{10}H_{14}$	1.1×10^{-3}		Wang et al. (2017)	Q	80, 238
(1-ethyl-3,5-dimethylbenzene)	9.3×10^{-4}		Wang et al. (2017)	Q	80, 239
[934-74-7]	2.2×10^{-3}		Wang et al. (2017)	Q	80, 240
LMAUULKNZLEMGN-UHFFFAOYSA-N	3.3×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.3×10^{-3}		Yaws (1999)	?	21
1-methyl-2-(1-methylethyl)-benzene	1.6×10^{-3}		Plyasunov and Shock (2000)	L	
$C_{10}H_{14}$	8.7×10^{-4}		Duchowicz et al. (2020)	V	186
(*o*-cymene)	9.0×10^{-4}		HSDB (2015)	V	
[527-84-4]	1.2×10^{-3}		Yaws (2003)	X	258
WWRCMNKATXZARA-UHFFFAOYSA-N	1.2×10^{-3}		Yaws (2003)	X	237
	1.3×10^{-3}		Dupeux et al. (2022)	Q	259
	6.1×10^{-4}		Duchowicz et al. (2020)	Q	
	4.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.2×10^{-3}		Hilal et al. (2008)	Q	
	6.6×10^{-4}		Modarresi et al. (2007)	Q	67
	5.3×10^{-4}		Katritzky et al. (1998)	Q	
	1.2×10^{-3}		Yaws (1999)	?	21

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methyl-3-(1-methylethyl)-benzene	1.4×10^{-3}		Plyasunov and Shock (2000)	L	
$C_{10}H_{14}$	1.4×10^{-3}		Duchowicz et al. (2020)	V	186
(m-cymene)	1.4×10^{-3}		HSDB (2015)	V	
[535-77-3]	9.0×10^{-4}		Copolovici and Niinemets (2005)	V	
XCYJPXQACVEIOS-UHFFFAOYSA-N	1.2×10^{-3}		Yaws (2003)	X	258
	1.2×10^{-3}		Yaws (2003)	X	237
	8.2×10^{-4}		Dupeux et al. (2022)	Q	259
	6.1×10^{-4}		Duchowicz et al. (2020)	Q	
	4.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-3}		Gharagheizi et al. (2010)	Q	246
	8.6×10^{-4}		Hilal et al. (2008)	Q	
	4.5×10^{-4}		Modarresi et al. (2007)	Q	67
	1.2×10^{-3}		Yaws (1999)	?	21
1-methyl-4-(1-methylethyl)-benzene	9.6×10^{-4}		Plyasunov and Shock (2000)	L	
$C_{10}H_{14}$	1.3×10^{-3}		Mackay and Shiu (1981)	L	
(p-cymene; p-isopropyltoluene)	1.8×10^{-3}	4900	Hiatt (2013)	M	
[99-87-6]	1.0×10^{-3}	2600	Kondoh and Nakajima (1997)	M	
HFPZCAJZSCWRBC-UHFFFAOYSA-N	9.0×10^{-4}		Duchowicz et al. (2020)	V	186
	8.0×10^{-4}		Duchowicz et al. (2020)	V	186
	1.1×10^{-3}		Martins et al. (2017)	V	315
	9.0×10^{-4}		HSDB (2015)	V	
	1.2×10^{-3}		Mackay et al. (2006a)	V	
	1.1×10^{-3}		Copolovici and Niinemets (2005)	V	
	9.1×10^{-4}		Niinemets and Reichstein (2002)	V	
	1.3×10^{-3}		Abraham et al. (1994a)	V	
	1.2×10^{-3}		Mackay et al. (1992a)	V	
	1.2×10^{-3}		Eastcott et al. (1988)	V	
	1.3×10^{-3}		Yaws (2003)	X	258
	1.3×10^{-3}		Yaws (2003)	X	237
	7.6×10^{-4}		Dupeux et al. (2022)	Q	259
	6.1×10^{-4}		Duchowicz et al. (2020)	Q	
	6.1×10^{-4}		Duchowicz et al. (2020)	Q	
	4.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-3}		Gharagheizi et al. (2010)	Q	246
	8.8×10^{-4}		Hilal et al. (2008)	Q	
	5.4×10^{-4}		Modarresi et al. (2007)	Q	67
	5.5×10^{-4}		Modarresi et al. (2007)	Q	67
		5300	Kühne et al. (2005)	Q	
	8.0×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	1.4×10^{-3}		English and Carroll (2001)	Q	230, 274
	5.4×10^{-4}		Katritzky et al. (1998)	Q	
	6.5×10^{-4}		Nirmalakhandan et al. (1997)	Q	

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
		4500	Kühne et al. (2005)	?	
	1.3×10^{-3}		Yaws (1999)	?	21
4-*tert*-butyltoluene	7.8×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	6.4×10^{-4}		HSDB (2015)	Q	99
[98-51-1]	2.7×10^{-4}		Gharagheizi et al. (2012)	Q	
QCWXDVFBZVHKLV-UHFFFAOYSA-N	6.4×10^{-4}		Zhang et al. (2010)	Q	287, 288
	5.2×10^{-4}		Zhang et al. (2010)	Q	287, 289
	1.3×10^{-3}		Zhang et al. (2010)	Q	287, 290
	4.7×10^{-4}		Zhang et al. (2010)	Q	287, 291
	8.2×10^{-4}		Gharagheizi et al. (2010)	Q	246
pentylbenzene	6.0×10^{-4}	6000	Brockbank (2013)	L	1, 359
$C_6H_5C_5H_{11}$	5.1×10^{-4}	5900	Plyasunov and Shock (2000)	L	
[538-68-1]	1.7×10^{-3}		Mackay and Shiu (1981)	L	
PWATWSYOIIXYMA-UHFFFAOYSA-N	6.1×10^{-4}		Ryu and Park (1999)	M	
	3.9×10^{-4}		Duchowicz et al. (2020)	V	186
	5.9×10^{-4}		Mackay et al. (2006a)	V	
	5.9×10^{-4}		Mackay et al. (1992a)	V	
	1.6×10^{-3}		Eastcott et al. (1988)	V	
	6.0×10^{-4}		Abraham (1984)	V	
	3.0×10^{-3}	7800	Ben-Naim and Wilf (1980)	V	1
	5.3×10^{-4}	5900	Owens et al. (1986)	T	
	4.4×10^{-4}		Yaws (2003)	X	237
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	5.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	6.0×10^{-4}		Gharagheizi et al. (2010)	Q	246
	6.1×10^{-4}		Hilal et al. (2008)	Q	
	4.3×10^{-4}		Modarresi et al. (2007)	Q	67
	6.1×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	4.4×10^{-4}		Yao et al. (2002)	Q	229
	5.8×10^{-4}		English and Carroll (2001)	Q	230, 260
	5.7×10^{-4}		Katritzky et al. (1998)	Q	
	6.4×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	4.4×10^{-4}		Yaws (1999)	?	21
	5.9×10^{-4}		Yaws and Yang (1992)	?	21
	6.0×10^{-4}		Abraham et al. (1990)	?	
pentamethylbenzene	7.7×10^{-3}		Hilal et al. (2008)	Q	
$C_{11}H_{16}$	7.0×10^{-4}		Modarresi et al. (2007)	Q	67
[700-12-9]					
BEZDDPMMPIDMGJ-UHFFFAOYSA-N					

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Table A2.5: Mononuclear aromatics (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
1,2-dimethyl-3-propylbenzene	8.7×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[17059-44-8]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
IRUSTUOJENXLMN-UHFFFAOYSA-N					
1,2-dimethyl-4-propylbenzene	8.8×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[3982-66-9]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
FZJVYOOQGFZCSY-UHFFFAOYSA-N					
1,3-dimethyl-2-propylbenzene	8.9×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[17059-45-9]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
POVRSTNZQPBWAS-UHFFFAOYSA-N					
1,3-dimethyl-4-propylbenzene	9.0×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[61827-85-8]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
HPAXKQMKDWCLGU-UHFFFAOYSA-N					
1,3-dimethyl-5-propylbenzene	9.3×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.3×10^{-4}		Gharagheizi et al. (2012)	Q	
[3982-64-7]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
NBICXWXPZRNMPF-UHFFFAOYSA-N					
1,4-dimethyl-2-propylbenzene	9.2×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.4×10^{-4}		Gharagheizi et al. (2012)	Q	
[3042-50-0]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
PWEDYOIWLPZSRP-UHFFFAOYSA-N					
1,2-dimethyl-3-isopropylbenzene	8.4×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.4×10^{-4}		Gharagheizi et al. (2012)	Q	
[22539-65-7]	9.4×10^{-4}		Gharagheizi et al. (2010)	Q	246
GDEQPEBFOWYWSA-UHFFFAOYSA-N					
1,2-dimethyl-4-isopropylbenzene	8.5×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.3×10^{-4}		Gharagheizi et al. (2012)	Q	
[4132-77-8]	9.4×10^{-4}		Gharagheizi et al. (2010)	Q	246
MGMSKQZIAGFMRU-UHFFFAOYSA-N					
1,3-dimethyl-2-isopropylbenzene	8.7×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.1×10^{-4}		Gharagheizi et al. (2012)	Q	
[14411-75-7]	9.4×10^{-4}		Gharagheizi et al. (2010)	Q	246
IVCIQLTVLDOHKA-UHFFFAOYSA-N					
1,3-dimethyl-4-isopropylbenzene	8.7×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.1×10^{-4}		Gharagheizi et al. (2012)	Q	
[4706-89-2]	9.4×10^{-4}		Gharagheizi et al. (2010)	Q	246
AADQFNAACHHRLT-UHFFFAOYSA-N					

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3-dimethyl-5-isopropylbenzene	9.2×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	1.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[4706-90-5]	9.4×10^{-4}		Gharagheizi et al. (2010)	Q	246
RMKJTYPFCFNTGQ-UHFFFAOYSA-N					
1,4-dimethyl-2-isopropylbenzene	9.0×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	1.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[4132-72-3]	9.4×10^{-4}		Gharagheizi et al. (2010)	Q	246
CLSBTDGUHSQYTO-UHFFFAOYSA-N					
1-ethyl-2-propylbenzene	9.4×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	3.5×10^{-4}		Gharagheizi et al. (2012)	Q	
[16021-20-8]	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
DMUVQFCRCMDZPW-UHFFFAOYSA-N	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	8.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
1-ethyl-3-propylbenzene	9.6×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	3.3×10^{-4}		Gharagheizi et al. (2012)	Q	
[20024-91-3]	8.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
QCYGXOCMWHSXSU-UHFFFAOYSA-N					
1-ethyl-4-propylbenzene	9.2×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	3.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[20024-90-2]	8.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
ADQDTIAWIXUACV-UHFFFAOYSA-N					
1-ethyl-2-isopropylbenzene	9.8×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.5×10^{-4}		Gharagheizi et al. (2012)	Q	
[18970-44-0]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
ZAJYARZMPOEGLK-UHFFFAOYSA-N					
1-ethyl-3-isopropylbenzene	9.6×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[4920-99-4]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
GSLSBTNLESMZTN-UHFFFAOYSA-N					
1-ethyl-4-isopropylbenzene	9.1×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	3.0×10^{-4}		Gharagheizi et al. (2012)	Q	
[4218-48-8]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
GUUDUUDWUWUTPD-UHFFFAOYSA-N					
1-methyl-2,3-diethylbenzene	9.0×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[13632-93-4]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
LRJOXARIJKBUFE-UHFFFAOYSA-N					
1-methyl-2,4-diethylbenzene	9.1×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.5×10^{-4}		Gharagheizi et al. (2012)	Q	
[1758-85-6]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
PZMJNJDRDKPVLB-UHFFFAOYSA-N					

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methyl-2,5-diethylbenzene	9.0×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[13632-94-5]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
ZEHGGUIGEDITMM-UHFFFAOYSA-N					
1-methyl-2,6-diethylbenzene	8.8×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[13632-95-6]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
XZZNTLNFQVAKFD-UHFFFAOYSA-N					
1-methyl-3,5-diethylbenzene	9.5×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	8.7×10^{-4}		Wang et al. (2017)	Q	80, 238
[2050-24-0]	5.8×10^{-4}		Wang et al. (2017)	Q	80, 239
HILAULICMJUOLK-UHFFFAOYSA-N	2.0×10^{-3}		Wang et al. (2017)	Q	80, 240
	2.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
1-methyl-2-butylbenzene	9.0×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	4.1×10^{-4}		Gharagheizi et al. (2012)	Q	
[1595-11-5]	8.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
NUJILYKLNKQOOX-UHFFFAOYSA-N					
1-methyl-3-butylbenzene	9.2×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	3.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[1595-04-6]	8.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
OAPCPUDMDJIBOQ-UHFFFAOYSA-N					
1-methyl-4-butylbenzene	9.1×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	4.0×10^{-4}		Gharagheizi et al. (2012)	Q	
[1595-05-7]	8.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
SBBKUBSYOVDBBC-UHFFFAOYSA-N					
1-methyl-2-isobutylbenzene	9.1×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[36301-29-8]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
XNMPJDZAHSMAMN-UHFFFAOYSA-N					
1-methyl-3-isobutylbenzene	9.3×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[5160-99-6]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
SDHYGAUOCHFYSR-UHFFFAOYSA-N					
1-methyl-4-isobutylbenzene	9.1×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[5161-04-6]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
VCGBZXLLPCGFQM-UHFFFAOYSA-N					
1-methyl-2-*sec*-butylbenzene	9.1×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.9×10^{-4}		Gharagheizi et al. (2012)	Q	
[1595-06-8]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
AMBAWAHKHZZAAY-UHFFFAOYSA-N					

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Table A2.5: Mononuclear aromatics (. . . continued)

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1-methyl-3-*sec*-butylbenzene	9.3×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[1772-10-7]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
RMNILBOMCXQZFC-UHFFFAOYSA-N					
1-methyl-4-*sec*-butylbenzene	9.0×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	3.0×10^{-4}		Gharagheizi et al. (2012)	Q	
[1595-16-0]	9.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
LWCFXYMSEGQWNB-UHFFFAOYSA-N					
1-methyl-2-*tert*-butyl benzene	7.2×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	3.4×10^{-4}		Gharagheizi et al. (2012)	Q	
[1074-92-6]	8.2×10^{-4}		Gharagheizi et al. (2010)	Q	246
AXHVNJGQOJFMHT-UHFFFAOYSA-N					
1-methyl-3-*tert*-butylbenzene	8.2×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.5×10^{-4}		Gharagheizi et al. (2012)	Q	
[1075-38-3]	8.2×10^{-4}		Gharagheizi et al. (2010)	Q	246
JTIAYWZZZOZUTK-UHFFFAOYSA-N					
1-methyl-3,4-diethylbenzene	9.2×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	2.4×10^{-4}		Gharagheizi et al. (2012)	Q	
[13732-80-4]	7.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
MJQJAQGFUBIGIK-UHFFFAOYSA-N					
1-phenyl-2,2-dimethylpropane	3.8×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	3.4×10^{-4}		Gharagheizi et al. (2012)	Q	
[1007-26-7]	4.5×10^{-4}		Gharagheizi et al. (2010)	Q	246
CJGXJKVMUHXVHL-UHFFFAOYSA-N					
1-phenyl-2-methylbutane	4.0×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	4.5×10^{-4}		Gharagheizi et al. (2012)	Q	
[3968-85-2]	5.5×10^{-4}		Gharagheizi et al. (2010)	Q	246
IFDLFCDWOFLKEB-UHFFFAOYSA-N					
1-phenyl-3-methylbutane	3.9×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	4.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[2049-94-7]	5.5×10^{-4}		Gharagheizi et al. (2010)	Q	246
XNXIYYFOYIUJIW-UHFFFAOYSA-N					
2-phenyl-3-methylbutane	4.1×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	3.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[4481-30-5]	5.3×10^{-4}		Gharagheizi et al. (2010)	Q	246
NQRMTOKLHZNAQH-UHFFFAOYSA-N					
2-phenylpentane	4.3×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	3.7×10^{-4}		Gharagheizi et al. (2012)	Q	
[2719-52-0]	5.5×10^{-4}		Gharagheizi et al. (2010)	Q	246
LTHAIAJHDPJXLG-UHFFFAOYSA-N					

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-phenylpentane	4.3×10^{-4}		Yaws (2003)	X	237
$C_{11}H_{16}$	3.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[1196-58-3]	5.5×10^{-4}		Gharagheizi et al. (2010)	Q	246
PBWHJRFXUPLZDS-UHFFFAOYSA-N					
(1,1-dimethylpropyl)-benzene	5.4×10^{-4}		Hine and Mookerjee (1975)	V	
$C_6H_5C_5H_{11}$	3.5×10^{-4}		Yaws (2003)	X	237
(*tert*-amylbenzene)	4.1×10^{-4}		Gharagheizi et al. (2012)	Q	
[2049-95-8]	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
QHTJSSMHBLGUHV-UHFFFAOYSA-N	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	4.5×10^{-4}		Gharagheizi et al. (2010)	Q	246
	9.9×10^{-4}		Hilal et al. (2008)	Q	
	5.8×10^{-4}		English and Carroll (2001)	Q	230, 231
	4.2×10^{-4}		Suzuki et al. (1992)	Q	232
	5.1×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
hexylbenzene	4.0×10^{-4}	6500	Brockbank (2013)	L	1
$C_6H_5C_6H_{13}$	4.0×10^{-4}	6300	Plyasunov and Shock (2000)	L	
[1077-16-3]	3.5×10^{-4}		Duchowicz et al. (2020)	V	186
LTEQMZWBSYACLV-UHFFFAOYSA-N	4.6×10^{-4}		Mackay et al. (2006a)	V	
	4.6×10^{-4}		Mackay et al. (1992a)	V	
	4.5×10^{-4}		Meylan and Howard (1991)	V	
	5.1×10^{-4}		Eastcott et al. (1988)	V	
	4.5×10^{-4}		Abraham (1984)	V	
	7.7×10^{-3}	9000	Ben-Naim and Wilf (1980)	V	1
	4.1×10^{-4}	6300	Owens et al. (1986)	T	
	3.9×10^{-4}		Yaws (2003)	X	237
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	6.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	5.3×10^{-4}		Gharagheizi et al. (2010)	Q	246
	4.8×10^{-4}		Hilal et al. (2008)	Q	
	4.3×10^{-4}		Modarresi et al. (2007)	Q	67
	4.6×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	3.7×10^{-4}		Yao et al. (2002)	Q	229
	4.2×10^{-4}		English and Carroll (2001)	Q	230, 231
	5.0×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	4.0×10^{-4}		Meylan and Howard (1991)	Q	
	3.9×10^{-4}		Yaws (1999)	?	21
	4.6×10^{-4}		Yaws and Yang (1992)	?	21
	4.3×10^{-4}		Abraham et al. (1990)	?	
hexamethylbenzene	8.6×10^{-3}		Hilal et al. (2008)	Q	
$C_{12}H_{18}$	1.5×10^{-3}		Modarresi et al. (2007)	Q	67
[87-85-4]					
YUWFEBAXEOLKSG-UHFFFAOYSA-N					

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Table A2.5: Mononuclear aromatics (. . . continued)

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1,2,3-triethylbenzene	3.5×10^{-4}		Yaws (2003)	X	237
$C_{12}H_{18}$	1.4×10^{-4}		Gharagheizi et al. (2012)	Q	
[42205-08-3]	6.0×10^{-4}		Gharagheizi et al. (2010)	Q	246
VIDOPANCAUPXNH-UHFFFAOYSA-N					
1,2,4-triethylbenzene	7.2×10^{-4}		Yaws (2003)	X	237
$C_{12}H_{18}$	1.4×10^{-4}		Gharagheizi et al. (2012)	Q	
[877-44-1]	6.0×10^{-4}		Gharagheizi et al. (2010)	Q	246
WNLWIOJSURYFIB-UHFFFAOYSA-N	7.2×10^{-4}		Yaws (1999)	?	21
1,3,5-triethylbenzene	1.0×10^{-3}		Plyasunov and Shock (2000)	L	
$C_{12}H_{18}$	3.4×10^{-4}		Yaws (2003)	X	237
[102-25-0]	1.4×10^{-4}		Gharagheizi et al. (2012)	Q	
WJYMPXJVHNDZHD-UHFFFAOYSA-N	6.0×10^{-4}		Gharagheizi et al. (2010)	Q	246
4-*tert*-butyl-*o*-xylene	5.8×10^{-4}		Zhang et al. (2010)	Q	287, 288
$C_{12}H_{18}$	7.2×10^{-4}		Zhang et al. (2010)	Q	287, 289
[7397-06-0]	9.0×10^{-4}		Zhang et al. (2010)	Q	287, 290
QRPPSTNABSMSCS-UHFFFAOYSA-N	2.7×10^{-4}		Zhang et al. (2010)	Q	287, 291
1-(1,1-dimethylethyl)-3,5-dimethylbenzene	5.8×10^{-4}		Zhang et al. (2010)	Q	287, 288
$C_{12}H_{18}$	4.5×10^{-4}		Zhang et al. (2010)	Q	287, 289
[98-19-1]	7.7×10^{-4}		Zhang et al. (2010)	Q	287, 290
FZSPYHREEHYLCB-UHFFFAOYSA-N	2.7×10^{-4}		Zhang et al. (2010)	Q	287, 291
o-diisopropylbenzene	4.8×10^{-4}		HSDB (2015)	Q	99
$C_{12}H_{18}$					
[25321-09-9]					
OKIRBHVFJGXOIS-UHFFFAOYSA-N					
m-diisopropylbenzene	9.5×10^{-4}		Yaws (2003)	X	237
$C_{12}H_{18}$	7.2×10^{-4}		Gharagheizi et al. (2010)	Q	246
[99-62-7]	9.6×10^{-4}		Yaws (1999)	?	21
UNEATYXSUBPPKP-UHFFFAOYSA-N					
p-diisopropylbenzene	1.0×10^{-3}		Yaws (2003)	X	237
$C_{12}H_{18}$	1.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[100-18-5]	7.2×10^{-4}		Gharagheizi et al. (2010)	Q	246
SPPWGCYEYAMHDT-UHFFFAOYSA-N	1.0×10^{-3}		Yaws (1999)	?	21
4-phenylcyclohexene	7.9×10^{-3}		Ebert et al. (2023)	?	318
$C_{12}H_{14}$					
[4994-16-5]					
XWCWNUSFQVJNDI-UHFFFAOYSA-N					

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Table A2.5: Mononuclear aromatics (. . . continued)

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heptylbenzene	2.7×10^{-4}		Brockbank (2013)	L	
$C_6H_5C_7H_{15}$	6.5×10^{-4}		Duchowicz et al. (2020)	V	186
[1078-71-3]	2.2×10^{-2}	11000	Ben-Naim and Wilf (1980)	V	1
LBNXAWYDQUGHGX-UHFFFAOYSA-N	6.5×10^{-4}		Yaws (2003)	X	237
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	1.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	5.0×10^{-4}		Gharagheizi et al. (2010)	Q	246
	3.9×10^{-4}		Hilal et al. (2008)	Q	
	3.5×10^{-4}		Yao et al. (2002)	Q	229
	1.5×10^{-3}		Yaws (1999)	?	21
5-*tert*-butyl-1,2,3-trimethylbenzene	5.3×10^{-4}		Zhang et al. (2010)	Q	287, 288
$C_{13}H_{20}$	9.2×10^{-4}		Zhang et al. (2010)	Q	287, 289
[98-23-7]	9.0×10^{-4}		Zhang et al. (2010)	Q	287, 290
ZQVJKYPEIPJEIP-UHFFFAOYSA-N	1.5×10^{-4}		Zhang et al. (2010)	Q	287, 291
octylbenzene	1.8×10^{-4}		Brockbank (2013)	L	
$C_6H_5C_8H_{17}$	2.3×10^{-4}		Duchowicz et al. (2020)	V	186
[2189-60-8]	5.4×10^{-2}	12000	Ben-Naim and Wilf (1980)	V	1
CDKDZKXSXLNROY-UHFFFAOYSA-N	8.7×10^{-4}		Yaws (2003)	X	237
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	1.7×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
	3.2×10^{-4}		Hilal et al. (2008)	Q	
	2.0×10^{-3}		Yaws (1999)	?	21
nonylbenzene	1.4×10^{-4}		Brockbank (2013)	L	
$C_{15}H_{24}$	1.8×10^{-3}		Gharagheizi et al. (2012)	Q	
[1081-77-2]	3.3×10^{-3}		Yaws (1999)	?	21
LIXVMPBOGDCSRM-UHFFFAOYSA-N					
3,5-di-*tert*-butyltoluene	3.7×10^{-3}	9100	Hiatt (2013)	M	
$C_{15}H_{24}$					
[15181-11-0]					
WIXDSJRJFDWTNY-UHFFFAOYSA-N					
1,3,5-tris(1-methylethyl)benzene	2.5×10^{-4}		Zhang et al. (2010)	Q	287, 288
$C_{15}H_{24}$	1.8×10^{-4}		Zhang et al. (2010)	Q	287, 289
[717-74-8]	5.2×10^{-4}		Zhang et al. (2010)	Q	287, 290
VUMCUSHVMYIRMB-UHFFFAOYSA-N	2.6×10^{-4}		Zhang et al. (2010)	Q	287, 291
ethyl(phenylethyl)-benzene	1.1×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{16}H_{18}$	1.2×10^{-2}		Zhang et al. (2010)	Q	287, 289
[64800-83-5]	6.4×10^{-2}		Zhang et al. (2010)	Q	287, 290
BDEIYMXBPHSOSG-UHFFFAOYSA-N	1.8×10^{-2}		Zhang et al. (2010)	Q	287, 291
4-(1-phenylethyl)-*m*-xylene	1.3×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{16}H_{18}$	1.6×10^{-2}		Zhang et al. (2010)	Q	287, 289
[6165-52-2]	5.2×10^{-2}		Zhang et al. (2010)	Q	287, 290
JOUBGGHXBLOLFY-UHFFFAOYSA-N	1.5×10^{-2}		Zhang et al. (2010)	Q	287, 291

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Table A2.5: Mononuclear aromatics (. . . continued)

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decylbenzene	7.6×10^{-5}		Brockbank (2013)	L	
$C_{16}H_{26}$	8.6×10^{-5}		Plyasunov and Shock (2000)	L	
(1-phenyldecane)	6.5×10^{-5}		Duchowicz et al. (2020)	V	186
[104-72-3]	1.3×10^{-4}		HSDB (2015)	V	
UZILCZKGXMQEQR-UHFFFAOYSA-N	8.6×10^{-5}		Sherblom et al. (1992)	V	
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	1.3×10^{-4}		Zhang et al. (2010)	Q	287, 288
	1.4×10^{-4}		Zhang et al. (2010)	Q	287, 289
	3.4×10^{-4}		Zhang et al. (2010)	Q	287, 290
	2.8×10^{-4}		Zhang et al. (2010)	Q	287, 291
	7.9×10^{-3}		Yaws (1999)	?	21
2-phenyldecane $C_{16}H_{26}$ [4537-13-7] DDTJIQUCOLHYDL-UHFFFAOYSA-N	1.0×10^{-4}		Sherblom et al. (1992)	V	
3-phenyldecane $C_{16}H_{26}$ [4621-36-7] PYVIFMPVFLOTLN-UHFFFAOYSA-N	1.1×10^{-4}		Sherblom et al. (1992)	V	
4-phenyldecane $C_{16}H_{26}$ [4537-12-6] QTDBKYLPIZUTFN-UHFFFAOYSA-N	9.2×10^{-5}		Sherblom et al. (1992)	V	
5-phenyldecane $C_{16}H_{26}$ [4537-11-5] CDOBABYRHNVZQG-UHFFFAOYSA-N	8.4×10^{-5}		Sherblom et al. (1992)	V	
undecylbenzene $C_{17}H_{28}$ (1-phenylundecane) [6742-54-7] XBEADGFTLHRJRB-UHFFFAOYSA-N	9.9×10^{-5}		HSDB (2015)	Q	99
2-phenylundecane $C_{17}H_{28}$ [4536-88-3] YHJBCRBYDBNEIK-UHFFFAOYSA-N	8.2×10^{-5}		Sherblom et al. (1992)	V	
3-phenylundecane $C_{17}H_{28}$ [4536-87-2] NVHBFHMWJJMQTG-UHFFFAOYSA-N	9.0×10^{-5}		Sherblom et al. (1992)	V	

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-phenylundecane $C_{17}H_{28}$ [4536-86-1] NSQAXMRLBNXEHK-UHFFFAOYSA-N	5.9×10^{-5}		Sherblom et al. (1992)	V	
5-phenylundecane $C_{17}H_{28}$ [4537-15-9] RRPCXIBGXYGQNC-UHFFFAOYSA-N	6.1×10^{-5}		Sherblom et al. (1992)	V	
6-phenylundecane $C_{17}H_{28}$ [4537-14-8] WCABIRIFXVXGQH-UHFFFAOYSA-N	6.4×10^{-5}		Sherblom et al. (1992)	V	
dodecylbenzene $C_{18}H_{30}$ (1-phenyldodecane) [123-01-3] KWKXNDCHNDYVRT-UHFFFAOYSA-N	7.6×10^{-5}		HSDB (2015)	Q	99
2-phenyldodecane $C_{18}H_{30}$ [2719-61-1] VRPRIAVYSREHAN-UHFFFAOYSA-N	1.1×10^{-4}		Sherblom et al. (1992)	V	
3-phenyldodecane $C_{18}H_{30}$ [2400-00-2] PGVOXXHNGYYHHB-UHFFFAOYSA-N	1.3×10^{-4}		Sherblom et al. (1992)	V	
4-phenyldodecane $C_{18}H_{30}$ [2719-64-4] RHDHXBLZBVAPTL-UHFFFAOYSA-N	8.3×10^{-5}		Sherblom et al. (1992)	V	
5-phenyldodecane $C_{18}H_{30}$ [2719-63-3] NPAWGLOPXKCTCV-UHFFFAOYSA-N	7.8×10^{-5}		Sherblom et al. (1992)	V	
6-phenyldodecane $C_{18}H_{30}$ [2719-62-2] ZYHJQFMTTFCBKH-UHFFFAOYSA-N	6.0×10^{-5}		Sherblom et al. (1992)	V	
tridecylbenzene $C_{19}H_{32}$ (1-phenyltridecane) [123-02-4] MCVUKOYZUCWLQQ-UHFFFAOYSA-N	1.1×10^{-4} 5.5×10^{-5}		Sherblom et al. (1992) HSDB (2015)	V Q	 99

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-phenyltridecane $C_{19}H_{32}$ [4534-53-6] FCXPVFLEDIQLLO-UHFFFAOYSA-N	2.7×10^{-4}		Sherblom et al. (1992)	V	
3-phenyltridecane $C_{19}H_{32}$ [4534-52-5] VZZMNLVGDGMQQV-UHFFFAOYSA-N	2.1×10^{-4}		Sherblom et al. (1992)	V	
4-phenyltridecane $C_{19}H_{32}$ [4534-51-4] RZGVZPAWCGDMCK-UHFFFAOYSA-N	2.0×10^{-4}		Sherblom et al. (1992)	V	
5-phenyltridecane $C_{19}H_{32}$ [4534-50-3] MZTIRLOLMGVVEK-UHFFFAOYSA-N	1.5×10^{-4}		Sherblom et al. (1992)	V	
6-phenyltridecane $C_{19}H_{32}$ [4534-49-0] OTSYFFDVDLHIKX-UHFFFAOYSA-N	1.5×10^{-4}		Sherblom et al. (1992)	V	
tetradecylbenzene $C_{20}H_{34}$ (1-phenyltetradecane) [1459-10-5] JZALLXAUNPOCEU-UHFFFAOYSA-N	4.2×10^{-5}		HSDB (2015)	Q	99
2-phenyltetradecane $C_{20}H_{34}$ [4534-59-2] GDFUGKICRHMMOT-UHFFFAOYSA-N	6.7×10^{-4}		Sherblom et al. (1992)	V	
3-phenyltetradecane $C_{20}H_{34}$ [4534-58-1] ILOABSZOHZMWLD-UHFFFAOYSA-N	6.2×10^{-4}		Sherblom et al. (1992)	V	
4-phenyltetradecane $C_{20}H_{34}$ [4534-57-0] YXLRHYCRTUAPMC-UHFFFAOYSA-N	4.0×10^{-4}		Sherblom et al. (1992)	V	
5-phenyltetradecane $C_{20}H_{34}$ [4534-56-9] RAWFVRXBPRHWLJ-UHFFFAOYSA-N	5.0×10^{-4}		Sherblom et al. (1992)	V	

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Table A2.5: Mononuclear aromatics (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
6-phenyltetradecane $C_{20}H_{34}$ [4534-55-8] MTDIFFBFSKQPIA-UHFFFAOYSA-N	3.6×10^{-4}		Sherblom et al. (1992)	V	
pentadecylbenzene $C_{21}H_{36}$ [2131-18-2] JIRNEODMTPGRGV-UHFFFAOYSA-N	1.2×10^{-5}		HSDB (2015)	Q	99
ethenylbenzene	3.6×10^{-3}	3700	Brockbank (2013)	L	1
C_8H_8	2.9×10^{-3}	4200	Plyasunov and Shock (2000)	L	
(styrene)	2.7×10^{-3}		Kim and Kim (2014)	M	
[100-42-5]	4.4×10^{-3}	4600	Hiatt (2013)	M	
PPBRXRYQALVLMV-UHFFFAOYSA-N	3.4×10^{-3}		Dohnal and Hovorka (1999)	M	
	2.5×10^{-3}		Welke et al. (1998)	M	
	3.8×10^{-3}	4100	Kondoh and Nakajima (1997)	M	
	2.9×10^{-3}	4800	Bissonette et al. (1990)	M	
	1.8×10^{-3}		Sato and Nakajima (1979a)	M	14
	3.6×10^{-3}		Lide and Frederikse (1995)	V	
	3.3×10^{-3}		Abraham et al. (1994a)	V	
	3.3×10^{-3}		Mackay et al. (1993)	V	
	3.8×10^{-3}		Yaws (2003)	X	258
	3.8×10^{-3}		Yaws (2003)	X	237
	3.8×10^{-3}	4200	Goldstein (1982)	X	298
	3.8×10^{-3}	3800	Fogg and Sangster (2003)	C	
	3.3×10^{-3}		Dupeux et al. (2022)	Q	259
	1.3×10^{-3}		Keshavarz et al. (2022)	Q	
	1.1×10^{-2}		Duchowicz et al. (2020)	Q	299
	8.7×10^{-3}		Wang et al. (2017)	Q	80, 238
	2.6×10^{-3}		Wang et al. (2017)	Q	80, 239
	7.6×10^{-3}		Wang et al. (2017)	Q	80, 240
	1.6×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	2.6×10^{-3}		Gharagheizi et al. (2010)	Q	246
	3.2×10^{-3}		Hilal et al. (2008)	Q	
	4.4×10^{-3}		Modarresi et al. (2007)	Q	67
		4800	Kühne et al. (2005)	Q	
	3.8×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	3.3×10^{-3}		English and Carroll (2001)	Q	230, 231
	1.2×10^{-4}		Katritzky et al. (1998)	Q	
	3.7×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	3.6×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		3700	Kühne et al. (2005)	?	
	3.8×10^{-3}		Yaws (1999)	?	21
	1.9×10^{-3}		Abraham and Weathersby (1994)	?	21

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.7×10^{-3}		Yaws and Yang (1992)	?	21
			Shiu and Ma (2000)	W	360
(*E*)-1-propenylbenzene C_9H_{10} [873-66-5] QROGIFZRVHSFLM-QHHAFSJGSA-N	2.9×10^{-3}		Hilal et al. (2008)	Q	
1-propenylbenzene C_9H_{10} [637-50-3] QROGIFZRVHSFLM-UHFFFAOYSA-N	3.7×10^{-3}		HSDB (2015)	Q	99
2-propenylbenzene	1.4×10^{-3}		Sato and Nakajima (1979a)	M	14
C_9H_{10}	2.2×10^{-3}		Hilal et al. (2008)	Q	
(allylbenzene)	1.5×10^{-3}		Yaffe et al. (2003)	Q	248, 249
[300-57-2]	2.9×10^{-3}		Nirmalakhandan et al. (1997)	Q	
HJWLCRVIBGQPNF-UHFFFAOYSA-N	1.4×10^{-3}		Abraham and Weathersby (1994)	?	21
1-ethenyl-3-methylbenzene	3.0×10^{-3}		Yaws (2003)	X	237
C_9H_{10}	7.0×10^{-3}		Gharagheizi et al. (2012)	Q	
(*m*-methylstyrene)	3.8×10^{-3}		Gharagheizi et al. (2010)	Q	246
[100-80-1]	3.1×10^{-3}		Hilal et al. (2008)	Q	
JZHGRUMIRATHIU-UHFFFAOYSA-N	1.6×10^{-3}		Modarresi et al. (2007)	Q	67
	3.0×10^{-3}		Yaws (1999)	?	21
	2.6×10^{-3}		Yaws and Yang (1992)	?	21
1-ethenyl-4-methylbenzene	3.1×10^{-3}		Duchowicz et al. (2020)	V	186
C_9H_{10}	3.1×10^{-3}		HSDB (2015)	V	
(*p*-methylstyrene)	3.1×10^{-3}		Yaws (2003)	X	237
[622-97-9]	5.5×10^{-3}		Duchowicz et al. (2020)	Q	
JLBJTVDPSNHSKJ-UHFFFAOYSA-N	7.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.8×10^{-3}		Gharagheizi et al. (2010)	Q	246
	3.4×10^{-3}		Hilal et al. (2008)	Q	
	2.8×10^{-3}		Modarresi et al. (2007)	Q	67
	1.5×10^{-3}		Yao et al. (2002)	Q	229
	3.1×10^{-3}		Yaws (1999)	?	21
	3.5×10^{-3}		Yaws and Yang (1992)	?	21
(1-methylethenyl)-benzene	3.9×10^{-3}		Duchowicz et al. (2020)	V	186
C_9H_{10}	3.8×10^{-3}		HSDB (2015)	V	
(α-methyl styrene)	3.3×10^{-3}		Abraham et al. (1994a)	V	
[98-83-9]	3.6×10^{-3}		Duchowicz et al. (2020)	Q	
XYLMUPLGERFSHI-UHFFFAOYSA-N	2.4×10^{-3}		Hilal et al. (2008)	Q	
	3.9×10^{-3}		English and Carroll (2001)	Q	230, 231

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Table A2.5: Mononuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
phenylacetylene	1.6×10^{-2}		Duchowicz et al. (2020)	V	186
C_8H_6	5.7×10^{-3}		Yaws (2003)	X	237
[536-74-3]	2.2×10^{-2}		Duchowicz et al. (2020)	Q	
UEXCJVNBTNXOEH-UHFFFAOYSA-N	2.0×10^{-2}		Gharagheizi et al. (2012)	Q	
	5.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
	3.9×10^{-3}		Hilal et al. (2008)	Q	
	6.5×10^{-3}		Modarresi et al. (2007)	Q	67
	1.5×10^{-3}		Yaffe et al. (2003)	Q	248, 249
α-methylstyrene dimer	1.1×10^{-2}		HSDB (2015)	Q	99
$C_{18}H_{20}$	5.7×10^{-3}		Zhang et al. (2010)	Q	287, 288
[6144-04-3]	7.2×10^{-3}		Zhang et al. (2010)	Q	287, 289
ATSCZMXECPRPEA-BUHFOSPRSA-N	2.4×10^{-1}		Zhang et al. (2010)	Q	287, 290
	9.0×10^{-2}		Zhang et al. (2010)	Q	287, 291

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A2.6 Terpenes and terpenoids

Table A2.6: Terpenes and terpenoids

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methyl-4-(1-methylethyl)-cyclohexane	5.6×10^{-6}		Duchowicz et al. (2020)	V	186
$C_{10}H_{20}$	5.6×10^{-6}		Copolovici and Niinemets (2005)	V	
(p-menthane)	2.1×10^{-4}		Duchowicz et al. (2020)	Q	
[99-82-1]					
CFJYNSNXFXLKNS-UHFFFAOYSA-N					
α-pinene	7.0×10^{-5}	4700	Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	2.9×10^{-4}	1800	Leng et al. (2013)	M	
[80-56-8]	7.4×10^{-5}	4400	Copolovici and Niinemets (2005)	M	
GRWFGVWFFZKLTI-UHFFFAOYSA-N	5.8×10^{-4}		Karl et al. (2003)	M	87
	1.4×10^{-2}		van Ruth et al. (2002)	M	14
	7.4×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 361
	2.1×10^{-3}		van Ruth et al. (2001)	M	14
	7.0×10^{-5}		Fichan et al. (1999)	M	
	4.7×10^{-5}		Falk et al. (1990)	M	14
	3.4×10^{-5}		Duchowicz et al. (2020)	V	186
	3.4×10^{-5}		HSDB (2015)	V	
	7.4×10^{-5}		Copolovici and Niinemets (2005)	V	
	7.4×10^{-5}		Niinemets and Reichstein (2002)	V	
	2.8×10^{-5}	10000	Li et al. (1998)	V	
	3.5×10^{-5}		Hilal et al. (2008)	C	
	2.2×10^{-4}		Dupeux et al. (2022)	Q	259
	3.0×10^{-4}		Duchowicz et al. (2020)	Q	
	7.6×10^{-4}		Wang et al. (2017)	Q	80, 238
	2.4×10^{-5}		Wang et al. (2017)	Q	80, 239
	5.6×10^{-4}		Wang et al. (2017)	Q	80, 240
	3.1×10^{-5}		Hilal et al. (2008)	Q	
β-pinene	2.1×10^{-4}		Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	1.6×10^{-4}		Helburn et al. (2008)	M	
[127-91-3]	1.5×10^{-4}	4500	Copolovici and Niinemets (2005)	M	
WTARULDDTDQWMU-UHFFFAOYSA-N	4.9×10^{-4}		Karl et al. (2003)	M	87
	4.7×10^{-5}		Falk et al. (1990)	M	14
	1.5×10^{-4}		Copolovici and Niinemets (2005)	V	
	1.5×10^{-4}		Niinemets and Reichstein (2002)	V	
	4.3×10^{-4}		Dupeux et al. (2022)	Q	259
	4.5×10^{-4}		Wang et al. (2017)	Q	80, 238
	3.2×10^{-5}		Wang et al. (2017)	Q	80, 239
	1.1×10^{-3}		Wang et al. (2017)	Q	80, 240
	6.2×10^{-5}		HSDB (2015)	Q	99

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Table A2.6: Terpenes and terpenoids (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methyl-4-(1-methylethyl)-1,3-cyclohexadiene	5.1×10^{-4}		Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	3.8×10^{-4}		Schuhfried et al. (2015)	M	
(α-terpinene)	2.9×10^{-4}	4800	Copolovici and Niinemets (2005)	M	
[99-86-5]	4.5×10^{-4}		Karl et al. (2003)	M	87
YHQGMYUVUMAZJR-UHFFFAOYSA-N	2.8×10^{-4}		Copolovici and Niinemets (2005)	V	
	5.1×10^{-4}		Niinemets and Reichstein (2002)	V	
	5.4×10^{-4}		Dupeux et al. (2022)	Q	259
1-methyl-4-(1-methylethyl)-1,4-cyclohexadiene	5.7×10^{-4}	4300	Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	4.5×10^{-4}		Schuhfried et al. (2015)	M	
(γ-terpinene)	3.8×10^{-4}	4800	Copolovici and Niinemets (2005)	M	
[99-85-4]	4.4×10^{-4}		Duchowicz et al. (2020)	V	186
YKFLAYDHMOASIY-UHFFFAOYSA-N	3.8×10^{-4}		Copolovici and Niinemets (2005)	V	
	2.8×10^{-4}		Niinemets and Reichstein (2002)	V	
	5.4×10^{-4}	8000	Li et al. (1998)	V	
	6.2×10^{-4}		Dupeux et al. (2022)	Q	259
	2.1×10^{-4}		Duchowicz et al. (2020)	Q	
	3.4×10^{-4}		Katritzky et al. (1998)	Q	
1-methyl-4-(1-methylethenyl)-cyclohexene	4.7×10^{-4}	4700	Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	4.8×10^{-4}	4600	Leng et al. (2013)	M	
(limonene)	2.6×10^{-4}		Copolovici and Niinemets (2007)	M	
[138-86-3]	7.0×10^{-4}		Fichan et al. (1999)	M	
XMGQYMWWDOXHJM-UHFFFAOYSA-N	2.4×10^{-4}		Welke et al. (1998)	M	
	7.0×10^{-4}		Falk et al. (1990)	M	14
	3.1×10^{-4}		Duchowicz et al. (2020)	V	186
	3.1×10^{-4}		HSDB (2015)	V	
	3.5×10^{-4}		Copolovici and Niinemets (2005)	V	
	6.4×10^{-4}	3000	van Roon et al. (2005)	V	
	3.5×10^{-4}		Niinemets and Reichstein (2002)	V	
	1.7×10^{-4}	10000	Li et al. (1998)	V	
	7.3×10^{-4}		Dupeux et al. (2022)	Q	259
	6.4×10^{-4}		Duchowicz et al. (2020)	Q	
	5.9×10^{-4}		Wang et al. (2017)	Q	80, 238
	1.1×10^{-4}		Wang et al. (2017)	Q	80, 239
	1.5×10^{-3}		Wang et al. (2017)	Q	80, 240
	1.1×10^{-4}		Hilal et al. (2008)	Q	
	1.9×10^{-4}		Modarresi et al. (2007)	Q	67

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Table A2.6: Terpenes and terpenoids (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(R)-1-methyl-4-(1-methylethenyl)-cyclohexene	3.8×10^{-4}		Schuhfried et al. (2015)	M	
$C_{10}H_{16}$	2.6×10^{-4}		Helburn et al. (2008)	M	
(R-(+)-limonene; D-limonene)	3.5×10^{-4}	4500	Copolovici and Niinemets (2005)	M	
[5989-27-5]	3.8×10^{-4}		Duchowicz et al. (2020)	V	186
XMGQYMWWDOXHJM-SNVBAGLBSA-N	3.9×10^{-4}		HSDB (2015)	V	
	3.8×10^{-4}		Mackay et al. (2006a)	V	
	3.8×10^{-4}		Yaws (2003)	X	258
	3.8×10^{-4}		Yaws (2003)	X	237
	7.3×10^{-4}		Dupeux et al. (2022)	Q	259
	6.4×10^{-4}		Duchowicz et al. (2020)	Q	
	1.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	3.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.9×10^{-4}		Modarresi et al. (2007)	Q	67
	3.8×10^{-4}		Yaws (1999)	?	21
(S)-1-methyl-4-(1-methylethenyl)-cyclohexene	3.7×10^{-4}		Schuhfried et al. (2015)	M	
$C_{10}H_{16}$	3.5×10^{-4}	4400	Copolovici and Niinemets (2005)	M	
(S-(-)-limonene)					
[5989-54-8]					
XMGQYMWWDOXHJM-JTQLQIEISA-N					
3,7,7-trimethyl-bicyclo[4.1.0]hept-3-ene	1.6×10^{-4}		Falk et al. (1990)	M	14
$C_{10}H_{16}$	7.3×10^{-5}		Copolovici and Niinemets (2005)	V	
(3-carene)	7.3×10^{-5}		Niinemets and Reichstein (2002)	V	
[13466-78-9]					
BQOFWKZOCNGFEC-UHFFFAOYSA-N					
7-methyl-3-methylene-1,6-octadiene	4.0×10^{-4}		Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	3.6×10^{-4}		Schuhfried et al. (2015)	M	
(myrcene)	8.7×10^{-4}		Fichan et al. (1999)	M	
[123-35-3]	1.5×10^{-4}		Duchowicz et al. (2020)	V	186
UAHWPYUMFXYFJY-UHFFFAOYSA-N	1.1×10^{-4}		HSDB (2015)	V	
	1.6×10^{-4}		Copolovici and Niinemets (2005)	V	
	7.2×10^{-4}	2800	van Roon et al. (2005)	V	
	1.6×10^{-4}		Niinemets and Reichstein (2002)	V	
	1.3×10^{-4}		Dupeux et al. (2022)	Q	259
	7.1×10^{-4}		Duchowicz et al. (2020)	Q	
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	6.2×10^{-5}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-5}		Raventos-Duran et al. (2010)	Q	245

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Table A2.6: Terpenes and terpenoids (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methyl-4-(1-methylethylidene)- cyclohexene	7.9×10^{-4}	5500	Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	3.8×10^{-4}	5300	Copolovici and Niinemets (2005)	M	
(α-terpinolene)	7.0×10^{-4}		HSDB (2015)	V	
[586-62-9]	3.7×10^{-4}		Copolovici and Niinemets (2005)	V	
MOYAFQVGZZPNRA-UHFFFAOYSA-N	3.8×10^{-4}		Niinemets and Reichstein (2002)	V	
	5.7×10^{-4}	12000	Li et al. (1998)	V	
α-phellandrene	1.8×10^{-4}		Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	1.8×10^{-4}	4500	Copolovici and Niinemets (2005)	M	
[99-83-2]	1.8×10^{-4}		Copolovici and Niinemets (2005)	V	
OGLDWXZKYODSOB-UHFFFAOYSA-N	1.4×10^{-4}		Niinemets and Reichstein (2002)	V	
	5.3×10^{-4}		Dupeux et al. (2022)	Q	259
(R)-(−)-α-phellandrene	3.4×10^{-4}		Schuhfried et al. (2015)	M	
$C_{10}H_{16}$					
[4221-98-1]					
OGLDWXZKYODSOB-SNVBAGLBSA-N					
β-phellandrene	1.8×10^{-4}	5100	Copolovici and Niinemets (2005)	M	
$C_{10}H_{16}$	1.8×10^{-4}		Copolovici and Niinemets (2005)	V	
[555-10-2]	1.8×10^{-4}		Niinemets and Reichstein (2002)	V	
LFJQCDVYDGGFCH-UHFFFAOYSA-N	6.1×10^{-4}		Dupeux et al. (2022)	Q	259
3,7-dimethyl-1,3,6-octatriene	4.0×10^{-4}		Copolovici and Niinemets (2005)	V	
$C_{10}H_{16}$					
(β-ocimene)					
[13877-91-3]					
IHPKGUQCSIINRJ-UHFFFAOYSA-N					
(Z)-3,7-dimethyl-1,3,6-octatriene	4.0×10^{-4}		Niinemets and Reichstein (2002)	V	
$C_{10}H_{16}$					
(*cis*-β-ocimene)					
[3338-55-4]					
IHPKGUQCSIINRJ-NTMALXAHSA-N					
(E)-3,7-dimethyl-1,3,6-octatriene	3.0×10^{-4}		Niinemets and Reichstein (2002)	V	
$C_{10}H_{16}$					
(*trans*-β-ocimene)					
[3779-61-1]					
IHPKGUQCSIINRJ-CSKARUKUSA-N					
2,2-dimethyl-3-methylene- bicyclo[2.2.1]heptane	2.3×10^{-4}		Plyasunov and Shock (2000)	L	
$C_{10}H_{16}$	1.0×10^{-4}		HSDB (2015)	V	
(camphene)	3.1×10^{-4}		Copolovici and Niinemets (2005)	V	
[79-92-5]	6.3×10^{-4}		Niinemets and Reichstein (2002)	V	
CRPUJAZIXJMDBK-UHFFFAOYSA-N					

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Table A2.6: Terpenes and terpenoids (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methylene-1-(1-methylethyl)- bicyclo[3.1.0]hexane $C_{10}H_{16}$ (sabinene) [3387-41-5] NDVASEGYNIMXJL-UHFFFAOYSA-N	1.5×10^{-4} 1.6×10^{-4} 1.6×10^{-4}		Plyasunov and Shock (2000) Copolovici and Niinemets (2005) Niinemets and Reichstein (2002)	L V V	
tricyclo[3.3.1.1(3,7)]decane $C_{10}H_{16}$ (adamantane) [281-23-2] ORILYTVJVMAKLC-UHFFFAOYSA-N	8.0×10^{-4} 1.1×10^{-4}	3400	van Roon et al. (2005) Hilal et al. (2008)	V Q	
β-caryophyllene $C_{15}H_{24}$ [87-44-5] NPNUFJAVOOONJE-IOMPXFEGSA-N	3.7×10^{-4} 2.6×10^{-3} 6.5×10^{-4} 3.4×10^{-5} 1.0×10^{-2}	4500	Copolovici and Niinemets (2015) Dupeux et al. (2022) Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	M Q Q Q Q	 259 80, 238 80, 239 80, 240
α-cedrene $C_{15}H_{24}$ [469-61-4] IRAQOCYXUMOFCW-KYEXWDHISA-N	2.8×10^{-4}	4900	Copolovici and Niinemets (2015)	M	
α-farnesene $C_{15}H_{24}$ [502-61-4] CXENHBSYCFFKJS-VDQVFBMKSA-N	3.4×10^{-4} 8.1×10^{-6}	4300	Copolovici and Niinemets (2015) Schuhfried et al. (2015)	M M	
α-humulene $C_{15}H_{24}$ [6753-98-6] FAMPSKZZVDUYOS-HRGUGZIWSA-N	2.9×10^{-4}	4700	Copolovici and Niinemets (2015)	M	
γ-gurjunene $C_{15}H_{24}$ [22567-17-5] DUYRYUZIBGFLDD-UHFFFAOYSA-N	3.3×10^{-4}	3700	Copolovici and Niinemets (2015)	M	
isosativene $C_{15}H_{24}$ [24959-83-9] CGZBLYYTRIVVTD-UHFFFAOYSA-N	3.9×10^{-4}	3600	Copolovici and Niinemets (2015)	M	
α-longipinene $C_{15}H_{24}$ [5989-08-2] HICYDYJTCDBHMZ-UHFFFAOYSA-N	3.4×10^{-4}	4100	Copolovici and Niinemets (2015)	M	

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Table A2.6: Terpenes and terpenoids (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
α-neoclovene $C_{15}H_{24}$ [4545-68-0] ZCJQJJWNFDNQGZ-UHFFFAOYSA-N	2.9×10^{-4}	3100	Copolovici and Niinemets (2015)	M	
β-neoclovene $C_{15}H_{24}$ [56684-96-9] BUDWHMNUSAOQBI-UHFFFAOYSA-N	2.9×10^{-4}	4600	Copolovici and Niinemets (2015)	M	
γ-neoclovene $C_{15}H_{24}$ ZYKFQRCKKGFKQR-UHFFFAOYSA-N	2.9×10^{-4}	3200	Copolovici and Niinemets (2015)	M	
valencene $C_{15}H_{24}$ [4630-07-3] QEBNYNLSCGVZOH-UHFFFAOYSA-N	3.2×10^{-4}	4500	Copolovici and Niinemets (2015)	M	

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A2.7 Polynuclear aromatics

Table A2.7: Polynuclear aromatics

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bis(1-methylethyl)-1,1'-biphenyl	4.5×10^{-3}		HSDB (2015)	Q	99
$C_{18}H_{22}$	6.4×10^{-3}		Zhang et al. (2010)	Q	287, 288
[36876-13-8]	5.0×10^{-3}		Zhang et al. (2010)	Q	287, 289
NUEUMFZLNOCRCQ-UHFFFAOYSA-N	3.2×10^{-2}		Zhang et al. (2010)	Q	287, 290
	2.0×10^{-2}		Zhang et al. (2010)	Q	287, 291
1,1-bis(3,4-dimethylphenyl)ethane	1.0×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{18}H_{22}$	1.8×10^{-2}		Zhang et al. (2010)	Q	287, 289
[1742-14-9]	6.5×10^{-2}		Zhang et al. (2010)	Q	287, 290
NCSVCMFDHINRJE-UHFFFAOYSA-N	4.8×10^{-3}		Zhang et al. (2010)	Q	287, 291
1-benzyl-2-(2-methylbenzyl)benzene	2.1×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_{21}H_{20}$	2.5×10^{-1}		Zhang et al. (2010)	Q	287, 289
[100404-06-6]	1.4		Zhang et al. (2010)	Q	287, 290
SMOZJCPUZPHHKQ-UHFFFAOYSA-N	4.1×10^{-1}		Zhang et al. (2010)	Q	287, 291
2,5-dibenzyltoluene	2.1×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_{21}H_{20}$	2.9×10^{-1}		Zhang et al. (2010)	Q	287, 289
[56310-11-3]	4.5		Zhang et al. (2010)	Q	287, 290
INLIRICAUXXHSB-UHFFFAOYSA-N	4.1×10^{-1}		Zhang et al. (2010)	Q	287, 291
biphenyl	3.6×10^{-2}	7000	Brockbank (2013)	L	1
$(C_6H_5)_2$	3.6×10^{-2}		Mackay and Shiu (1981)	L	
[92-52-4]	3.4×10^{-2}		Destaillats and Charles (2002)	M	
ZUOUZKKEUPVFJK-UHFFFAOYSA-N			Dewulf et al. (1999)	M	362
	3.2×10^{-2}		Shiu and Mackay (1997)	M	
	5.1×10^{-2}		Fendinger and Glotfelty (1990)	M	
	3.3×10^{-2}		Mackay and Shiu (1981)	M	
	2.4×10^{-2}		Mackay et al. (1979)	M	
	3.5×10^{-2}		Mackay et al. (2006a)	V	
	3.5×10^{-2}		Mackay et al. (2006b)	V	
	3.6×10^{-2}		Shiu and Ma (2000)	V	
	3.5×10^{-2}		Shiu and Mackay (1997)	V	
	3.6×10^{-2}		Abraham et al. (1994a)	V	
	1.9×10^{-2}		Mackay et al. (1992a)	V	
	1.2×10^{-2}		Eastcott et al. (1988)	V	
	1.9×10^{-2}		Shiu and Mackay (1986)	V	
	7.3×10^{-2}		Burkhard et al. (1985)	V	
	2.0×10^{1}	6200	Bopp (1983)	V	
	3.5×10^{-2}		Cabani et al. (1981)	V	
	6.4×10^{-3}		Mackay and Leinonen (1975)	V	
	1.2×10^{-2}		Bohon and Claussen (1951)	V	
	7.6×10^{-3}	2900	Paasivirta et al. (1999)	T	
	1.7×10^{-2}		Yaws (2003)	X	258
	3.9×10^{-2}		Dupeux et al. (2022)	Q	259

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	2.8×10^{-2}		Duchowicz et al. (2020)	Q	299
	4.5×10^{-2}		Schröder et al. (2010)	Q	363
	1.3×10^{-2}		Hilal et al. (2008)	Q	
	5.0×10^{-2}		Modarresi et al. (2007)	Q	67
		5100	Kühne et al. (2005)	Q	
	3.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.5×10^{-2}		English and Carroll (2001)	Q	230, 231
	4.4×10^{-4}		Katritzky et al. (1998)	Q	
	8.0×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	2.9×10^{-2}		Arbuckle (1983)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		6000	Kühne et al. (2005)	?	
	1.2×10^{-2}		Yaws and Yang (1992)	?	21
2-methyl-1,1'-biphenyl $C_{13}H_{12}$ [643-58-3] ALLIZEAXNXSFGD-UHFFFAOYSA-N	2.2×10^{-2}		HSDB (2015)	Q	99
	1.0×10^{-2}		Hilal et al. (2008)	Q	
3-methyl-1,1'-biphenyl $C_{13}H_{12}$ [643-93-6] NPDIDUXTRAITDE-UHFFFAOYSA-N	1.5×10^{-2}		Hilal et al. (2008)	Q	
4-methyl-1,1'-biphenyl $C_{13}H_{12}$ [644-08-6] ZZLCFHIKESPLTH-UHFFFAOYSA-N	1.6×10^{-2}		Hilal et al. (2008)	Q	
diphenylmethane $C_{13}H_{12}$ (1,1'-methylenebisbenzene) [101-81-5] CZZYITDELCSZES-UHFFFAOYSA-N	7.7×10^{-2}		Duchowicz et al. (2020)	V	186
	7.6×10^{-2}		HSDB (2015)	V	
	1.1		Mackay et al. (2006a)	V	
	1.1		Mackay et al. (1993)	V	
	4.5×10^{-2}		Meylan and Howard (1991)	V	
	4.7×10^{-2}		Cabani et al. (1981)	V	
	1.0		Mackay et al. (1992b)	X	364
	4.3×10^{-2}		Yaws (2003)	X	237
	2.1×10^{-2}		Duchowicz et al. (2020)	Q	
	5.7×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.2×10^{-2}		Hilal et al. (2008)	Q	
	1.6×10^{-2}		Modarresi et al. (2007)	Q	67
	2.1×10^{-2}		Meylan and Howard (1991)	Q	
	4.3×10^{-2}		Yaws (1999)	?	21

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-diphenylethane	5.9×10^{-2}		Mackay et al. (2006a)	V	
$C_{14}H_{14}$	5.9×10^{-2}		Mackay et al. (1993)	V	
(dibenzyl)	5.9×10^{-2}		Mackay et al. (1992b)	X	364
[103-29-7]					
QWUWMCYKGHVNAV-UHFFFAOYSA-N					
3-isopropyl-1,1'-biphenyl	5.8×10^{-3}		Ebert et al. (2023)	?	365
$C_{15}H_{16}$					
[20282-30-8]					
LIWRTHVZRZXVFX-UHFFFAOYSA-N					
4-isopropyl-1,1'-biphenyl	4.2×10^{-3}		Ebert et al. (2023)	?	365
$C_{15}H_{16}$					
[7116-95-2]					
KWSHGRJUSUJPQD-UHFFFAOYSA-N					
o-terphenyl	1.6×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{18}H_{14}$	1.6×10^{-1}		HSDB (2015)	V	
[84-15-1]	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
OIAQMFOKAXHPNH-UHFFFAOYSA-N	3.1×10^{-1}		Zhang et al. (2010)	Q	287, 288
	8.2×10^{-2}		Zhang et al. (2010)	Q	287, 289
	7.3×10^{-1}		Zhang et al. (2010)	Q	287, 290
	4.0		Zhang et al. (2010)	Q	287, 291
m-terphenyl	2.8		Duchowicz et al. (2020)	V	186
$C_{18}H_{14}$	2.8		HSDB (2015)	V	
[92-06-8]	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
YJTKZCDBKVTVBY-UHFFFAOYSA-N	1.2		Schröder et al. (2010)	Q	363
p-terphenyl	6.0		Duchowicz et al. (2020)	V	186
$C_{18}H_{14}$			Mackay et al. (2006a)	V	292
[92-94-4]	2.0×10^{-2}		Yaws (2003)	X	237
XJKSTNDFUHDPQJ-UHFFFAOYSA-N	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
	2.9×10^{-1}		HSDB (2015)	Q	99
	3.1×10^{-1}		Zhang et al. (2010)	Q	287, 288
	2.4×10^{-1}		Zhang et al. (2010)	Q	287, 289
	1.1		Zhang et al. (2010)	Q	287, 290
	4.0		Zhang et al. (2010)	Q	287, 291
	2.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
indene	6.2×10^{-3}		HSDB (2015)	Q	99
C_9H_8					
[95-13-6]					
YBYIRNPNPLQARY-UHFFFAOYSA-N					
5-ethylidene-2-norbornene	7.6×10^{-5}		HSDB (2015)	Q	99
C_9H_{12}					
[16219-75-3]					
OJOWICOBYCXEKR-KRXBUXKQSA-N					

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Table A2.7: Polynuclear aromatics (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
indane	4.3×10^{-3}		Plyasunov and Shock (2000)	L	
C_9H_{10}	4.3×10^{-3}		Mackay et al. (2006a)	V	
[496-11-7]	4.7×10^{-3}		Abraham et al. (1994a)	V	
PQNFLJBBNBOBRQ-UHFFFAOYSA-N	4.5×10^{-3}		Yaws (2003)	X	258
	4.5×10^{-3}		Yaws (2003)	X	237
	2.4×10^{-3}		Dupeux et al. (2022)	Q	259
	9.6×10^{-2}		Keshavarz et al. (2022)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	Q	299
	4.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	5.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-3}		Modarresi et al. (2007)	Q	67
	4.8×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	7.2×10^{-3}		English and Carroll (2001)	Q	230, 231
	5.8×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	4.5×10^{-3}		Yaws (1999)	?	21
azulene $C_{10}H_8$ [275-51-4] CUFNKYGDVFVPHO-UHFFFAOYSA-N	1.5×10^{-1}	7800	Hiatt (2013)	M	
naphthalene	2.1×10^{-2}	4400	Schwardt et al. (2021)	L	1
$C_{10}H_8$	2.1×10^{-2}	5400	Brockbank (2013)	L	1
[91-20-3]	2.1×10^{-2}		Ma et al. (2010b)	L	366
UFWIBTONFRDIAS-UHFFFAOYSA-N	2.2×10^{-2}		Ma et al. (2010b)	L	367
	2.2×10^{-2}	5300	Fogg and Sangster (2003)	L	
	2.3×10^{-2}		Mackay and Shiu (1981)	L	
	3.3×10^{-2}	6100	Hiatt (2013)	M	
	6.0×10^{-2}		Lee et al. (2012)	M	
	4.0×10^{-2}		Bobadilla et al. (2003)	M	
	2.4×10^{-2}		Destaillats and Charles (2002)	M	
	1.3×10^{-2}	3600	Dewulf et al. (1999)	M	
	1.8×10^{-2}		Altschuh et al. (1999)	M	
	2.2×10^{-2}		De Maagd et al. (1998)	M	12
	2.2×10^{-2}		Shiu and Mackay (1997)	M	
	1.7×10^{-2}	5100	Kondoh and Nakajima (1997)	M	
	2.3×10^{-2}	5700	Alaee et al. (1996)	M	
	2.1×10^{-2}		Zhang and Pawliszyn (1993)	M	
	1.3×10^{-2}		Fendinger and Glotfelty (1990)	M	
	2.7×10^{-2}		Yurteri et al. (1987)	M	12
	2.6×10^{-2}		Webster et al. (1985)	M	
	2.0×10^{-2}		Mackay et al. (1979)	M	
	1.8×10^{-2}		Southworth (1979)	M	
	2.2×10^{-2}	5400	Schwarz and Wasik (1977)	M	
	2.3×10^{-2}		Mackay et al. (2006a)	V	
	2.3×10^{-2}		Shiu and Ma (2000)	V	

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.2×10^{-2}		De Maagd et al. (1998)	V	12
	2.3×10^{-2}		Shiu and Mackay (1997)	V	
	2.0×10^{-2}		Lide and Frederikse (1995)	V	
	2.3×10^{-2}		Abraham et al. (1994a)	V	
	9.0×10^{-3}		Hwang et al. (1992)	V	
	7.2×10^{-3}		Eastcott et al. (1988)	V	
	2.3×10^{-2}		Cabani et al. (1981)	V	
	2.4×10^{-2}		Hine and Mookerjee (1975)	V	
	8.4×10^{-3}		Mackay and Leinonen (1975)	V	
	2.5×10^{-2}	5100	Wauchope and Haque (1972)	V	
	2.3×10^{-2}	5600	Wauchope and Haque (1972)	V	
	1.9×10^{-2}		Bohon and Claussen (1951)	V	
	1.1×10^{-2}	2100	Paasivirta et al. (1999)	T	
	2.1×10^{-2}		Mackay et al. (1979)	T	
	7.1×10^{-3}		Yaws (2003)	X	258
	2.1×10^{-2}	3600	Goldstein (1982)	X	298
	2.7×10^{-2}		McCarty (1980)	X	368
	2.0×10^{-2}		Smith et al. (1993)	C	
	2.0×10^{-2}		Ryan et al. (1988)	C	
	1.8×10^{-2}		Dupeux et al. (2022)	Q	259
	1.3×10^{-1}		Keshavarz et al. (2022)	Q	
	2.4×10^{-2}		Duchowicz et al. (2020)	Q	184
	1.8×10^{-2}		Parnis et al. (2015)	Q	369
	2.7×10^{-2}		Schröder et al. (2013)	Q	370
	1.5×10^{-2}		Schröder et al. (2010)	Q	363
	2.1×10^{-2}		Hilal et al. (2008)	Q	
	4.0×10^{-2}		Modarresi et al. (2007)	Q	67
		5200	Kühne et al. (2005)	Q	
	2.4×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.1×10^{-2}		English and Carroll (2001)	Q	230, 231
	3.3×10^{-4}		Katritzky et al. (1998)	Q	
	5.6×10^{-2}		Russell et al. (1992)	Q	279
	4.3×10^{-2}		Suzuki et al. (1992)	Q	232
	3.2×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	3.4×10^{-2}		Arbuckle (1983)	Q	
	2.2×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	3.6×10^{-2}		MacBean (2012a)	?	
		5400	Kühne et al. (2005)	?	
	8.0×10^{-3}		Yaws and Yang (1992)	?	21
	2.3×10^{-2}		Abraham et al. (1990)	?	
naphthalene-d8 $C_{10}D_8$ [1146-65-2] UFWIBTONFRDIAS-PGRXLJNUSA-N	3.5×10^{-2}	5300	Hiatt (2013)	M	

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Table A2.7: Polynuclear aromatics (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methylnaphthalene	2.0×10^{-2}	5800	Brockbank (2013)	L	1
$C_{10}H_7CH_3$	2.2×10^{-2}	6100	Fogg and Sangster (2003)	L	
[90-12-0]	2.2×10^{-2}		Mackay and Shiu (1981)	L	
QPUYECUOLPXSFR-UHFFFAOYSA-N	4.4×10^{-2}	5900	Hiatt (2013)	M	
	1.9×10^{-2}		Altschuh et al. (1999)	M	
	2.1×10^{-2}	6100	Bamford et al. (1999a)	M	
	4.1×10^{-2}		Shiu and Mackay (1997)	M	
	1.6×10^{-2}		Fendinger and Glotfelty (1990)	M	
	3.8×10^{-2}		Mackay and Shiu (1981)	M	
	2.8×10^{-2}	4900	Schwarz and Wasik (1977)	M	
	2.2×10^{-2}		Mackay et al. (2006a)	V	
	2.2×10^{-2}		Shiu and Ma (2000)	V	
	2.2×10^{-2}		Shiu and Mackay (1997)	V	
	2.5×10^{-2}		Abraham et al. (1994a)	V	
	2.5×10^{-2}		Eastcott et al. (1988)	V	
	2.2×10^{-2}		Cabani et al. (1981)	V	
	2.2×10^{-2}		Yaws (2003)	X	237
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	Q	
	1.6×10^{-2}		Parnis et al. (2015)	Q	369
	2.3×10^{-2}		Schröder et al. (2013)	Q	370
	1.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.8×10^{-2}		Hilal et al. (2008)	Q	
	3.0×10^{-2}		Modarresi et al. (2007)	Q	67
		5500	Kühne et al. (2005)	Q	
	3.8×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.5×10^{-2}		English and Carroll (2001)	Q	230, 260
	1.2×10^{-3}		Katritzky et al. (1998)	Q	
	2.3×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		5700	Kühne et al. (2005)	?	
	2.2×10^{-2}		Yaws (1999)	?	21
	2.7×10^{-2}		Yaws and Yang (1992)	?	21
1-methylnaphthalene-d10	4.6×10^{-2}	5400	Hiatt (2013)	M	
$C_{10}D_7CD_3$					
[38072-94-5]					
QPUYECUOLPXSFR-UZHHFJDZSA-N					
2-methylnaphthalene	2.0×10^{-2}	5100	Brockbank (2013)	L	1
$C_{10}H_7CH_3$	1.8×10^{-2}	5600	Fogg and Sangster (2003)	L	
[91-57-6]	3.5×10^{-2}	5500	Hiatt (2013)	M	
QIMMUPPBPVKWKM-UHFFFAOYSA-N	1.6×10^{-2}		Altschuh et al. (1999)	M	
	1.9×10^{-2}	5400	Bamford et al. (1999a)	M	
	2.2×10^{-2}		De Maagd et al. (1998)	M	12
	5.0×10^{-5}	1200	Hansen et al. (1993)	M	281
	3.1×10^{-2}		Fendinger and Glotfelty (1990)	M	
	2.0×10^{-2}		Mackay et al. (2006a)	V	

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.6×10^{-2}		De Maagd et al. (1998)	V	12
	2.0×10^{-2}		Shiu and Mackay (1997)	V	
	2.4×10^{-2}		Meylan and Howard (1991)	V	
	2.0×10^{-2}		Eastcott et al. (1988)	V	
	2.4×10^{-2}		Mackay and Shiu (1981)	V	
	2.0×10^{-2}		Mackay et al. (1992b)	X	364
	2.3×10^{-2}		Yaws (2003)	X	237
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	Q	
	1.6×10^{-2}		Parnis et al. (2015)	Q	369
	2.2×10^{-2}		Schröder et al. (2013)	Q	370
	1.6×10^{-2}		Ghargheizi et al. (2010)	Q	246
	2.6×10^{-2}		Hilal et al. (2008)	Q	
	2.4×10^{-2}		Modarresi et al. (2007)	Q	67
		5500	Kühne et al. (2005)	Q	
	2.4×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.2×10^{-3}		Katritzky et al. (1998)	Q	
	1.7×10^{-2}		Meylan and Howard (1991)	Q	
	1.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		5700	Kühne et al. (2005)	?	
	2.3×10^{-2}		Yaws (1999)	?	21
	2.0×10^{-2}		Yaws and Yang (1992)	?	21
			Shiu and Ma (2000)	W	360
1-ethylnaphthalene $C_{10}H_7C_2H_5$ [1127-76-0] ZMXIYERNXPIYFR-UHFFFAOYSA-N	2.0×10^{-2}	5900	Brockbank (2013)	L	1
	2.6×10^{-2}		Mackay and Shiu (1981)	L	
	1.4×10^{-2}		Altschuh et al. (1999)	M	
	2.2×10^{-2}	4800	Schwarz and Wasik (1977)	M	
	2.6×10^{-2}		Mackay et al. (2006a)	V	
	2.7×10^{-2}		Eastcott et al. (1988)	V	
	2.3×10^{-2}		Cabani et al. (1981)	V	
	2.6×10^{-2}		Mackay et al. (1992b)	X	364
	2.0×10^{-2}		Yaws (2003)	X	237
	2.2×10^{-2}		Keshavarz et al. (2022)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	Q	184
	1.9×10^{-2}		Schröder et al. (2013)	Q	370
	1.6×10^{-2}		Ghargheizi et al. (2010)	Q	246
	2.8×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	67
	4.8×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	9.5×10^{-3}		English and Carroll (2001)	Q	230, 231
	2.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.4×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	2.0×10^{-2}		Yaws (1999)	?	21
	2.7×10^{-2}		Yaws and Yang (1992)	?	21

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-ethylnaphthalene	1.2×10^{-2}		Mackay and Shiu (1981)	L	
$C_{10}H_7C_2H_5$	1.8×10^{-2}		Altschuh et al. (1999)	M	
[939-27-5]	1.3×10^{-2}		Mackay et al. (2006a)	V	
RJTJVVYSTUQWNI-UHFFFAOYSA-N	1.6×10^{-2}		Eastcott et al. (1988)	V	
	1.3×10^{-2}		Mackay et al. (1992b)	X	364
	8.8×10^{-3}		Yaws (2003)	X	237
	2.2×10^{-2}		Keshavarz et al. (2022)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	Q	299
	1.9×10^{-2}		Schröder et al. (2013)	Q	370
	3.6×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
	1.9×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	67
	1.2×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.8×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	1.6×10^{-2}		Yaws and Yang (1992)	?	21
1,2,3,4-tetrahydronaphthalene	6.4×10^{-3}	5300	Plyasunov and Shock (2000)	L	
$C_{10}H_{12}$	5.1×10^{-3}	5400	Ashworth et al. (1988)	M	278
(tetralin)	7.3×10^{-3}		Duchowicz et al. (2020)	V	186
[119-64-2]	2.1×10^{-3}		Mackay et al. (1993)	V	
CXWXQJXEFPUFDZ-UHFFFAOYSA-N	5.8×10^{-3}		Yaws (2003)	X	237, 297
	1.2×10^{-2}		Duchowicz et al. (2020)	Q	
	5.8×10^{-3}		HSDB (2015)	Q	99
	3.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	4.3×10^{-3}		Modarresi et al. (2007)	Q	67
		4900	Kühne et al. (2005)	Q	
		5300	Kühne et al. (2005)	?	
	7.2×10^{-3}		Yaws (1999)	?	21, 297
1,2-dimethylnaphthalene	4.8×10^{-2}		Yaws (2003)	X	258
$C_{12}H_{12}$	4.8×10^{-2}		Yaws (2003)	X	237
[573-98-8]	2.6×10^{-2}		Dupeux et al. (2022)	Q	259
QNLZIZAQLLYXTC-UHFFFAOYSA-N	4.2×10^{-2}		Schröder et al. (2013)	Q	370
	1.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
1,3-dimethylnaphthalene	1.7×10^{-2}		Duchowicz et al. (2020)	V	186
$C_{12}H_{12}$	2.6×10^{-2}		Cabani et al. (1981)	V	
[575-41-7]	6.1×10^{-3}		Duchowicz et al. (2020)	Q	
QHJMFSMPSZREIF-UHFFFAOYSA-N	2.0×10^{-2}		Schröder et al. (2013)	Q	370
	2.8×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.9×10^{-2}		Hilal et al. (2008)	Q	
	4.6×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	1.1×10^{-2}		English and Carroll (2001)	Q	230, 231
	1.9×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.4×10^{-2}		Yaws and Yang (1992)	?	21

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Table A2.7: Polynuclear aromatics (. . . continued)

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1,4-dimethylnaphthalene	2.6×10^{-2}		Duchowicz et al. (2020)	V	186
$C_{12}H_{12}$	3.2×10^{-2}		Mackay et al. (2006a)	V	
[571-58-4]	4.7×10^{-2}		Cabani et al. (1981)	V	
APQSQLNWAIULLK-UHFFFAOYSA-N	6.1×10^{-3}		Duchowicz et al. (2020)	Q	
	2.0×10^{-2}		Schröder et al. (2013)	Q	370
	2.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.4×10^{-2}		Hilal et al. (2008)	Q	
	3.7×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	1.9×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.3×10^{-2}		Maniere et al. (2011)	?	165
	2.0×10^{-2}		Yaws and Yang (1992)	?	21
1,5-dimethylnaphthalene	2.8×10^{-2}		Shiu and Mackay (1997)	M	
$C_{12}H_{12}$	1.3×10^{-2}		Yaws (2003)	X	237
[571-61-9]	2.2×10^{-2}		Keshavarz et al. (2022)	Q	
SDDBCEWUYXVGCQ-UHFFFAOYSA-N	6.1×10^{-3}		Duchowicz et al. (2020)	Q	184
	1.4×10^{-2}		Parnis et al. (2015)	Q	369
	2.1×10^{-2}		Schröder et al. (2013)	Q	370
	2.7×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
	3.3×10^{-2}		Hilal et al. (2008)	Q	
	2.4×10^{-2}		Modarresi et al. (2007)	Q	67
	2.9×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.1×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	2.8×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	1.6×10^{-2}		Yaws and Yang (1992)	?	21
1,6-dimethylnaphthalene	2.3×10^{-2}		HSDB (2015)	Q	99
$C_{12}H_{12}$	3.8×10^{-2}		Schröder et al. (2013)	Q	370
[575-43-9]					
CBMXCNPQDUJNHT-UHFFFAOYSA-N					
1,7-dimethylnaphthalene	3.9×10^{-2}		Ebert et al. (2023)	?	371
$C_{12}H_{12}$					
[575-37-1]					
SPUWFVKLHHEKGV-UHFFFAOYSA-N					
1,8-dimethylnaphthalene	2.6×10^{-2}		Schröder et al. (2013)	Q	370
$C_{12}H_{12}$					
[569-41-5]					
XAABPYINPXYOLM-UHFFFAOYSA-N					
2,3-dimethylnaphthalene	1.6×10^{-2}		Mackay et al. (2006a)	V	
$C_{12}H_{12}$	6.4×10^{-2}		Eastcott et al. (1988)	V	
[581-40-8]	4.4×10^{-2}		Cabani et al. (1981)	V	
WWGUMAYGTYQSGA-UHFFFAOYSA-N	1.3×10^{-2}		Yaws (2003)	X	237
	1.1×10^{-2}		Meylan and Howard (1991)	C	
	2.2×10^{-2}		Keshavarz et al. (2022)	Q	
	6.1×10^{-3}		Duchowicz et al. (2020)	Q	299
	2.5×10^{-2}		Schröder et al. (2013)	Q	370

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.0×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
	3.6×10^{-2}		Hilal et al. (2008)	Q	
	2.0×10^{-2}		Modarresi et al. (2007)	Q	67
	4.6×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.3×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.5×10^{-2}		Meylan and Howard (1991)	Q	
	1.1×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	1.7×10^{-2}		Yaws and Yang (1992)	?	21
2,6-dimethylnaphthalene $C_{12}H_{12}$ [581-42-0] YGYNBBAUIYTWBF-UHFFFAOYSA-N	7.8×10^{-3}		Mackay et al. (2006a)	V	
	6.2×10^{-2}		Eastcott et al. (1988)	V	
	3.4×10^{-2}		Cabani et al. (1981)	V	
	2.0×10^{-2}		Schröder et al. (2013)	Q	370
	2.8×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.2×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	67
	3.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.9×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	8.2×10^{-3}		Yaws and Yang (1992)	?	21
2,7-dimethylnaphthalene $C_{12}H_{12}$ [582-16-1] LRQYSMQNJLZKPS-UHFFFAOYSA-N	2.1×10^{-2}		Schröder et al. (2013)	Q	370
acenaphthene $C_{12}H_{10}$ [83-32-9] CWRYPZZKDGJXCA-UHFFFAOYSA-N	5.4×10^{-2}	6500	Schwardt et al. (2021)	L	1
	7.2×10^{-2}	5400	Brockbank (2013)	L	1
	7.2×10^{-2}		Ma et al. (2010b)	L	366
	7.0×10^{-2}		Ma et al. (2010b)	L	367
	5.5×10^{-2}	6500	Fogg and Sangster (2003)	L	
	4.2×10^{-2}		Mackay and Shiu (1981)	L	
	2.6×10^{-1}		Lee et al. (2012)	M	
	5.4×10^{-2}	6600	Bamford et al. (1999a)	M	
	6.2×10^{-2}		Shiu and Mackay (1997)	M	
	1.1×10^{-1}		Zhang and Pawliszyn (1993)	M	
	1.6×10^{-1}		Fendinger and Glotfelty (1990)	M	
	6.4×10^{-3}		Mackay and Shiu (1981)	M	
	4.1×10^{-2}		Warner et al. (1980)	M	
	6.8×10^{-2}		Mackay et al. (1979)	M	
	8.2×10^{-2}		Mackay et al. (2006a)	V	
	8.2×10^{-2}		Shiu and Ma (2000)	V	
	8.2×10^{-2}		Shiu and Mackay (1997)	V	
	1.2×10^{-2}		Hwang et al. (1992)	V	
	9.5×10^{-2}		Eastcott et al. (1988)	V	
	8.2×10^{-2}		Cabani et al. (1981)	V	
	1.2×10^{-1}		Hine and Mookerjee (1975)	V	
	1.2×10^{-1}	6000	Wauchope and Haque (1972)	V	
	3.4×10^{-2}	2900	Paasivirta et al. (1999)	T	

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.1×10^{-2}	2800	Goldstein (1982)	X	298
	5.2×10^{-2}		McCarty (1980)	X	368
	6.4×10^{-2}		HSDB (2015)	C	
	4.1×10^{-2}		Smith et al. (1993)	C	
	4.0×10^{-2}		Ryan et al. (1988)	C	
	4.1×10^{-2}		Shen (1982)	C	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	4.8×10^{-2}		Duchowicz et al. (2020)	Q	
	9.2×10^{-2}		Abraham et al. (2019)	Q	
	3.4×10^{-2}		Parnis et al. (2015)	Q	369
	9.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.9×10^{-2}		Schröder et al. (2010)	Q	363
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	4.4×10^{-2}		Modarresi et al. (2007)	Q	67
		5500	Kühne et al. (2005)	Q	
	6.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	9.9×10^{-2}		Suzuki et al. (1992)	Q	232
	1.1×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	7.9×10^{-2}		Arbuckle (1983)	Q	
	5.4×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		6600	Kühne et al. (2005)	?	
acenaphthylene $C_{12}H_8$ [208-96-8] HXGDTGSAIMULJN-UHFFFAOYSA-N	8.5×10^{-2}	6300	Brockbank (2013)	L	1
	8.2×10^{-2}		Ma et al. (2010b)	L	366
	1.0×10^{-1}		Ma et al. (2010b)	L	367
	9.1×10^{-2}	6700	Fogg and Sangster (2003)	L	
	7.9×10^{-2}	6600	Bamford et al. (1999a)	M	
	8.8×10^{-2}		Fendinger and Glotfelty (1990)	M	
	8.7×10^{-2}		Warner et al. (1980)	M	
	8.7×10^{-1}		HSDB (2015)	V	
	1.2×10^{-1}		Mackay et al. (2006a)	V	
	1.2×10^{-1}		Shiu and Mackay (1997)	V	
	1.2×10^{-1}	5000	Paasivirta et al. (1999)	T	
	8.7×10^{-2}		Smith et al. (1993)	C	
	8.4×10^{-2}		Ryan et al. (1988)	C	
	8.7×10^{-2}		Shen (1982)	C	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	5.7×10^{-2}		Duchowicz et al. (2020)	Q	184
	6.2×10^{-2}		Parnis et al. (2015)	Q	369
	1.1×10^{-1}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	67
		5600	Kühne et al. (2005)	Q	
	8.6×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	8.7×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		6600	Kühne et al. (2005)	?	
			Shiu and Ma (2000)	W	360

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
1,2,4-trimethylnaphthalene $C_{13}H_{14}$ [2717-42-2] JCNGSJUYPCVGAM-UHFFFAOYSA-N	1.3×10^{-2}		Parnis et al. (2015)	Q	369
1,3,7-trimethylnaphthalene $C_{13}H_{14}$ [2131-38-6] HXDVFWJRDVUZFT-UHFFFAOYSA-N	6.0×10^{-2}		Ebert et al. (2023)	?	371
1,3,8-trimethylnaphthalene $C_{13}H_{14}$ [17057-91-9] XYTKCJHHXQVFCK-UHFFFAOYSA-N	6.7×10^{-2}		Ebert et al. (2023)	?	371
1,4,5-trimethylnaphthalene $C_{13}H_{14}$ [2131-41-1] FSAWRQYDMHSDRN-UHFFFAOYSA-N	1.8×10^{-2} 4.3×10^{-2} 2.3×10^{-2}		Mackay et al. (2006a) Eastcott et al. (1988) Schröder et al. (2013)	V V Q	 370
1,4,6-trimethylnaphthalene $C_{13}H_{14}$ [2131-42-2] VGKRZAKNKJAKDN-UHFFFAOYSA-N	4.3×10^{-2}		Ebert et al. (2023)	?	371
2,3,6-trimethylnaphthalene $C_{13}H_{14}$ [829-26-5] UNBZRJCHIWTUHB-UHFFFAOYSA-N	2.8×10^{-2}		Ebert et al. (2023)	?	371
1-(1-methylethyl)naphthalene $C_{13}H_{14}$ (1-isopropylnaphthalene) [6158-45-8] PMPBFICDXLLSRM-UHFFFAOYSA-N	3.3×10^{-2}		Schröder et al. (2013)	Q	370
2-(1-methylethyl)naphthalene $C_{13}H_{14}$ (2-isopropylnaphthalene) [2027-17-0] TVYVQNHYIHAJTD-UHFFFAOYSA-N	1.2×10^{-2} 3.1×10^{-2}		HSDB (2015) Schröder et al. (2013)	Q Q	99 370
2-ethyl-6-methylnaphthalene $C_{13}H_{14}$ [7372-86-3] ZOYUJOHRFWIQTH-UHFFFAOYSA-N	1.2×10^{-2}		Parnis et al. (2015)	Q	369

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-benzindene	1.3×10^{-1}	6100	Brockbank (2013)	L	1
$C_{13}H_{10}$	1.1×10^{-1}		Ma et al. (2010b)	L	366
(fluorene)	1.1×10^{-1}		Ma et al. (2010b)	L	367
[86-73-7]	1.1×10^{-1}	6000	Fogg and Sangster (2003)	L	
NIHNNTQXNPWCJQ-UHFFFAOYSA-N	1.2×10^{-1}		Mackay and Shiu (1981)	L	
	3.2×10^{-1}		Lee et al. (2012)	M	
	1.0×10^{-1}	6200	Bamford et al. (1999a)	M	
	7.9×10^{-2}	7400	Bamford et al. (1999b)	M	
	1.5×10^{-1}		De Maagd et al. (1998)	M	12
	1.0×10^{-1}		Shiu and Mackay (1997)	M	
	1.6×10^{-1}		Fendinger and Glotfelty (1990)	M	
	9.9×10^{-2}		Mackay and Shiu (1981)	M	
	8.4×10^{-2}		Warner et al. (1980)	M	
	1.3×10^{-1}		Mackay et al. (2006a)	V	
	1.3×10^{-1}		Shiu and Ma (2000)	V	
	1.7×10^{-1}		De Maagd et al. (1998)	V	12
	1.3×10^{-1}		Shiu and Mackay (1997)	V	
	1.5×10^{-2}		Hwang et al. (1992)	V	
	1.1×10^{-1}		Eastcott et al. (1988)	V	
	1.3×10^{-1}		Cabani et al. (1981)	V	
	1.3×10^{-1}	6400	Wauchope and Haque (1972)	V	
	2.3×10^{-2}	3700	Paasivirta et al. (1999)	T	
	8.4×10^{-2}	3000	Goldstein (1982)	X	298
	4.7×10^{-2}		McCarty (1980)	X	368
	9.9×10^{-2}		HSDB (2015)	C	
	8.4×10^{-2}		Smith et al. (1993)	C	
	8.4×10^{-2}		Ryan et al. (1988)	C	
	8.4×10^{-2}		Shen (1982)	C	
	3.2×10^{-1}		Keshavarz et al. (2022)	Q	
	5.7×10^{-2}		Duchowicz et al. (2020)	Q	299
	1.1×10^{-1}		Abraham et al. (2019)	Q	
	1.0×10^{-1}		Parnis et al. (2015)	Q	369
	9.0×10^{-2}		Schröder et al. (2010)	Q	363
	9.2×10^{-2}		Hilal et al. (2008)	Q	
	4.1×10^{-2}		Modarresi et al. (2007)	Q	67
		5100	Kühne et al. (2005)	Q	
	1.2×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	5.4×10^{-2}		English and Carroll (2001)	Q	230, 274
	2.0×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		5400	Kühne et al. (2005)	?	
	1.2×10^{-1}		Abraham et al. (1990)	?	
1-methyl-9H-fluorene	1.5×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{14}H_{12}$	2.9×10^{-2}		Duchowicz et al. (2020)	Q	
[1730-37-6]					
GKEUODMJRFDLJY-UHFFFAOYSA-N					

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Table A2.7: Polynuclear aromatics (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-9H-fluorene $C_{14}H_{12}$ [1430-97-3] RKJHJMAZNPASHY-UHFFFAOYSA-N	8.6×10^{-2}		Parnis et al. (2015)	Q	369
9-methyl-9H-fluorene $C_{14}H_{12}$ [2523-37-7] ZVEJRZRAUYJYCO-UHFFFAOYSA-N	9.1×10^{-2}		Parnis et al. (2015)	Q	369
1,2,5,6-tetramethylnaphthalene $C_{14}H_{16}$ [2131-43-3] ONIJFQFZCKJNDH-UHFFFAOYSA-N	1.3×10^{-2}		Parnis et al. (2015)	Q	369
1,4,6,7-tetramethylnaphthalene $C_{14}H_{16}$ [13764-18-6] VPSPONOBLZCLIU-UHFFFAOYSA-N	8.6×10^{-2}		Ebert et al. (2023)	?	371
1-methyl-7-(1-methylethyl)-naphthalene $C_{14}H_{16}$ [490-65-3] UZVVHZJKXPCUQU-UHFFFAOYSA-N	1.2×10^{-2}		Parnis et al. (2015)	Q	369
(E)-stilbene $C_{14}H_{12}$ (*trans*-1,2-diphenylethene) [103-30-0] PJANXHGTPQOBST-VAWYXSNFSA-N	1.4×10^{-2} 1.4×10^{-2} 2.5×10^{-2} 2.5×10^{-2} 2.5×10^{-2} 1.1×10^{-1}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006a) Mackay et al. (1992b) Duchowicz et al. (2020) Abraham et al. (2019)	V V V X Q Q	186 364
phenanthrene $C_{14}H_{10}$ [85-01-8] YNPNZTXNASCQKK-UHFFFAOYSA-N	2.1×10^{-1} 3.4×10^{-1} 2.3×10^{-1} 2.3×10^{-1} 2.3×10^{-1} 2.5×10^{-1} 1.8×10^{-1} 2.7×10^{-1} 2.3×10^{-1} 1.6×10^{-1} 3.4×10^{-1} 2.8×10^{-1} 2.1×10^{-1} 2.5×10^{-1} 4.2×10^{-1} 2.7×10^{-1} 2.5×10^{-1}	4500 7100 4200 7700 6000 7600 3800 	Schwardt et al. (2021) Brockbank (2013) Ma et al. (2010b) Ma et al. (2010b) Fogg and Sangster (2003) Mackay and Shiu (1981) Lee et al. (2012) Odabasi et al. (2006) Bamford et al. (1999a) Bamford et al. (1999b) De Maagd et al. (1998) Shiu and Mackay (1997) Alaee et al. (1996) Zhang and Pawliszyn (1993) Fendinger and Glotfelty (1990) Mackay and Shiu (1981) Mackay et al. (1979)	L L L L L L M M M M M M M M M M M	1 1 366 367 12

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Table A2.7: Polynuclear aromatics (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.8×10^{-1}		Southworth (1979)	M	
	3.1×10^{-1}		Mackay et al. (2006a)	V	
	3.1×10^{-1}		Shiu and Ma (2000)	V	
	3.8×10^{-1}		De Maagd et al. (1998)	V	12
	3.1×10^{-1}		Shiu and Mackay (1997)	V	
	3.2×10^{-2}		Hwang et al. (1992)	V	
	2.8×10^{-1}		Eastcott et al. (1988)	V	
	3.2×10^{-1}		Cabani et al. (1981)	V	
	2.0×10^{-1}		Southworth (1979)	V	
	3.9×10^{-1}		Hine and Mookerjee (1975)	V	
	2.8×10^{-1}	6500	Wauchope and Haque (1972)	V	
	9.3×10^{-2}	4900	Paasivirta et al. (1999)	T	
	9.0×10^{-2}		Yaws (2003)	X	258
	9.0×10^{-2}		Yaws (2003)	X	237
	9.3×10^{-2}	4700	Goldstein (1982)	X	298
	7.6×10^{-2}		McCarty (1980)	X	368
	2.5×10^{-1}		Smith et al. (1993)	C	294
	2.5×10^{-1}		Ryan et al. (1988)	C	
	2.5×10^{-1}		Dupeux et al. (2022)	Q	259
	4.3×10^{-1}		Keshavarz et al. (2022)	Q	
	9.2×10^{-2}		Duchowicz et al. (2020)	Q	184
	2.1×10^{-1}		Parnis et al. (2015)	Q	369
	7.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
	1.7×10^{-1}		Schröder et al. (2010)	Q	363
	2.6×10^{-1}		Hilal et al. (2008)	Q	
	6.4×10^{-1}		Modarresi et al. (2007)	Q	67
		4800	Kühne et al. (2005)	Q	
	2.5×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	9.2×10^{-1}		Suzuki et al. (1992)	Q	232
	4.8×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	2.6×10^{-1}		Arbuckle (1983)	Q	
	2.3×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		5300	Kühne et al. (2005)	?	
	2.7×10^{-1}		Abraham et al. (1990)	?	
9,10-dihydrophenanthrene	1.2×10^{-1}	7500	Reza and Trejo (2004)	M	
$C_{14}H_{12}$	3.2×10^{-1}		Duchowicz et al. (2020)	V	186
[776-35-2]	5.8×10^{-2}		Duchowicz et al. (2020)	Q	
XXPBFNVKTVJZKF-UHFFFAOYSA-N	9.0×10^{-2}		Schröder et al. (2010)	Q	363
	4.1×10^{-2}		Hilal et al. (2008)	Q	
		5400	Kühne et al. (2005)	Q	
		7500	Kühne et al. (2005)	?	

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
anthracene	1.8×10^{-1}	4800	Schwardt et al. (2021)	L	1
$C_{14}H_{10}$	3.3×10^{-1}	6700	Brockbank (2013)	L	1
[120-12-7]	2.0×10^{-1}		Ma et al. (2010b)	L	366
MWPLVEDNUUSJAV-UHFFFAOYSA-N	2.0×10^{-1}		Ma et al. (2010b)	L	367
	1.7×10^{-1}	5700	Fogg and Sangster (2003)	L	
	1.7×10^{-1}		Mackay and Shiu (1981)	L	
	1.6×10^{-1}		Lee et al. (2012)	M	
	2.3×10^{-1}	5600	Reza and Trejo (2004)	M	
	1.8×10^{-1}	6000	Bamford et al. (1999a)	M	
	1.5×10^{-1}	6500	Bamford et al. (1999b)	M	
	1.3×10^{-1}		Shiu and Mackay (1997)	M	
	2.0×10^{-1}	3500	Alaee et al. (1996)	M	
	1.1×10^{-1}		Zhang and Pawliszyn (1993)	M	
	5.1×10^{-1}		Fendinger and Glotfelty (1990)	M	
	2.7×10^{-1}		Webster et al. (1985)	M	
	1.4×10^{-2}		Mackay and Shiu (1981)	M	
	1.5×10^{-1}		Southworth (1979)	M	
	2.5×10^{-1}		Mackay et al. (2006a)	V	
	2.5×10^{-1}		Shiu and Ma (2000)	V	
	2.5×10^{-1}		Shiu and Mackay (1997)	V	
	3.0×10^{-2}		Hwang et al. (1992)	V	
	6.1×10^{-1}		Eastcott et al. (1988)	V	
	5.1×10^{-1}		Cabani et al. (1981)	V	
	3.4×10^{-2}		Southworth (1979)	V	
	5.6×10^{-1}		Hine and Mookerjee (1975)	V	
	2.6×10^{1}	7000	Wauchope and Haque (1972)	V	
	4.6×10^{-3}	3100	Paasivirta et al. (1999)	T	
	3.5×10^{-1}	4000	Goldstein (1982)	X	298
	7.0×10^{-3}		McCarty (1980)	X	368
	1.1×10^{-1}		Smith et al. (1993)	C	
	3.7×10^{-2}		Ryan et al. (1988)	C	
	1.0×10^{-1}		Smith et al. (1981a)	C	
	4.3×10^{-1}		Keshavarz et al. (2022)	Q	
	9.2×10^{-2}		Duchowicz et al. (2020)	Q	
	1.9×10^{-1}		Parnis et al. (2015)	Q	369
	1.5×10^{-1}		Schröder et al. (2010)	Q	363
	3.3×10^{-1}		Hilal et al. (2008)	Q	
	4.5×10^{-1}		Modarresi et al. (2007)	Q	67
		6400	Kühne et al. (2005)	Q	
	1.7×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	7.0×10^{-1}		Russell et al. (1992)	Q	279
	9.0×10^{-1}		Suzuki et al. (1992)	Q	232
	9.0×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.8×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		5100	Kühne et al. (2005)	?	

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
9,10-dihydroanthracene $C_{14}H_{12}$ [613-31-0] WPDAVTSOEQEGMS-UHFFFAOYSA-N	1.5×10^{-1}		Schröder et al. (2010)	Q	363
2,3-dihydro-1,1,3,3,5-pentamethyl-1H-indene	7.5×10^{-4}		Zhang et al. (2010)	Q	287, 288
$C_{14}H_{20}$	1.9×10^{-3}		Zhang et al. (2010)	Q	287, 289
[81-03-8]	2.1×10^{-3}		Zhang et al. (2010)	Q	287, 290
NNXHDILUOAXSPU-UHFFFAOYSA-N	3.9×10^{-4}		Zhang et al. (2010)	Q	287, 291
1-methylanthracene $C_{15}H_{12}$ [610-48-0] KZNJSFHJUQDYHE-UHFFFAOYSA-N	1.7×10^{-1}		Parnis et al. (2015)	Q	369
2-methylanthracene $C_{15}H_{12}$ [613-12-7] GYMFBYTZOGMSQJ-UHFFFAOYSA-N	1.6×10^{-2}		Duchowicz et al. (2020)	V	186
	4.7×10^{-2}		Duchowicz et al. (2020)	Q	
9-methylanthracene	2.5×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{15}H_{12}$	6.1×10^{-1}		Mackay et al. (2006a)	V	
[779-02-2]	9.4×10^{-3}		Eastcott et al. (1988)	V	
CPGPAVAKSZHMBP-UHFFFAOYSA-N	4.7×10^{-2}		Duchowicz et al. (2020)	Q	
	1.9×10^{-1}		Parnis et al. (2015)	Q	369
	4.2×10^{-1}		Hilal et al. (2008)	Q	
9-methyl-phenanthrene $C_{15}H_{12}$ [883-20-5] DALBHIYZSZZWBS-UHFFFAOYSA-N	1.9×10^{-1}		Parnis et al. (2015)	Q	369
9-ethylfluorene $C_{15}H_{14}$ [2294-82-8] QBBCCEYJCKGWIK-UHFFFAOYSA-N	7.4×10^{-2}		Parnis et al. (2015)	Q	369
1,7-dimethylfluorene $C_{15}H_{14}$ [442-66-0] NHPVHXMCRWRSNW-UHFFFAOYSA-N	9.1×10^{-2}		Parnis et al. (2015)	Q	369
1-methylphenanthrene	2.0×10^{-1}	4600	Bamford et al. (1999a)	M	
$C_{15}H_{12}$	5.8×10^{-1}		Keshavarz et al. (2022)	Q	
[832-69-9]	4.7×10^{-2}		Duchowicz et al. (2020)	Q	184
DOWJXOHBNXRUOD-UHFFFAOYSA-N	1.9×10^{-1}		Parnis et al. (2015)	Q	369
	3.3×10^{-1}		Hilal et al. (2008)	Q	
	3.8×10^{-1}		Modarresi et al. (2007)	Q	67
		5200	Kühne et al. (2005)	Q	
	2.0×10^{-1}		Duchowicz et al. (2020)	?	185, 21

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		4600	Kühne et al. (2005)	?	
1,3-diisopropylnaphthalene $C_{16}H_{20}$ [57122-16-4] JDBFIFNXALGSOF-UHFFFAOYSA-N	1.6×10^{-2}		Schröder et al. (2013)	Q	370
1,5-diisopropylnaphthalene $C_{16}H_{20}$ [27351-96-8] GFZWCYSEPXDDRI-UHFFFAOYSA-N	1.6×10^{-2}		Schröder et al. (2013)	Q	370
1,7-diisopropylnaphthalene $C_{16}H_{20}$ [94133-80-9] XNSUVOOWWSAQMZ-UHFFFAOYSA-N	7.8×10^{-3}		Ebert et al. (2023)	?	318
2,6-diisopropylnaphthalene $C_{16}H_{20}$ [24157-81-1] GWLLTEXUIOFAFE-UHFFFAOYSA-N	1.3×10^{-2}		Schröder et al. (2013)	Q	370
2,7-diisopropylnaphthalene $C_{16}H_{20}$ [40458-98-8] YGDMAJYAQCDTNG-UHFFFAOYSA-N	1.3×10^{-2}		Schröder et al. (2013)	Q	370
2-ethylanthracene $C_{16}H_{14}$ [52251-71-5] ZXAGXLDEMUNQSH-UHFFFAOYSA-N	1.9×10^{-1} 4.7×10^{-2}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
1,3-dimethylphenanthrene $C_{16}H_{14}$ [16664-45-2] UJUUQKOWULNFNG-UHFFFAOYSA-N	1.7×10^{-1}		Parnis et al. (2015)	Q	369
3,6-dimethylphenanthrene $C_{16}H_{14}$ [1576-67-6] OMIBPZBOAJFEJS-UHFFFAOYSA-N	1.8×10^{-1}		Parnis et al. (2015)	Q	369
2,3-dimethylanthracene $C_{16}H_{14}$ [613-06-9] OGVRJXPGSVLDRD-UHFFFAOYSA-N	2.1×10^{-1}		Parnis et al. (2015)	Q	369
9,10-dimethylanthracene $C_{16}H_{14}$ [781-43-1] JTGMTYWYUZDRBK-UHFFFAOYSA-N	1.8 3.4×10^{-1} 1.5×10^{-1}		Mackay et al. (2006a) HSDB (2015) Parnis et al. (2015)	V Q Q	 99 369

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
9-propyl-9H-fluorene $C_{16}H_{16}$ [4037-45-0] ZTBWLZNGULENBG-UHFFFAOYSA-N	6.1×10^{-2}		Parnis et al. (2015)	Q	369
pyrene $C_{16}H_{10}$ [129-00-0] BBEAQIROQSPTKN-UHFFFAOYSA-N	5.9×10^{-1}	5500	Schwardt et al. (2021)	L	1
	1.1	6900	Brockbank (2013)	L	1
	7.5×10^{-1}		Ma et al. (2010b)	L	366
	7.5×10^{-1}		Ma et al. (2010b)	L	367
	6.6×10^{-1}	4800	Fogg and Sangster (2003)	L	
	8.3×10^{-1}		Mackay and Shiu (1981)	L	
	4.1×10^{-1}		Lee et al. (2012)	M	
	8.5×10^{-1}	6300	Reza and Trejo (2004)	M	
	2.0		Altschuh et al. (1999)	M	
	5.9×10^{-1}	5500	Bamford et al. (1999a)	M	
	5.0×10^{-1}		De Maagd et al. (1998)	M	12
	1.1		De Maagd et al. (1998)	M	12
	8.3×10^{-1}		Shiu and Mackay (1997)	M	
	9.1×10^{-1}		Mackay and Shiu (1981)	M	
	5.3×10^{-1}		Southworth (1979)	M	
	1.1		Mackay et al. (2006a)	V	
	1.1		Shiu and Ma (2000)	V	
	1.4		De Maagd et al. (1998)	V	12
	1.1		Shiu and Mackay (1997)	V	
	3.6×10^{-2}		Hwang et al. (1992)	V	
	1.1		Eastcott et al. (1988)	V	
	7.6×10^{-1}		Cabani et al. (1981)	V	
	9.4×10^{-1}		Southworth (1979)	V	
	2.2	7600	Wauchope and Haque (1972)	V	
	1.4×10^{-1}	5700	Paasivirta et al. (1999)	T	
	1.9		Smith et al. (1993)	C	372
	1.4×10^{-3}		Ryan et al. (1988)	C	
	7.6		Petrasek et al. (1983)	C	
	7.8×10^{-1}		Keshavarz et al. (2022)	Q	
	3.0×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.3		Abraham et al. (2019)	Q	
	4.7×10^{-1}		Parnis et al. (2015)	Q	369
	3.6×10^{-1}		Schröder et al. (2010)	Q	363
	2.3×10^{-1}		Hilal et al. (2008)	Q	
	2.3		Modarresi et al. (2007)	Q	67
		5200	Kühne et al. (2005)	Q	
	8.4×10^{-1}		English and Carroll (2001)	Q	230, 231
	5.4×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	8.3×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		5500	Kühne et al. (2005)	?	
	9.0×10^{-1}		Abraham et al. (1990)	?	

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Table A2.7: Polynuclear aromatics (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benzo[jk]fluorene	5.8×10^{-1}	5900	Schwardt et al. (2021)	L	1
$C_{16}H_{10}$	7.0×10^{-1}	6900	Brockbank (2013)	L	1
(fluoranthene)	6.9×10^{-1}		Ma et al. (2010b)	L	366
[206-44-0]	7.5×10^{-1}		Ma et al. (2010b)	L	367
GVEPBJHOBDJJJI-UHFFFAOYSA-N	5.4×10^{-1}	4800	Fogg and Sangster (2003)	L	
	4.5×10^{-3}		Mackay and Shiu (1981)	L	
	3.4×10^{-1}		Lee et al. (2012)	M	
	5.1×10^{-1}	4900	Bamford et al. (1999a)	M	
	9.1×10^{-1}		De Maagd et al. (1998)	M	12
	1.1	6900	ten Hulscher et al. (1992)	M	
	1.9	8700	Abou-Naccoul et al. (2014)	V	
	1.0		Mackay et al. (2006a)	V	
	1.0		Shiu and Ma (2000)	V	
	1.4		De Maagd et al. (1998)	V	12
	1.0		Shiu and Mackay (1997)	V	
	2.1		McLachlan et al. (1990)	V	373
	1.1		Eastcott et al. (1988)	V	
	4.0×10^{-1}	5400	Paasivirta et al. (1999)	T	
	1.5		Smith et al. (1993)	C	
	1.0		Ryan et al. (1988)	C	
	9.9×10^{-1}		Petrasek et al. (1983)	C	
	7.8×10^{-1}		Keshavarz et al. (2022)	Q	
	3.0×10^{-1}		Duchowicz et al. (2020)	Q	
	1.1		Abraham et al. (2019)	Q	
	5.8×10^{-1}		Parnis et al. (2015)	Q	369
	4.6×10^{-1}		Schröder et al. (2010)	Q	363
	4.4×10^{-1}		Hilal et al. (2008)	Q	
	2.2×10^{-1}		Modarresi et al. (2007)	Q	67
		5100	Kühne et al. (2005)	Q	
	1.1		Duchowicz et al. (2020)	?	185, 21
		5000	Kühne et al. (2005)	?	
1,2,3,4-tetrahydro-1,1,3,4,4,6-hexamethylnaphthalene	4.2×10^{-4}		Zhang et al. (2010)	Q	287, 288
$C_{16}H_{24}$	1.3×10^{-3}		Zhang et al. (2010)	Q	287, 289
[2084-69-7]	3.2×10^{-3}		Zhang et al. (2010)	Q	287, 290
JIVANURAWUCQIG-UHFFFAOYSA-N	2.7×10^{-4}		Zhang et al. (2010)	Q	287, 291
[2.2]paracyclophane	2.9×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{16}H_{16}$	8.4×10^{-2}		Zhang et al. (2010)	Q	287, 289
[1633-22-3]	9.5×10^{-1}		Zhang et al. (2010)	Q	287, 290
OOLUVSIJOMLOCB-UHFFFAOYSA-N	4.3×10^{-2}		Zhang et al. (2010)	Q	287, 291

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benzo[a]fluorene	3.7×10^{-1}	4400	Bamford et al. (1999a)	M	
$C_{17}H_{12}$	1.1		Keshavarz et al. (2022)	Q	
[238-84-6]	2.2×10^{-1}		Duchowicz et al. (2020)	Q	184
HKMTVMBEALTRRR-UHFFFAOYSA-N	4.6×10^{-1}		Modarresi et al. (2007)	Q	67
		6300	Kühne et al. (2005)	Q	
	3.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		4400	Kühne et al. (2005)	?	
			Shiu and Ma (2000)	W	360
1-methylpyrene	3.1		HSDB (2015)	Q	99
$C_{17}H_{12}$	4.5×10^{-1}		Parnis et al. (2015)	Q	369
[2381-21-7]					
KBSPJIWZDWBDGM-UHFFFAOYSA-N					
2-methylpyrene	3.1		HSDB (2015)	Q	99
$C_{17}H_{12}$					
[3442-78-2]					
VIRFPLJXRDHVEI-UHFFFAOYSA-N					
2-methylfluoranthene	5.4×10^{-1}		Parnis et al. (2015)	Q	369
$C_{17}H_{12}$					
[30997-39-8]					
VVRCMNWZFPMXQZ-UHFFFAOYSA-N					
9-n-propylphenanthrene	1.3×10^{-1}		Parnis et al. (2015)	Q	369
$C_{17}H_{16}$					
[17024-03-2]					
PIWHTUVAMGYSIC-UHFFFAOYSA-N					
1,2,6-trimethylphenanthrene	1.8×10^{-1}		Parnis et al. (2015)	Q	369
$C_{17}H_{16}$					
[30436-55-6]					
MYWOJODOMFBVCB-UHFFFAOYSA-N					
9-butyl-9H-fluorene	5.1×10^{-2}		Parnis et al. (2015)	Q	369
$C_{17}H_{18}$					
[3952-42-9]					
RBDADLSAYYPJAN-UHFFFAOYSA-N					
11H-benzo[b]fluorene	2.5		Duchowicz et al. (2020)	V	186
$C_{17}H_{12}$	2.2×10^{-1}		Duchowicz et al. (2020)	Q	
[243-17-4]					
HAPOJKSPCGLOOD-UHFFFAOYSA-N					
2,7-dimethylpyrene	2.9		HSDB (2015)	Q	99
$C_{18}H_{14}$	3.9×10^{-1}		Parnis et al. (2015)	Q	369
[15679-24-0]					
GSKHIRFMTJUBSM-UHFFFAOYSA-N					

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Table A2.7: Polynuclear aromatics (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chrysene	1.5×10^{1}	12000	Brockbank (2013)	L	1
$C_{18}H_{12}$	2.3		Ma et al. (2010b)	L	366
[218-01-9]	2.7		Ma et al. (2010b)	L	367
WDECIBYCCFPHNR-UHFFFAOYSA-N	2.1		Lee et al. (2012)	M	
	1.9	13000	Bamford et al. (1999a)	M	
	9.4		Zhang and Pawliszyn (1993)	M	
	1.0×10^{1}		HSDB (2015)	V	
	1.5×10^{1}		Mackay et al. (2006a)	V	
	1.5×10^{1}		Shiu and Ma (2000)	V	
	2.2		Eastcott et al. (1988)	V	
	2.0×10^{-1}	6400	Paasivirta et al. (1999)	T	
	9.4		Smith et al. (1993)	C	
	4.6×10^{-3}		Ryan et al. (1988)	C	
	6.6		Petrasek et al. (1983)	C	
	1.4		Keshavarz et al. (2022)	Q	
	3.6×10^{-1}		Duchowicz et al. (2020)	Q	299
	2.4		Parnis et al. (2015)	Q	369
	2.0		Schröder et al. (2010)	Q	363
	3.6		Hilal et al. (2008)	Q	
	5.0		Modarresi et al. (2007)	Q	67
	1.9		Duchowicz et al. (2020)	?	185, 21
naphthacene	2.0×10^{1}		Duchowicz et al. (2020)	V	186
$C_{18}H_{12}$	3.6×10^{2}		Mackay et al. (2006a)	V	
(2,3-benzanthracene)	2.5×10^{2}		Mackay et al. (1992b)	X	364
[92-24-0]	3.6×10^{-1}		Duchowicz et al. (2020)	Q	
IFLREYGFSNHWGE-UHFFFAOYSA-N	4.2		Ferreira (2001)	Q	12
triphenylene	6.4×10^{1}		Duchowicz et al. (2020)	V	186
$C_{18}H_{12}$			Mackay et al. (2006a)	V	292
(benzo[l]phenanthrene)	1.0×10^{2}		Mackay et al. (1992b)	X	364
[217-59-4]	3.6×10^{-1}		Duchowicz et al. (2020)	Q	
SLGBZMMZGDRARJ-UHFFFAOYSA-N	8.6		Schröder et al. (2010)	Q	363
	2.9		Hilal et al. (2008)	Q	
	4.7		Modarresi et al. (2007)	Q	67
	3.1		Ferreira (2001)	Q	12
benz[a]anthracene	1.4		Ma et al. (2010b)	L	366
$C_{18}H_{12}$	1.6		Ma et al. (2010b)	L	367
[56-55-3]	9.0×10^{-1}	7900	Fogg and Sangster (2003)	L	
DXBHBZVCASKNBY-UHFFFAOYSA-N	1.7		Lee et al. (2012)	M	
	8.2×10^{-1}	8300	Bamford et al. (1999a)	M	
	9.9		Zhang and Pawliszyn (1993)	M	
	1.2		Southworth (1979)	M	
	1.7		Mackay et al. (2006a)	V	
	2.4		Eastcott et al. (1988)	V	
	7.5×10^{1}		Smith and Bomberger (1980)	V	24
	4.0		Southworth (1979)	V	
	1.5×10^{-1}	6100	Paasivirta et al. (1999)	T	

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.5		Smith et al. (1993)	C	79
	9.8		Ryan et al. (1988)	C	
	8.2×10^{1}		Petrasek et al. (1983)	C	
	1.4		Keshavarz et al. (2022)	Q	
	3.6×10^{-1}		Duchowicz et al. (2020)	Q	
	2.2		Parnis et al. (2015)	Q	369
	1.6		Schröder et al. (2010)	Q	363
	4.4		Hilal et al. (2008)	Q	
	5.0		Modarresi et al. (2007)	Q	67
		6100	Kühne et al. (2005)	Q	
	5.6		Ferreira (2001)	Q	12
	8.2×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		8300	Kühne et al. (2005)	?	
			Shiu and Ma (2000)	W	360
4,5-dimethylpyrene $C_{18}H_{14}$ [15679-25-1] MCZKPUHBCIHFBZ-UHFFFAOYSA-N	4.5×10^{-1}		Parnis et al. (2015)	Q	369
3-ethylfluoranthene $C_{18}H_{14}$ [20496-16-6] JXUOLJXLPIIRTP-UHFFFAOYSA-N	4.8×10^{-1}		Parnis et al. (2015)	Q	369
1,2,6,9-tetramethylphenanthrene $C_{18}H_{18}$ [204256-39-3] XFJWRZAPBOJONX-UHFFFAOYSA-N	1.6×10^{-1}		Parnis et al. (2015)	Q	369
1,9-dimethyl-5-ethylphenanthrene $C_{18}H_{18}$ MDZYWNWRMJIOPN-UHFFFAOYSA-N	1.0×10^{-1}		Parnis et al. (2015)	Q	369
1,9-dimethyl-7-ethylphenanthrene $C_{18}H_{18}$ NFFCDFHAMXFVEK-UHFFFAOYSA-N	1.4×10^{-1}		Parnis et al. (2015)	Q	369
1,2,3,4-tetrahydro-5-(1-phenylethyl)-naphthalene	1.6×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{18}H_{20}$	1.0×10^{-1}		Zhang et al. (2010)	Q	287, 289
[60466-61-7]	2.0×10^{-1}		Zhang et al. (2010)	Q	287, 290
TXOHWLOHKUPUKO-UHFFFAOYSA-N	2.9×10^{-2}		Zhang et al. (2010)	Q	287, 291
4-methylchrysene $C_{19}H_{14}$ [3351-30-2] BLVHWJCLSMYFMT-UHFFFAOYSA-N	1.9		Parnis et al. (2015)	Q	369

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5-methylchrysene $C_{19}H_{14}$ [3697-24-3] GOHBXWHNJHENRX-UHFFFAOYSA-N	5.2		HSDB (2015)	Q	99
6-methylchrysene $C_{19}H_{14}$ [1705-85-7] ASVDRLYVNFOSCI-UHFFFAOYSA-N	2.2		Parnis et al. (2015)	Q	369
1-propylpyrene $C_{19}H_{16}$ [42211-33-6] HIOZPFGGCXEPAP-UHFFFAOYSA-N	3.2×10^{-1}		Parnis et al. (2015)	Q	369
7-methylbenz[a]anthracene $C_{19}H_{14}$ [2541-69-7] DIIFUCUPDHMNIV-UHFFFAOYSA-N	5.2		HSDB (2015)	Q	99
10-methylbenz[a]anthracene $C_{19}H_{14}$ [2381-15-9] WUMGYHICFXGLAB-UHFFFAOYSA-N	5.2		HSDB (2015)	Q	99
12-methylbenz[a]anthracene $C_{19}H_{14}$ [2422-79-9] ACYOLKMEHHTLAB-UHFFFAOYSA-N	5.2		HSDB (2015)	Q	99
6-ethylchrysene $C_{20}H_{16}$ [2732-58-3] ZJSYTTGSPQNXKT-UHFFFAOYSA-N	1.8		Parnis et al. (2015)	Q	369
3,9-dimethylbenz[a]anthracene $C_{20}H_{16}$ [316-51-8] DBPDWIZRMPUWRH-UHFFFAOYSA-N	1.9		Parnis et al. (2015)	Q	369
1-butylpyrene $C_{20}H_{18}$ [35980-18-8] UFOTZLIYHMGVAV-UHFFFAOYSA-N	2.8×10^{-1}		Parnis et al. (2015)	Q	369
7,12-dimethyl-benz[a]anthracene $C_{20}H_{16}$ [57-97-6] ARSRBNBHOADGJU-UHFFFAOYSA-N	2.6 5.1×10^{3} 9.2×10^{-2} 4.9 1.5		Duchowicz et al. (2020) Mackay et al. (2006a) Duchowicz et al. (2020) HSDB (2015) Parnis et al. (2015)	V V Q Q Q	186 99 369

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
9,10-dimethyl-benz[a]anthracene $C_{20}H_{16}$ [58429-99-5] GKVUDAZMZLMNJQ-UHFFFAOYSA-N			Mackay et al. (2006a)	V	292
benzo[b]fluoranthene	1.5×10^{1}	5400	Brockbank (2013)	L	1
$C_{20}H_{12}$	1.5×10^{1}		Ma et al. (2010b)	L	366
[205-99-2]	1.5×10^{1}		Ma et al. (2010b)	L	367
FTOVXSOBNPWTSH-UHFFFAOYSA-N	1.5×10^{1}	5400	ten Hulscher et al. (1992)	M	
	1.4×10^{1}	7500	Paasivirta et al. (1999)	T	
	8.3×10^{-1}		Smith et al. (1993)	C	
	1.4		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	184
	6.0		Parnis et al. (2015)	Q	369
	5.6		Hilal et al. (2008)	Q	
	2.1		Modarresi et al. (2007)	Q	67
		4700	Kühne et al. (2005)	Q	
	2.0×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.5×10^{1}		Duchowicz et al. (2020)	?	185, 21
		5400	Kühne et al. (2005)	?	
benzo[k]fluoranthene	1.7×10^{1}		Ma et al. (2010b)	L	366
$C_{20}H_{12}$	1.8×10^{1}		Ma et al. (2010b)	L	367
[207-08-9]	1.0×10^{1}		Lee et al. (2012)	M	
HAXBIWFMXWRORI-UHFFFAOYSA-N	1.7×10^{1}	5900	ten Hulscher et al. (1992)	M	
			Mackay et al. (2006a)	V	292
	8.3×10^{1}		De Maagd et al. (1998)	V	12
	6.2×10^{1}		Shiu and Mackay (1997)	V	
	1.5	6900	Paasivirta et al. (1999)	T	
	9.6×10^{-3}	1900	Goldstein (1982)	X	298
	2.5×10^{-1}		Smith et al. (1993)	C	
	2.6		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	299
	5.9		Parnis et al. (2015)	Q	369
	8.0		Hilal et al. (2008)	Q	
	2.4		Modarresi et al. (2007)	Q	67
		6300	Kühne et al. (2005)	Q	
	2.0×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	1.7×10^{1}		Duchowicz et al. (2020)	?	185, 21
		5800	Kühne et al. (2005)	?	
benzo[a]pyrene	4.5	8500	Brockbank (2013)	L	1
$C_{20}H_{12}$	2.0×10^{1}		Ma et al. (2010b)	L	366
(benz[a]pyrene)	1.3×10^{1}		Ma et al. (2010b)	L	367
[50-32-8]	6.2		Lee et al. (2012)	M	
FMMWHPNWAFZXNH-UHFFFAOYSA-N	1.3×10^{1}		Altschuh et al. (1999)	M	
	2.2×10^{1}	4700	ten Hulscher et al. (1992)	M	
	2.2×10^{1}		Mackay et al. (2006a)	V	
	2.9×10^{1}		De Maagd et al. (1998)	V	12

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Table A2.7: Polynuclear aromatics (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{1}		Shiu and Mackay (1997)	V	
	1.3×10^{2}		McLachlan et al. (1990)	V	373
	1.8×10^{1}		Eastcott et al. (1988)	V	
	7.5		Smith and Bomberger (1980)	V	24
	1.9×10^{1}		Southworth (1979)	V	
	8.2×10^{-1}	8200	Paasivirta et al. (1999)	T	
	1.6×10^{-3}	110	Goldstein (1982)	X	298
	2.0×10^{1}		Smith et al. (1993)	C	
	8.2×10^{-4}		Ryan et al. (1988)	C	
	2.6		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	299
	5.1		Parnis et al. (2015)	Q	369
	2.9		Hilal et al. (2008)	Q	
	1.5×10^{1}		Modarresi et al. (2007)	Q	67
		4900	Kühne et al. (2005)	Q	
	2.9×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.2×10^{1}		Duchowicz et al. (2020)	?	185, 21
		4700	Kühne et al. (2005)	?	
			Shiu and Ma (2000)	W	360
benzo[e]pyrene	3.3×10^{1}		Duchowicz et al. (2020)	V	186
$C_{20}H_{12}$	3.3×10^{1}		HSDB (2015)	V	
[192-97-2]	2.1×10^{1}		Mackay et al. (2006a)	V	
TXVHTIQJNYSSKO-UHFFFAOYSA-N	2.7	8300	Paasivirta et al. (1999)	T	
	1.2		Duchowicz et al. (2020)	Q	
	1.5×10^{1}		Ferreira (2001)	Q	12
			Shiu and Ma (2000)	W	360
perylene	2.7		Duchowicz et al. (2020)	V	186
$C_{20}H_{12}$			Mackay et al. (2006a)	V	292
(dibenz[de,kl]anthracene)	2.3		Riederer (1990)	V	
[198-55-0]	2.5×10^{-1}	6300	Paasivirta et al. (1999)	T	
CSHWQDPOILHKBI-UHFFFAOYSA-N	3.3×10^{2}		Mackay et al. (1992b)	X	364
	1.2		Duchowicz et al. (2020)	Q	
	5.7		Parnis et al. (2015)	Q	369
	2.3		Hilal et al. (2008)	Q	
	1.1×10^{1}		Ferreira (2001)	Q	12
1,2-benzfluoranthene	6.9		Hilal et al. (2008)	Q	
$C_{20}H_{12}$					
[203-33-8]					
OQDXASJSCOTNQS-UHFFFAOYSA-N					
benzo[j]fluoranthene	4.9×10^{1}		HSDB (2015)	Q	99
$C_{20}H_{12}$					
[205-82-3]					
KHNYNFUTFKJLDD-UHFFFAOYSA-N					

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3,6-trimethylchrysene $C_{21}H_{18}$ [1586755-28-3] UGLPREDFUVNEMJ-UHFFFAOYSA-N	1.8		Parnis et al. (2015)	Q	369
6-propylchrysene $C_{21}H_{18}$ [6910-41-4] PGBSMHMYMMBHFF-UHFFFAOYSA-N	1.5		Parnis et al. (2015)	Q	369
20-methylcholanthrene	1.9		Duchowicz et al. (2020)	V	186
$C_{21}H_{16}$	1.9		HSDB (2015)	V	
[56-49-5]			Mackay et al. (2006a)	V	292
PPQNQXQZIWHJRB-UHFFFAOYSA-N	3.7×10^{-1}		Duchowicz et al. (2020)	Q	
6-butylchrysene $C_{22}H_{20}$ [6901-71-9] XJQKMLMKECCWEO-UHFFFAOYSA-N	1.3		Parnis et al. (2015)	Q	369
dibenz[a,h]anthracene	7.0×10^{1}		Duchowicz et al. (2020)	V	186
$C_{22}H_{14}$	1.8×10^{2}	12000	Abou-Naccoul et al. (2014)	V	
[53-70-3]	5.8×10^{3}		Mackay et al. (2006a)	V	
LHRCREOYAASXPZ-UHFFFAOYSA-N	1.3×10^{2}		Eastcott et al. (1988)	V	
	1.2	7800	Paasivirta et al. (1999)	T	
	1.4×10^{2}		Smith et al. (1993)	C	
	1.4		Duchowicz et al. (2020)	Q	
	1.4×10^{2}		HSDB (2015)	Q	99
	2.6×10^{1}		Parnis et al. (2015)	Q	369
	1.2×10^{1}		Hilal et al. (2008)	Q	
	8.3×10^{1}		Ferreira (2001)	Q	12
indeno[1,2,3-cd]pyrene	2.9×10^{1}		Ma et al. (2010b)	L	366
$C_{22}H_{12}$	2.0×10^{1}		Ma et al. (2010b)	L	367
[193-39-5]	2.8×10^{1}	3600	ten Hulscher et al. (1992)	M	
SXQBHARYMNFBPS-UHFFFAOYSA-N	2.5	7400	Paasivirta et al. (1999)	T	
	1.4×10^{2}		Smith et al. (1993)	C	
	4.7		Keshavarz et al. (2022)	Q	
	3.7		Duchowicz et al. (2020)	Q	184
	1.3×10^{1}		Parnis et al. (2015)	Q	369
	5.0		Hilal et al. (2008)	Q	
	9.4		Modarresi et al. (2007)	Q	67
		5100	Kühne et al. (2005)	Q	
	2.8×10^{1}		Duchowicz et al. (2020)	?	185, 21
		3600	Kühne et al. (2005)	?	

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
benzo[ghi]perylene	3.0×10^{1}		Ma et al. (2010b)	L	366
$C_{22}H_{12}$	2.4×10^{1}		Ma et al. (2010b)	L	367
[191-24-2]	3.0×10^{1}	3200	ten Hulscher et al. (1992)	M	
GYFAGKUZYNFMBN-UHFFFAOYSA-N	1.8×10^{1}		De Maagd et al. (1998)	V	12
	1.3×10^{1}		Shiu and Mackay (1997)	V	
	6.9×10^{1}		Eastcott et al. (1988)	V	
	4.0	9200	Paasivirta et al. (1999)	T	
	1.3×10^{1}		Mackay et al. (1992b)	X	364
	1.8×10^{2}		Smith et al. (1993)	C	
	4.7		Keshavarz et al. (2022)	Q	
	3.7		Duchowicz et al. (2020)	Q	
	1.1×10^{1}		Parnis et al. (2015)	Q	369
	2.6		Hilal et al. (2008)	Q	
	6.1×10^{1}		Modarresi et al. (2007)	Q	67
		3700	Kühne et al. (2005)	Q	
	3.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	3.0×10^{1}		Duchowicz et al. (2020)	?	185, 21
		3300	Kühne et al. (2005)	?	
benzo[b]triphenylene	1.9×10^{1}	8600	Abou-Naccoul et al. (2014)	V	
$C_{22}H_{14}$	4.4×10^{3}		Mackay et al. (2006a)	V	
(dibenz[a,c]anthracene)	1.9×10^{1}		Hilal et al. (2008)	Q	
[215-58-7]	1.4×10^{2}		Ferreira (2001)	Q	12
RAASUWZPTOJQAY-UHFFFAOYSA-N					
dibenz[a,j]anthracene	8.6×10^{1}		Hilal et al. (2008)	Q	
$C_{22}H_{14}$	8.3×10^{1}		Ferreira (2001)	Q	12
[224-41-9]					
KLIHYVJAYWCEDM-UHFFFAOYSA-N					
picene	6.2		Hilal et al. (2008)	Q	
$C_{22}H_{14}$	7.7×10^{1}		Ferreira (2001)	Q	12
[213-46-7]					
GBROPGWFBFCKAG-UHFFFAOYSA-N					
benzo[c]chrysene	8.0×10^{1}		HSDB (2015)	Q	99
$C_{22}H_{14}$					
[194-69-4]					
YZWGEMSQAMDWEM-UHFFFAOYSA-N					
benzo[g]chrysene	8.0×10^{1}		HSDB (2015)	Q	99
$C_{22}H_{14}$					
[196-78-1]					
JZOIZKBKSZMVRV-UHFFFAOYSA-N					
dibenzo[a,e]pyrene	7.0×10^{2}		HSDB (2015)	Q	99
$C_{24}H_{14}$					
[192-65-4]					
KGHMWBNEMFNJFZ-UHFFFAOYSA-N					

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Table A2.7: Polynuclear aromatics (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dibenzo[a,h]pyrene $C_{24}H_{14}$ [189-64-0] RXUSYFJGDZFVND-UHFFFAOYSA-N	7.0×10^2		HSDB (2015)	Q	99
dibenzo[a,i]pyrene $C_{24}H_{14}$ [189-55-9] TUGYIJVAYAHHHM-UHFFFAOYSA-N	7.0×10^2		HSDB (2015)	Q	99
coronene $C_{24}H_{12}$ [191-07-1] VPUGDVKSAQVFFS-UHFFFAOYSA-N			Mackay et al. (2006a)	V	292
dibenz[a,e]aceanthrylene $C_{24}H_{14}$ [5385-75-1] JHOWUOKQHJHGMU-UHFFFAOYSA-N	7.0×10^2		HSDB (2015)	Q	99
dibenzo[b,k]chrysene $C_{26}H_{16}$ [217-54-9] DHCSBRKYHMINPB-UHFFFAOYSA-N	1.2×10^3		HSDB (2015)	Q	99

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A3 Organic species with oxygen (O)

A3.1 Carbon oxides

Table A3.1: Carbon oxides

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
carbon monoxide	9.7×10^{-6}	1300	Burkholder et al. (2019)	L	1
CO	8.0×10^{-6}	1400	Burkholder et al. (2019)	L	70
[630-08-0]	9.7×10^{-6}	1300	Burkholder et al. (2015)	L	1
UGFAIRIUMAVXCW-UHFFFAOYSA-N	8.0×10^{-6}	1400	Burkholder et al. (2015)	L	70
	9.7×10^{-6}	1300	Warneck and Williams (2012)	L	
	9.7×10^{-6}	1300	Sander et al. (2011)	L	1
	9.7×10^{-6}	1300	Sander et al. (2006)	L	1
	9.7×10^{-6}	1300	Fernández-Prini et al. (2003)	L	3
			Cargill (1990)	L	374
	9.4×10^{-6}	1300	Wilhelm et al. (1977)	L	
	9.7×10^{-6}	1300	Rettich et al. (1982)	M	375
	7.0×10^{-6}	1500	Schmidt (1979)	M	33, 34
	7.9×10^{-5}		Meadows and Spedding (1974)	M	
	8.3×10^{-6}		Power and Stegall (1970)	M	14
	7.9×10^{-6}	1200	Douglas (1967)	M	376, 377
	9.4×10^{-6}	1300	Winkler (1901)	M	378
	9.5×10^{-6}	1200	Bunsen (1855a)	M	43
	6.0×10^{-6}		Pierotti (1965)	T	
	1.0×10^{-5}		Hayer et al. (2022)	Q	20
	8.7×10^{-6}		Yaws (1999)	?	21
	9.4×10^{-6}	1300	Yaws et al. (1999)	?	21
	8.4×10^{-6}		Abraham and Weathersby (1994)	?	21
	9.4×10^{-6}	1400	Dean and Lange (1999)	?	379, 23
	8.6×10^{-6}		Yaws and Yang (1992)	?	21
carbon dioxide	3.4×10^{-4}	2300	Burkholder et al. (2019)	L	1
CO_2	2.8×10^{-4}	2600	Burkholder et al. (2019)	L	70
[124-38-9]	3.4×10^{-4}	2300	Burkholder et al. (2015)	L	1
CURLTUGMZLYLDI-UHFFFAOYSA-N	2.8×10^{-4}	2600	Burkholder et al. (2015)	L	70
	3.3×10^{-4}	2400	Sander et al. (2011)	L	1
	3.3×10^{-4}	2400	Sander et al. (2006)	L	1
	3.3×10^{-4}	2300	Fernández-Prini et al. (2003)	L	3
	3.4×10^{-4}	2300	Carroll et al. (1991)	L	
	3.4×10^{-4}	2400	Crovetto (1991)	L	
	3.4×10^{-4}	2300	Yoo et al. (1986)	L	1
	3.4×10^{-4}	2400	Edwards et al. (1978)	L	1
	3.3×10^{-4}	2400	Wilhelm et al. (1977)	L	
	3.4×10^{-4}	2400	Weiss (1974)	L	1
	3.4×10^{-4}	2300	Zheng et al. (1997)	M	380
	3.3×10^{-4}	2400	Murray and Riley (1971)	M	381
	2.4×10^{-4}		Power and Stegall (1970)	M	14
	3.3×10^{-4}	2400	Morrison and Billett (1952)	M	382
	3.3×10^{-4}		Orcutt and Seevers (1937a)	M	

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Table A3.1: Carbon oxides (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	3.3×10^{-4}	2300	Kunerth (1922)	M	
	3.3×10^{-4}	2500	Geffcken (1904)	M	
	3.4×10^{-4}	2400	Bohr (1899)	M	383
	3.4×10^{-4}	2500	Bunsen (1855a)	M	43
	6.5×10^{-4}		Duchowicz et al. (2020)	V	186
	3.4×10^{-4}	2400	Chen et al. (1979)	R	1
	3.1×10^{-4}	2400	Chameides (1984)	T	
	3.3×10^{-4}	2400	Edwards et al. (1975)	T	1
	3.4×10^{-4}		Perry and Chilton (1973)	X	29
	3.4×10^{-4}	2400	Lelieveld and Crutzen (1991)	C	
	3.4×10^{-4}	2400	Pandis and Seinfeld (1989)	C	
	3.9×10^{-4}		Nunn (1958)	C	12
	2.3×10^{-4}		Hayer et al. (2022)	Q	20
	4.0		Duchowicz et al. (2020)	Q	
		2900	Kühne et al. (2005)	Q	
			Scharlin (1996)	E	1, 384
		2400	Kühne et al. (2005)	?	
	4.5×10^{-4}		Yaws (1999)	?	21
	3.3×10^{-4}	2400	Yaws et al. (1999)	?	21
	2.6×10^{-4}		Abraham and Weathersby (1994)	?	21
	3.3×10^{-4}	2400	Dean and Lange (1999)	?	385, 23
	4.5×10^{-4}		Yaws and Yang (1992)	?	21
	3.4×10^{-4}	2400	Seinfeld (1986)	?	21
	3.3×10^{-4}	2400	Hoffmann and Jacob (1984)	?	21
carbon suboxide C_3O_2 [504-64-3] GNEVIACKFGQMHB-UHFFFAOYSA-N	1.1×10^{-2}		Keßel et al. (2017)	M	386

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A3.2 Alcohols (ROH)

Table A3.2: Alcohols (ROH)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methanol	2.0	5500	Burkholder et al. (2019)	L	1
CH_3OH	2.0	5500	Burkholder et al. (2015)	L	1
[67-56-1]	2.0	5400	Brockbank (2013)	L	1
OKKJLVBELUTLKV-UHFFFAOYSA-N	2.0	5600	Sander et al. (2011)	L	387, 1
	2.1	5300	Warneck (2006)	L	
	2.2	5200	Sander et al. (2006)	L	
	2.0	5500	Dohnal et al. (2006)	L	1
	1.7	4500	Fogg and Sangster (2003)	L	
	2.1	5400	Plyasunov and Shock (2000)	L	
	3.6×10^{-2}		St-Pierre et al. (2014)	M	173
	2.2	5300	O'Farrell and Waghorne (2010)	M	
	2.1		Vitenberg and Dobryakov (2008)	M	
	7.8×10^{-1}		Helburn et al. (2008)	M	
	2.2	5300	Lin and Chou (2006)	M	
	2.0	5600	Teja et al. (2001)	M	11, 338
	2.6	5900	Zhu et al. (2000)	M	
	2.0	5500	Gupta et al. (2000)	M	
	1.6		Altschuh et al. (1999)	M	
	2.1		Merk and Riederer (1997)	M	
	1.3		Kaneko et al. (1994)	M	14
	2.2		Li and Carr (1993)	M	
	2.6	3900	Pividal et al. (1992)	M	
	2.2	5200	Snider and Dawson (1985)	M	
	2.0		Richon et al. (1985)	M	
	1.3×10^{1}		Mazza (1980)	M	
	2.2		Rytting et al. (1978)	M	
	2.3		Burnett (1963)	M	
	2.3		Butler et al. (1935)	M	388
	7.6×10^{-2}		Abraham and Acree (2007)	V	
	1.8	6200	Fukuchi et al. (2002)	V	
	1.9		Hwang et al. (1992)	V	
	2.8		Riederer (1990)	V	
		5400	Abraham (1984)	V	
	2.2	5700	Glew and Moelwyn-Hughes (1953)	R	
	2.1	5400	Plyasunov et al. (2001)	T	
	1.5		Yaws (2003)	X	258
	1.5		Yaws (2003)	X	237
	1.6	5600	Schaffer and Daubert (1969)	X	298
	2.2		Gaffney and Senum (1984)	X	389
	2.1		Timmermans (1960)	X	390
	1.6		Dupeux et al. (2022)	Q	259
	2.1		Hayer et al. (2022)	Q	20
	5.0×10^{-1}		Keshavarz et al. (2022)	Q	
	2.8		Duchowicz et al. (2020)	Q	184
	3.4×10^{-1}		Wang et al. (2017)	Q	80, 238

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.1		Wang et al. (2017)	Q	80, 239
	6.6		Wang et al. (2017)	Q	80, 240
	2.1		Li et al. (2014)	Q	241
	2.0		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	2.5		Raventos-Duran et al. (2010)	Q	245
	2.6×10^{-1}		Gharagheizi et al. (2010)	Q	246
	2.0		Hilal et al. (2008)	Q	
	2.9		Modarresi et al. (2007)	Q	67
		6200	Kühne et al. (2005)	Q	
	2.2		Yaffe et al. (2003)	Q	248, 249
	1.1		Yao et al. (2002)	Q	229, 267
	2.6		English and Carroll (2001)	Q	230, 231
	1.6		Katritzky et al. (1998)	Q	
	1.5		Yaws et al. (1997)	Q	
	2.0		Suzuki et al. (1992)	Q	232
	1.8		Nirmalakhandan and Speece (1988)	Q	
	2.4		Taft et al. (1985)	Q	
	2.2		Duchowicz et al. (2020)	?	185, 21
		5000	Kühne et al. (2005)	?	
	1.9		Yaws (1999)	?	21
	1.1		Abraham and Weathersby (1994)	?	21
	1.4		Yaws and Yang (1992)	?	21
	2.2		Abraham et al. (1990)	?	
ethanol	1.9	6400	Burkholder et al. (2019)	L	1
C_2H_5OH	1.9	6400	Burkholder et al. (2015)	L	1
[64-17-5]	1.8	6300	Brockbank (2013)	L	1
LFQSCWFLJHTTHZ-UHFFFAOYSA-N	1.9	6400	Sander et al. (2011)	L	1
	1.9	6300	Warneck (2006)	L	
	2.0	6600	Sander et al. (2006)	L	
	1.8	6300	Dohnal et al. (2006)	L	1
	1.7	5700	Fogg and Sangster (2003)	L	
	1.9	6300	Plyasunov and Shock (2000)	L	
	1.9	6200	Dubowski (1979)	L	1
	1.8	5900	Willey et al. (2017)	M	
	2.2	5500	O'Farrell and Waghorne (2010)	M	
	1.8		Vitenberg and Dobryakov (2008)	M	
	1.9	5800	Falabella et al. (2006)	M	11, 338
	1.9		Straver and de Loos (2005)	M	
			Cheng et al. (2004)	M	328
	1.1		Ueberfeld et al. (2001)	M	
	1.8	5800	Gupta et al. (2000)	M	
	1.3		Altschuh et al. (1999)	M	
	1.0		Eger et al. (1999)	M	14
	1.9		Merk and Riederer (1997)	M	
	8.3×10^{-1}		Kaneko et al. (1994)	M	14
	1.9		Li and Carr (1993)	M	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	3.1	3900	Pividal et al. (1992)	M	
	1.9		Park et al. (1987)	M	
	1.9	6600	Snider and Dawson (1985)	M	
	2.0		Richon et al. (1985)	M	
	1.9	6000	Jones (1983)	M	1
	6.2		Mazza (1980)	M	
	1.9		Rytting et al. (1978)	M	
	2.3		Rohrschneider (1973)	M	
	2.1		Burnett (1963)	M	
	1.9	6500	Harger et al. (1950)	M	
	1.9		Butler et al. (1935)	M	
	4.7×10^{-2}		Abraham and Acree (2007)	V	
	1.7	6300	Fukuchi et al. (2002)	V	
	1.3		Hwang et al. (1992)	V	
		6300	Abraham (1984)	V	
	1.9	6300	Plyasunov et al. (2001)	T	
	1.4		Yaws (2003)	X	237
	1.5	6400	Schaffer and Daubert (1969)	X	298
	2.0		Gaffney and Senum (1984)	X	389
	1.6		Timmermans (1960)	X	390
	1.7		Hayer et al. (2022)	Q	20
	6.7×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1		Duchowicz et al. (2020)	Q	
	3.1×10^{-1}		Wang et al. (2017)	Q	80, 238
	2.0		Wang et al. (2017)	Q	80, 239
	2.3		Wang et al. (2017)	Q	80, 240
	1.6		Raventos-Duran et al. (2010)	Q	242, 243
	1.6		Raventos-Duran et al. (2010)	Q	244
	1.6		Raventos-Duran et al. (2010)	Q	245
	1.3		Gharagheizi et al. (2010)	Q	246
	1.1		Hilal et al. (2008)	Q	
	1.8		Modarresi et al. (2007)	Q	67
		6500	Kühne et al. (2005)	Q	
	2.0		Yaffe et al. (2003)	Q	248, 249
	1.4		Yao et al. (2002)	Q	229
	1.4		English and Carroll (2001)	Q	230, 231
	1.2		Katritzky et al. (1998)	Q	
	1.3		Yaws et al. (1997)	Q	
	1.4		Russell et al. (1992)	Q	279
	1.4		Suzuki et al. (1992)	Q	232
	1.6		Nirmalakhandan and Speece (1988)	Q	
	2.0		Duchowicz et al. (2020)	?	185, 21
	1.9		Bartelt-Hunt et al. (2008)	?	21
		6400	Kühne et al. (2005)	?	
	1.2		Yaws (1999)	?	21
	8.2×10^{-1}		Abraham and Weathersby (1994)	?	21
	1.2		Yaws and Yang (1992)	?	21

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.9		Abraham et al. (1990)	?	
1-propanol	1.4	6900	Burkholder et al. (2019)	L	391, 1
C_3H_7OH	1.4	6900	Burkholder et al. (2015)	L	392, 1
[71-23-8]	1.5	7000	Brockbank (2013)	L	1, 393
BDERNNFJNOPAEC-UHFFFAOYSA-N	1.4	6900	Sander et al. (2011)	L	394, 1
	1.3	7500	Sander et al. (2006)	L	
	1.4	6900	Dohnal et al. (2006)	L	1
	1.4	6200	Fogg and Sangster (2003)	L	
	1.5	6900	Plyasunov and Shock (2000)	L	
	1.5		Vitenberg and Dobryakov (2008)	M	
	1.2	6200	Falabella et al. (2006)	M	11, 338
	1.5		Straver and de Loos (2005)	M	
	3.2×10^{-1}		van Ruth et al. (2002)	M	14
	3.2×10^{-1}		van Ruth and Villeneuve (2002)	M	14, 361
	6.5×10^{-1}		van Ruth et al. (2001)	M	14
	1.2	6200	Gupta et al. (2000)	M	
	2.7		Altschuh et al. (1999)	M	
	1.5		Merk and Riederer (1997)	M	
	7.2×10^{-1}		Kaneko et al. (1994)	M	14
	1.4		Li and Carr (1993)	M	
	1.3	7500	Snider and Dawson (1985)	M	
	1.8		Richon et al. (1985)	M	
	3.7		Mazza (1980)	M	
	1.5		Rytting et al. (1978)	M	
	1.6		Burnett (1963)	M	
	1.4		Butler et al. (1935)	M	388
	3.1×10^{-2}		Abraham and Acree (2007)	V	
	1.8	7700	Fukuchi et al. (2002)	V	
	8.0×10^{-2}	4500	Djerki and Laub (1988)	V	
		6900	Abraham (1984)	V	
	1.5	6900	Plyasunov et al. (2001)	T	
	1.2		Yaws (2003)	X	258
	1.2		Dupeux et al. (2022)	Q	259
	1.5		Hayer et al. (2022)	Q	20
	9.0×10^{-1}		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	
	2.5×10^{-1}		Wang et al. (2017)	Q	80, 238
	1.3		Wang et al. (2017)	Q	80, 239
	1.2		Wang et al. (2017)	Q	80, 240
	1.2		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	1.2		Raventos-Duran et al. (2010)	Q	245
	7.0×10^{-1}		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	67
		6900	Kühne et al. (2005)	Q	
	1.2		Yaffe et al. (2003)	Q	248, 272
	1.1		Yao et al. (2002)	Q	229

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Table A3.2: Alcohols (ROH) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	1.2		English and Carroll (2001)	Q	230, 231
	1.7		Katritzky et al. (1998)	Q	
	1.2		Yaws et al. (1997)	Q	
	1.1		Russell et al. (1992)	Q	279
	1.1		Suzuki et al. (1992)	Q	232
	1.2		Nirmalakhandan and Speece (1988)	Q	
	1.3		Duchowicz et al. (2020)	?	185, 21
		7500	Kühne et al. (2005)	?	
	1.3		Yaws (1999)	?	21
	6.0×10^{-1}		Abraham and Weathersby (1994)	?	21
	1.1		Yaws and Yang (1992)	?	21
	1.5		Abraham et al. (1990)	?	
2-propanol C_3H_7OH (isopropanol) [67-63-0] KFZMGEQAYNKOFK-UHFFFAOYSA-N	1.2	7100	Burkholder et al. (2019)	L	1
	1.2	7100	Burkholder et al. (2015)	L	1
	1.2	6900	Brockbank (2013)	L	1
	1.3	7500	Sander et al. (2011)	L	
	1.3	7500	Sander et al. (2006)	L	
	1.2	6200	Fogg and Sangster (2003)	L	
	1.2	7000	Plyasunov and Shock (2000)	L	
	1.1	8400	Hiatt (2013)	M	
	6.8×10^{-1}		Helburn et al. (2008)	M	
	1.3	7300	Lin and Chou (2006)	M	
			Cheng et al. (2004)	M	328
			Cheng et al. (2003)	M	328
	1.8×10^{-1}		Ayuttaya et al. (2001)	M	340
	1.0×10^{-3}		Ayuttaya et al. (2001)	M	341
	5.7×10^{-1}		Ayuttaya et al. (2001)	M	342
	1.1		Kim et al. (2000)	M	
	9.2×10^{-1}		Altschuh et al. (1999)	M	
	1.2		Merk and Riederer (1997)	M	
	5.8×10^{-1}		Kaneko et al. (1994)	M	14
	7.9×10^{-1}	5700	Kolb et al. (1992)	M	277
	1.4		Pividal et al. (1992)	M	80
	9.8×10^{-1}		Yu (1992)	M	12
	1.2	7400	Snider and Dawson (1985)	M	
	2.1		Mazza (1980)	M	
	1.2		Rytting et al. (1978)	M	
	1.2		Butler et al. (1935)	M	
	1.2	7100	Fenclová et al. (2007)	V	1
	1.2	7600	Fukuchi et al. (2002)	V	
	1.7		Hine and Weimar (1965)	R	
	7.6×10^{-1}		Yaws (2003)	X	258
	2.4		Dupeux et al. (2022)	Q	259
	1.2		Hayer et al. (2022)	Q	20
	9.0×10^{-1}		Keshavarz et al. (2022)	Q	
	4.8×10^{-1}		Duchowicz et al. (2020)	Q	184
	2.8×10^{-1}		Wang et al. (2017)	Q	80, 238

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.0		Wang et al. (2017)	Q	80, 239
	1.2		Wang et al. (2017)	Q	80, 240
	1.2		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	1.2		Raventos-Duran et al. (2010)	Q	245
	4.3×10^{-1}		Hilal et al. (2008)	Q	
	7.0×10^{-1}		Modarresi et al. (2007)	Q	67
		6900	Kühne et al. (2005)	Q	
			Yaffe et al. (2003)	Q	356
	7.7×10^{-1}		Yao et al. (2002)	Q	229
	1.0		English and Carroll (2001)	Q	230, 274
	1.1		Katritzky et al. (1998)	Q	
	8.9×10^{-1}		Yaws et al. (1997)	Q	
	1.4		Russell et al. (1992)	Q	279
	9.7×10^{-1}		Suzuki et al. (1992)	Q	232
	1.1		Nirmalakhandan and Speece (1988)	Q	
	1.3		Taft et al. (1985)	Q	
	1.2		Duchowicz et al. (2020)	?	185, 21
		6000	Kühne et al. (2005)	?	
	8.0×10^{-1}		Yaws (1999)	?	21
	5.0×10^{-1}		Abraham and Weathersby (1994)	?	21
	8.8×10^{-1}		Yaws and Yang (1992)	?	21
	1.2		Abraham et al. (1990)	?	
glycidol $C_3H_6O_2$ [556-52-5] CTKINSOISVBQLD-UHFFFAOYSA-N	1.7×10^{3}		HSDB (2015)	Q	99
1-butanol C_4H_9OH [71-36-3] LRHPLDYGYMQRHN-UHFFFAOYSA-N	1.2	7500	Burkholder et al. (2019)	L	1
	1.2	7500	Burkholder et al. (2015)	L	1
	1.2	7500	Brockbank (2013)	L	1
	1.2	7500	Sander et al. (2011)	L	1
	1.3	7200	Sander et al. (2006)	L	
	1.2	7500	Dohnal et al. (2006)	L	1
	1.1	6300	Fogg and Sangster (2003)	L	
	1.2	7400	Plyasunov and Shock (2000)	L	
	1.0	7000	Wu et al. (2022a)	M	
	2.0		Chao et al. (2017)	M	
	1.0	6800	Shunthirasingham et al. (2013)	M	
	1.3		Vitenberg and Dobryakov (2008)	M	
	1.1	6000	Lei et al. (2007)	M	395
	8.2×10^{-1}	6200	Falabella et al. (2006)	M	11, 338
	9.4×10^{-1}	6100	Hovorka et al. (2002)	M	11
	4.5×10^{-1}		van Ruth et al. (2002)	M	14
	4.4×10^{-1}		van Ruth and Villeneuve (2002)	M	14, 361
	4.8×10^{-1}		van Ruth et al. (2001)	M	14
	1.1		Kim et al. (2000)	M	

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Table A3.2: Alcohols (ROH) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.2×10^{-1}	6200	Gupta et al. (2000)	M	
	1.2		Altschuh et al. (1999)	M	
	5.5×10^{-1}		Eger et al. (1999)	M	14
	1.1		Merk and Riederer (1997)	M	
	1.4×10^{-1}		Chaintreau et al. (1995)	M	
	5.1×10^{-1}		Kaneko et al. (1994)	M	14
	1.1		Li and Carr (1993)	M	
	6.1×10^{-1}	5600	Kolb et al. (1992)	M	277
	1.2	7200	Snider and Dawson (1985)	M	
	5.3×10^{-1}		Friant and Suffet (1979)	M	38
	1.2		Rytting et al. (1978)	M	
	1.1		Amoore and Buttery (1978)	M	
	1.1		Buttery et al. (1969)	M	
	1.4		Burnett (1963)	M	
	1.2		Butler et al. (1935)	M	388
	1.1		Chao et al. (2017)	V	
	1.1		Mackay et al. (2006c)	V	
	7.3×10^{-1}		Mackay et al. (1995)	V	
	8.3×10^{-1}		Hwang et al. (1992)	V	
	2.2×10^{-1}	4700	Djerki and Laub (1988)	V	
		7400	Abraham (1984)	V	
	1.2		Amoore and Buttery (1978)	V	
	1.2		Butler et al. (1935)	V	
	1.2		Yaws (2003)	X	258
	9.4×10^{-1}		Dupeux et al. (2022)	Q	259
	1.9		Hayer et al. (2022)	Q	20
	1.2		Keshavarz et al. (2022)	Q	
	1.3		Duchowicz et al. (2020)	Q	184
	2.0×10^{-1}		Wang et al. (2017)	Q	80, 238
	9.1×10^{-1}		Wang et al. (2017)	Q	80, 239
	1.3		Wang et al. (2017)	Q	80, 240
	1.2		Li et al. (2014)	Q	241
	9.4×10^{-1}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	5.6×10^{-1}		Hilal et al. (2008)	Q	
	1.0		Modarresi et al. (2007)	Q	67
		7200	Kühne et al. (2005)	Q	
	1.2		Yaffe et al. (2003)	Q	248, 272
	1.1		Yao et al. (2002)	Q	229
	9.5×10^{-1}		English and Carroll (2001)	Q	230, 260
	1.8		Katritzky et al. (1998)	Q	
	1.1		Yaws et al. (1997)	Q	
	8.6×10^{-1}		Russell et al. (1992)	Q	279
	8.4×10^{-1}		Suzuki et al. (1992)	Q	232
	9.9×10^{-1}		Nirmalakhandan and Speece (1988)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1		Duchowicz et al. (2020)	?	185, 21
		6900	Kühne et al. (2005)	?	
	1.1		Yaws (1999)	?	21
	1.2		Abraham et al. (1990)	?	
	1.8		Mackay and Yeun (1983)	?	
2-butanol	1.1	7600	Burkholder et al. (2019)	L	1
$C_4H_{10}O$	1.1	7600	Burkholder et al. (2015)	L	1
(*sec*-butanol)	9.5×10^{-1}	7600	Brockbank (2013)	L	1
[78-92-2]	1.1	7300	Sander et al. (2011)	L	
BTANRVKWQNVYAZ-UHFFFAOYSA-N	1.1	7300	Sander et al. (2006)	L	
	1.0	7400	Fogg and Sangster (2003)	L	
	9.9×10^{-1}	7600	Plyasunov and Shock (2000)	L	
	8.3×10^{-1}		Merk and Riederer (1997)	M	
	1.1	7300	Snider and Dawson (1985)	M	
	9.8×10^{-1}		Rytting et al. (1978)	M	
	9.6×10^{-1}		Butler et al. (1935)	M	
	9.5×10^{-1}	7600	Fenclová et al. (2007)	V	1
	1.1		Mackay et al. (2006c)	V	
	1.1		Mackay et al. (1995)	V	
	9.1×10^{-1}	7500	Cabani et al. (1975b)	T	
	6.7×10^{-1}		Yaws (2003)	X	258
	1.1		Dupeux et al. (2022)	Q	259
	1.2		Hayer et al. (2022)	Q	20
	1.2		Keshavarz et al. (2022)	Q	
	5.1×10^{-1}		Duchowicz et al. (2020)	Q	299
	2.3×10^{-1}		Wang et al. (2017)	Q	80, 238
	8.9×10^{-1}		Wang et al. (2017)	Q	80, 239
	7.3×10^{-1}		Wang et al. (2017)	Q	80, 240
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-1}		Hilal et al. (2008)	Q	
	4.9×10^{-1}		Modarresi et al. (2007)	Q	67
		7200	Kühne et al. (2005)	Q	
	1.2		Yaffe et al. (2003)	Q	248, 249
	6.2×10^{-1}		Yao et al. (2002)	Q	229
	8.4×10^{-1}		English and Carroll (2001)	Q	230, 231
	5.7×10^{-1}		Katritzky et al. (1998)	Q	
	1.2		Yaws et al. (1997)	Q	
	7.7×10^{-1}		Suzuki et al. (1992)	Q	232
	9.0×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	1.1		Duchowicz et al. (2020)	?	185, 21
		7100	Kühne et al. (2005)	?	
	1.2		Yaws (1999)	?	21
	9.9×10^{-1}		Abraham et al. (1990)	?	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-1-propanol	8.3×10^{-1}	7200	Burkholder et al. (2019)	L	1
$C_4H_{10}O$	8.3×10^{-1}	7200	Burkholder et al. (2015)	L	1
(isobutanol)	8.0×10^{-1}	7400	Brockbank (2013)	L	1
[78-83-1]	1.0		Sander et al. (2011)	L	
ZXEKIIBDNHEJCQ-UHFFFAOYSA-N	1.0		Sander et al. (2006)	L	
	8.5×10^{-1}	7200	Plyasunov and Shock (2000)	L	
	1.2		Chao et al. (2017)	M	
	2.2×10^{-1}		Kim and Kim (2014)	M	
			Cheng et al. (2004)	M	328
	6.7×10^{-1}	6100	Hovorka et al. (2002)	M	11
	1.1		Altschuh et al. (1999)	M	
	3.7×10^{-1}		Shiu and Mackay (1997)	M	
	7.8×10^{-1}		Merk and Riederer (1997)	M	
	4.4×10^{-1}		Kaneko et al. (1994)	M	14
	1.0		Snider and Dawson (1985)	M	
	8.0×10^{-1}		Rytting et al. (1978)	M	
	8.3×10^{-1}		Butler et al. (1935)	M	
	9.2×10^{-1}		Chao et al. (2017)	V	
	7.6×10^{-1}	7200	Fenclová et al. (2007)	V	1
	7.3×10^{-1}		Mackay et al. (2006c)	V	
	7.3×10^{-1}		Shiu and Mackay (1997)	V	
	7.3×10^{-1}		Mackay et al. (1995)	V	
	1.2		Keshavarz et al. (2022)	Q	
	5.1×10^{-1}		Duchowicz et al. (2020)	Q	
	2.3×10^{-1}		Wang et al. (2017)	Q	80, 238
	9.1×10^{-1}		Wang et al. (2017)	Q	80, 239
	7.6×10^{-1}		Wang et al. (2017)	Q	80, 240
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	5.1×10^{-1}		Hilal et al. (2008)	Q	
	6.1×10^{-1}		Modarresi et al. (2007)	Q	67
		7200	Kühne et al. (2005)	Q	
	3.7×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	6.2×10^{-1}		Yao et al. (2002)	Q	229
	5.7×10^{-1}		English and Carroll (2001)	Q	230, 231
	1.8		Katritzky et al. (1998)	Q	
	8.3×10^{-1}		Yaws et al. (1997)	Q	
	7.7×10^{-1}		Suzuki et al. (1992)	Q	232
	8.4×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	1.0		Duchowicz et al. (2020)	?	185, 21
		8100	Kühne et al. (2005)	?	
	8.4×10^{-1}		Yaws (1999)	?	21
	3.1×10^{-1}		Abraham and Weathersby (1994)	?	21
	8.0×10^{-1}		Abraham et al. (1990)	?	
	9.6×10^{-1}		Mackay and Yeun (1983)	?	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-2-propanol	7.9×10^{-1}	7600	Brockbank (2013)	L	1
$C_4H_{10}O$	6.9×10^{-1}	8300	Sander et al. (2011)	L	
(*tert*-butanol)	6.9×10^{-1}	8300	Sander et al. (2006)	L	
[75-65-0]	7.9×10^{-1}	7700	Plyasunov and Shock (2000)	L	
DKGAVHZHDRPRBM-UHFFFAOYSA-N	1.4	7900	Hiatt (2013)	M	
	1.1		Altschuh et al. (1999)	M	
	8.1×10^{-1}		Merk and Riederer (1997)	M	
			Koga (1995)	M	396
	6.8×10^{-1}	8300	Snider and Dawson (1985)	M	
	7.6×10^{-1}		Rytting et al. (1978)	M	
	8.3×10^{-1}		Butler et al. (1935)	M	
	8.0×10^{-1}	7700	Fenclová et al. (2007)	V	1
	2.4×10^{-1}		Yaws (2003)	X	258
	8.0×10^{-1}	6500	Pankow et al. (1996)	C	
	2.0		Dupeux et al. (2022)	Q	259
	1.2		Keshavarz et al. (2022)	Q	
	2.2×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.6×10^{-1}		Wang et al. (2017)	Q	80, 238
	6.6×10^{-1}		Wang et al. (2017)	Q	80, 239
	1.1		Wang et al. (2017)	Q	80, 240
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	4.1×10^{-1}		Modarresi et al. (2007)	Q	67
		7200	Kühne et al. (2005)	Q	
	7.9×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.9×10^{-1}		Yao et al. (2002)	Q	229
	9.0×10^{-1}		English and Carroll (2001)	Q	230, 231
	7.5×10^{-1}		Katritzky et al. (1998)	Q	
	7.3×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	3.0×10^{-1}		Yaws et al. (1997)	Q	
	6.1×10^{-1}		Suzuki et al. (1992)	Q	232
	7.0×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	1.1		Duchowicz et al. (2020)	?	185, 21
		8300	Kühne et al. (2005)	?	
	5.7×10^{-1}		Yaws (1999)	?	21
	7.7×10^{-1}		Abraham et al. (1990)	?	
			Burkholder et al. (2019)	W	397
			Burkholder et al. (2015)	W	398
1-pentanol	8.6×10^{-1}	7400	Brockbank (2013)	L	1
$C_5H_{11}OH$	1.0	7900	Dohnal et al. (2006)	L	1
(amyl alcohol)	8.9×10^{-1}	7800	Plyasunov and Shock (2000)	L	
[71-41-0]	8.1×10^{-1}	7100	Shunthirasingham et al. (2013)	M	
AMQJEAYHLZJPGS-UHFFFAOYSA-N	7.5×10^{-1}	6100	Lei et al. (2007)	M	395
	9.4×10^{-1}	6800	Falabella et al. (2006)	M	11, 338
	9.5×10^{-1}	6900	Gupta et al. (2000)	M	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.7×10^{-1}		Merk and Riederer (1997)	M	
	4.2×10^{-1}		Kaneko et al. (1994)	M	14
	8.4×10^{-1}		Li and Carr (1993)	M	
	9.0×10^{-1}		Rytting et al. (1978)	M	
	7.8×10^{-1}		Butler et al. (1935)	M	
	8.3×10^{-1}		Mackay et al. (2006c)	V	
	8.3×10^{-1}		Mackay et al. (1995)	V	
	6.1×10^{-1}	4900	Djerki and Laub (1988)	V	
		7800	Abraham (1984)	V	
	7.8×10^{-1}		Amoore and Buttery (1978)	V	
	7.6×10^{-1}		Butler et al. (1935)	V	
	7.6×10^{-1}		Yaws (2003)	X	258
	7.3×10^{-1}		Dupeux et al. (2022)	Q	259
	1.6		Keshavarz et al. (2022)	Q	
	1.4		Duchowicz et al. (2020)	Q	
	1.8×10^{-1}		Wang et al. (2017)	Q	80, 238
	6.6×10^{-1}		Wang et al. (2017)	Q	80, 239
	9.1×10^{-1}		Wang et al. (2017)	Q	80, 240
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	4.5×10^{-1}		Hilal et al. (2008)	Q	
	7.6×10^{-1}		Modarresi et al. (2007)	Q	67
		7600	Kühne et al. (2005)	Q	
	7.9×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	5.3×10^{-1}		Yao et al. (2002)	Q	229
	7.7×10^{-1}		English and Carroll (2001)	Q	230, 231
	1.3		Katritzky et al. (1998)	Q	
	7.7×10^{-1}		Yaws et al. (1997)	Q	
	6.2×10^{-1}		Russell et al. (1992)	Q	358
	6.5×10^{-1}		Suzuki et al. (1992)	Q	232
	7.9×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	7.6×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		7700	Kühne et al. (2005)	?	
	7.7×10^{-1}		Yaws (1999)	?	21
	8.1×10^{-1}		Yaws and Yang (1992)	?	21
	9.0×10^{-1}		Abraham et al. (1990)	?	
	9.6×10^{-1}		Mackay and Yeun (1983)	?	
2-pentanol	6.7×10^{-1}	7900	Brockbank (2013)	L	1
$C_5H_{12}O$	6.5×10^{-1}	8000	Plyasunov and Shock (2000)	L	
(*sec*-pentanol)	7.1×10^{-1}	8000	Fenclová et al. (2010)	M	1
[6032-29-7]	3.0×10^{-1}		van Ruth et al. (2002)	M	14
JYVLIDXNZAXMDK-UHFFFAOYSA-N	2.6×10^{-1}		van Ruth and Villeneuve (2002)	M	14, 361
	2.3×10^{-1}		van Ruth et al. (2001)	M	14
	6.6×10^{-1}		Merk and Riederer (1997)	M	
	6.7×10^{-1}		Butler et al. (1935)	M	
	6.6×10^{-1}		Mackay et al. (2006c)	V	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.6×10^{-1}		Mackay et al. (1995)	V	
	6.5×10^{-1}		Yaws (2003)	X	258
	7.6×10^{-1}		Dupeux et al. (2022)	Q	259
	1.6		Keshavarz et al. (2022)	Q	
	5.3×10^{-1}		Duchowicz et al. (2020)	Q	
	1.8×10^{-1}		Wang et al. (2017)	Q	80, 238
	6.3×10^{-1}		Wang et al. (2017)	Q	80, 239
	6.2×10^{-1}		Wang et al. (2017)	Q	80, 240
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-1}		Hilal et al. (2008)	Q	
	3.5×10^{-1}		Modarresi et al. (2007)	Q	67
		7600	Kühne et al. (2005)	Q	
	6.7×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	6.4×10^{-1}		Yao et al. (2002)	Q	229
	7.0×10^{-1}		English and Carroll (2001)	Q	230, 260
	9.0×10^{-1}		Katritzky et al. (1998)	Q	
	6.5×10^{-1}		Yaws et al. (1997)	Q	
	5.8×10^{-1}		Suzuki et al. (1992)	Q	232
	7.2×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	6.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		7900	Kühne et al. (2005)	?	
	6.5×10^{-1}		Yaws (1999)	?	21
	6.7×10^{-1}		Abraham et al. (1990)	?	
3-pentanol	6.0×10^{-1}	7600	Brockbank (2013)	L	1
$C_5H_{12}O$	5.5×10^{-1}		Plyasunov and Shock (2000)	L	
[584-02-1]	6.4×10^{-1}	8000	Fenclová et al. (2010)	M	1
AQIXEPGDORPWBJ-UHFFFAOYSA-N	5.0×10^{-1}		Duchowicz et al. (2020)	V	186
	6.3×10^{-1}	7900	Cabani et al. (1975b)	T	
	5.3×10^{-1}		Duchowicz et al. (2020)	Q	
	1.8×10^{-1}		Wang et al. (2017)	Q	80, 238
	6.6×10^{-1}		Wang et al. (2017)	Q	80, 239
	2.3×10^{-1}		Wang et al. (2017)	Q	80, 240
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.2×10^{-1}		Hilal et al. (2008)	Q	
	5.2×10^{-1}		Modarresi et al. (2007)	Q	67
		7600	Kühne et al. (2005)	Q	
	6.7×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	6.1×10^{-1}		Yao et al. (2002)	Q	229
	7.0×10^{-1}		English and Carroll (2001)	Q	230, 231
	5.0×10^{-1}		Katritzky et al. (1998)	Q	
	7.7×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	5.2×10^{-1}		Yaws et al. (1997)	Q	
		7500	Kühne et al. (2005)	?	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.3×10^{-1}		Yaws (1999)	?	21
	6.2×10^{-1}		Abraham et al. (1990)	?	
2-methyl-1-butanol	7.6×10^{-1}	7900	Brockbank (2013)	L	1
$C_5H_{12}O$	7.1×10^{-1}		Plyasunov and Shock (2000)	L	
[137-32-6]	7.8×10^{-1}	7700	Fenclová et al. (2010)	M	1
QPRQEDXDYOZYLA-UHFFFAOYSA-N	3.3×10^{-1}		Kaneko et al. (1994)	M	14
	7.0×10^{-1}		Butler et al. (1935)	M	
	8.4×10^{-1}		Yaws (2003)	X	258
	4.6×10^{-1}		Dupeux et al. (2022)	Q	259
	1.6		Keshavarz et al. (2022)	Q	
	5.3×10^{-1}		Duchowicz et al. (2020)	Q	299
	1.8×10^{-1}		Wang et al. (2017)	Q	80, 238
	7.6×10^{-1}		Wang et al. (2017)	Q	80, 239
	5.5×10^{-1}		Wang et al. (2017)	Q	80, 240
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-1}		Hilal et al. (2008)	Q	
	5.9×10^{-1}		Modarresi et al. (2007)	Q	67
		7600	Kühne et al. (2005)	Q	
	7.0×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	4.7×10^{-1}		English and Carroll (2001)	Q	230, 274
	1.9		Katritzky et al. (1998)	Q	
	8.3×10^{-1}		Yaws et al. (1997)	Q	
	6.0×10^{-1}		Suzuki et al. (1992)	Q	232
	6.9×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	7.0×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		6800	Kühne et al. (2005)	?	
	8.4×10^{-1}		Yaws (1999)	?	21
	7.0×10^{-1}		Abraham et al. (1990)	?	
(*S*)-2-methyl-1-butanol	3.9×10^{-1}		Hilal et al. (2008)	Q	
$C_5H_{12}O$					
[1565-80-6]					
QPRQEDXDYOZYLA-RXMQYKEDSA-N					
3-methyl-1-butanol	8.2×10^{-1}	8000	Brockbank (2013)	L	1
$C_5H_{12}O$	7.0×10^{-1}		Plyasunov and Shock (2000)	L	
(isopentanol)	6.7×10^{-1}	6900	Ammari and Schroen (2019)	M	11
[123-51-3]	8.2×10^{-1}	7700	Fenclová et al. (2010)	M	1
PHTQWCKDNZKARW-UHFFFAOYSA-N	3.3×10^{-1}		van Ruth et al. (2002)	M	14
	3.2×10^{-1}		van Ruth and Villeneuve (2002)	M	14, 361
	3.2×10^{-1}		van Ruth et al. (2001)	M	14
	7.5×10^{-1}		Yaws (2003)	X	258
	7.1×10^{-1}		Dupeux et al. (2022)	Q	259
	1.6		Keshavarz et al. (2022)	Q	
	1.2×10^{-1}		Abney (2021)	Q	399
	5.3×10^{-1}		Duchowicz et al. (2020)	Q	299

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.8×10^{-1}		Wang et al. (2017)	Q	80, 238
	7.4×10^{-1}		Wang et al. (2017)	Q	80, 239
	1.3		Wang et al. (2017)	Q	80, 240
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	4.6×10^{-1}		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	67
		7600	Kühne et al. (2005)	Q	
	6.1×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	7.0×10^{-1}		Yao et al. (2002)	Q	229
	4.7×10^{-1}		English and Carroll (2001)	Q	230, 231
	6.9×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	7.4×10^{-1}		Yaws et al. (1997)	Q	
	7.0×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		8200	Kühne et al. (2005)	?	
	7.4×10^{-1}		Yaws (1999)	?	21
	7.0×10^{-1}		Abraham et al. (1990)	?	
2-methyl-2-butanol $C_5H_{12}O$ (*tert*-pentanol) [75-85-4] MSXVEPNJUHWQHW-UHFFFAOYSA-N	6.5×10^{-1}	7900	Brockbank (2013)	L	1
	7.1×10^{-1}	8200	Plyasunov and Shock (2000)	L	
	7.2×10^{-1}	8200	Fenclová et al. (2010)	M	1
	7.0×10^{-1}		Merk and Riederer (1997)	M	
	7.1×10^{-1}		Butler et al. (1935)	M	
	1.6		Keshavarz et al. (2022)	Q	
	2.3×10^{-1}		Duchowicz et al. (2020)	Q	
	1.2×10^{-1}		Wang et al. (2017)	Q	80, 238
	6.6×10^{-1}		Wang et al. (2017)	Q	80, 239
	4.8×10^{-1}		Wang et al. (2017)	Q	80, 240
	7.2×10^{-1}		HSDB (2015)	Q	99
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.7×10^{-1}		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	67
		7600	Kühne et al. (2005)	Q	
	7.9×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	2.8×10^{-1}		Yao et al. (2002)	Q	229
	7.5×10^{-1}		English and Carroll (2001)	Q	230, 231
	6.9×10^{-1}		Katritzky et al. (1998)	Q	
	6.1×10^{-1}		Yaws et al. (1997)	Q	
	5.0×10^{-1}		Suzuki et al. (1992)	Q	232
	6.0×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	7.2×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		7200	Kühne et al. (2005)	?	
	5.6×10^{-2}		Yaws (1999)	?	21
	7.2×10^{-1}		Abraham et al. (1990)	?	

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Table A3.2: Alcohols (ROH) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-2-butanol	5.1×10^{-1}	7600	Brockbank (2013)	L	1
$C_5H_{12}O$	5.4×10^{-1}	7800	Fenclová et al. (2010)	M	1
[598-75-4]	5.6×10^{-1}		Duchowicz et al. (2020)	V	186
MXLMTQWGSQIYOW-UHFFFAOYSA-N	2.1×10^{-1}		Duchowicz et al. (2020)	Q	
	2.1×10^{-1}		Wang et al. (2017)	Q	80, 238
	6.9×10^{-1}		Wang et al. (2017)	Q	80, 239
	4.2×10^{-1}		Wang et al. (2017)	Q	80, 240
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-1}		Hilal et al. (2008)	Q	
	7.1×10^{-1}		Modarresi et al. (2007)	Q	67
		7600	Kühne et al. (2005)	Q	
	6.1×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	4.5×10^{-1}		Katritzky et al. (1998)	Q	
	5.4×10^{-1}		Yaws et al. (1997)	Q	
		7500	Kühne et al. (2005)	?	
	5.5×10^{-1}		Yaws (1999)	?	21
2,2-dimethyl-1-propanol	3.0×10^{-1}	7800	Brockbank (2013)	L	1, 400
$C_5H_{12}O$	1.9×10^{-1}		Duchowicz et al. (2020)	V	186
[75-84-3]	1.9×10^{-1}		HSDB (2015)	V	
KPSSIOMAKSHJJG-UHFFFAOYSA-N	5.7×10^{-1}		Yaws (2003)	X	258
	3.7×10^{-1}		Dupeux et al. (2022)	Q	259
	2.3×10^{-1}		Duchowicz et al. (2020)	Q	
	1.2×10^{-1}		Wang et al. (2017)	Q	80, 238
	5.9×10^{-1}		Wang et al. (2017)	Q	80, 239
	3.0×10^{-1}		Wang et al. (2017)	Q	80, 240
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-1}		Hilal et al. (2008)	Q	
	5.7×10^{-1}		Modarresi et al. (2007)	Q	67
		7600	Kühne et al. (2005)	Q	
	4.9×10^{-1}		Saxena and Hildemann (1996)	E	401
		7900	Kühne et al. (2005)	?	
1-hexanol	7.6×10^{-1}	7800	Brockbank (2013)	L	1
$C_6H_{14}O$	6.6×10^{-1}	8200	Plyasunov and Shock (2000)	L	
[111-27-3]	5.7×10^{-1}	7300	Shunthirasingham et al. (2013)	M	
ZSIAUFGUXNUGDI-UHFFFAOYSA-N	5.1×10^{-1}	6100	Lei et al. (2007)	M	395
	3.9×10^{-1}	5800	Falabella et al. (2006)	M	11, 338
	3.8×10^{-1}		Souchon et al. (2004)	M	
	2.5×10^{-1}		van Ruth et al. (2002)	M	14
	7.3×10^{-1}		van Ruth and Villeneuve (2002)	M	14, 361
	1.6×10^{-1}		van Ruth et al. (2001)	M	14
	3.9×10^{-1}	5800	Gupta et al. (2000)	M	
	9.8×10^{-1}		Altschuh et al. (1999)	M	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.5×10^{-1}		Eger et al. (1999)	M	14
	5.8×10^{-1}		Merk and Riederer (1997)	M	
	6.4×10^{-1}		Li and Carr (1993)	M	
	6.9×10^{-1}		Rytting et al. (1978)	M	
	5.8×10^{-1}		Buttery et al. (1969)	M	
	5.3×10^{-1}		Mackay et al. (2006c)	V	
	5.3×10^{-1}		Mackay et al. (1995)	V	
	7.6×10^{-1}		Hwang et al. (1992)	V	
	1.7	5100	Djerki and Laub (1988)	V	
		8200	Abraham (1984)	V	
	6.4×10^{-1}		Hine and Mookerjee (1975)	V	
	6.4×10^{-1}		Butler et al. (1935)	V	
	5.2×10^{-1}		Yaws (2003)	X	258
	5.8×10^{-1}		Dupeux et al. (2022)	Q	259
	2.1×10^{-1}		Keshavarz et al. (2022)	Q	
	1.4		Duchowicz et al. (2020)	Q	299
	1.4×10^{-1}		Wang et al. (2017)	Q	80, 238
	5.0×10^{-1}		Wang et al. (2017)	Q	80, 239
	8.5×10^{-1}		Wang et al. (2017)	Q	80, 240
	6.4×10^{-1}		Li et al. (2014)	Q	241
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.7×10^{-1}		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	67
		7900	Kühne et al. (2005)	Q	
	4.1×10^{-1}		Yao et al. (2002)	Q	229, 267
	6.2×10^{-1}		English and Carroll (2001)	Q	230, 231
	1.5		Katritzky et al. (1998)	Q	
	4.7×10^{-1}		Yaws et al. (1997)	Q	
	3.9×10^{-1}		Russell et al. (1992)	Q	279
	5.1×10^{-1}		Suzuki et al. (1992)	Q	232
	6.2×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	5.8×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		8400	Kühne et al. (2005)	?	
	4.7×10^{-1}		Yaws (1999)	?	21
	5.3×10^{-1}		Yaws and Yang (1992)	?	21
	6.9×10^{-1}		Abraham et al. (1990)	?	
2-hexanol $C_6H_{14}O$ [626-93-7] QNVRIHYSUZMSGM-UHFFFAOYSA-N	3.9×10^{-1}	8100	Brockbank (2013)	L	1
	5.2×10^{-1}		Plyasunov and Shock (2000)	L	
	4.8×10^{-1}		Merk and Riederer (1997)	M	
	4.0×10^{-1}		Duchowicz et al. (2020)	V	186
	4.2×10^{-1}		Yaws (2003)	X	258
	7.3×10^{-1}		Dupeux et al. (2022)	Q	259
	5.4×10^{-1}		Duchowicz et al. (2020)	Q	
	1.7×10^{-1}		Wang et al. (2017)	Q	80, 238
	4.6×10^{-1}		Wang et al. (2017)	Q	80, 239

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Table A3.2: Alcohols (ROH) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.6×10^{-1}		Wang et al. (2017)	Q	80, 240
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-1}		Hilal et al. (2008)	Q	
	2.8×10^{-1}		Modarresi et al. (2007)	Q	67
	4.0×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.8×10^{-1}		Yao et al. (2002)	Q	229
	1.1		Katritzky et al. (1998)	Q	
	4.2×10^{-1}		Yaws et al. (1997)	Q	
	4.2×10^{-1}		Yaws (1999)	?	21
3-hexanol	3.7×10^{-1}	8400	Brockbank (2013)	L	1
$C_6H_{14}O$	4.2×10^{-1}	8400	Plyasunov and Shock (2000)	L	
[623-37-0]	2.5×10^{-1}		Duchowicz et al. (2020)	V	186
ZOCHHNOQQHDWHG-UHFFFAOYSA-N	2.3×10^{-1}		Meylan and Howard (1991)	V	
	2.0×10^{-1}		Hine and Mookerjee (1975)	V	
	3.9×10^{-1}	8400	Cabani et al. (1975b)	T	
	2.2×10^{-1}		Yaws (2003)	X	237
	5.4×10^{-1}		Duchowicz et al. (2020)	Q	
	1.7×10^{-1}		Wang et al. (2017)	Q	80, 238
	5.3×10^{-1}		Wang et al. (2017)	Q	80, 239
	2.5×10^{-1}		Wang et al. (2017)	Q	80, 240
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-1}		Gharagheizi et al. (2010)	Q	246
	2.8×10^{-1}		Hilal et al. (2008)	Q	
	4.1×10^{-1}		Modarresi et al. (2007)	Q	67
	4.0×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	5.8×10^{-1}		English and Carroll (2001)	Q	230, 231
	4.1×10^{-1}		Yaws et al. (1997)	Q	
	4.8×10^{-1}		Suzuki et al. (1992)	Q	232
	5.6×10^{-1}		Meylan and Howard (1991)	Q	
	6.0×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	3.9×10^{-1}		Abraham et al. (1990)	?	
2-methyl-1-pentanol	4.6×10^{-1}		Plyasunov and Shock (2000)	L	
$C_6H_{14}O$	2.3×10^{-1}		Duchowicz et al. (2020)	V	186
[105-30-6]	2.3×10^{-1}		HSDB (2015)	V	
PFNHSEQQEPMLNI-UHFFFAOYSA-N	5.4×10^{-1}		Duchowicz et al. (2020)	Q	
	1.7×10^{-1}		Wang et al. (2017)	Q	80, 238
	6.0×10^{-1}		Wang et al. (2017)	Q	80, 239
	5.5×10^{-1}		Wang et al. (2017)	Q	80, 240
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	4.4×10^{-1}		Hilal et al. (2008)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.6×10^{-1}		Modarresi et al. (2007)	Q	67
	3.1×10^{-1}		Yaws et al. (1997)	Q	
	3.1×10^{-1}		Yaws (1999)	?	21
3-methyl-1-pentanol	7.5×10^{-1}	8600	Brockbank (2013)	L	1
$C_6H_{14}O$	1.7×10^{-1}		Wang et al. (2017)	Q	80, 238
[589-35-5]	6.8×10^{-1}		Wang et al. (2017)	Q	80, 239
IWTBVKIGCDZRPL-UHFFFAOYSA-N	9.6×10^{-1}		Wang et al. (2017)	Q	80, 240
	3.3×10^{-1}		Gharagheizi et al. (2012)	Q	
	3.8×10^{-1}		Hilal et al. (2008)	Q	
2-methyl-2-pentanol	2.8×10^{-1}		Duchowicz et al. (2020)	V	186
$C_6H_{14}O$	3.1×10^{-1}		Hine and Mookerjee (1975)	V	
[590-36-3]	2.4×10^{-1}		Duchowicz et al. (2020)	Q	
WFRBDWRZVBPBDO-UHFFFAOYSA-N	1.0×10^{-1}		Wang et al. (2017)	Q	80, 238
	5.1×10^{-1}		Wang et al. (2017)	Q	80, 239
	3.9×10^{-1}		Wang et al. (2017)	Q	80, 240
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.2×10^{-1}		Hilal et al. (2008)	Q	
	7.7×10^{-1}		Modarresi et al. (2007)	Q	67
	2.9×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	6.2×10^{-1}		English and Carroll (2001)	Q	230, 231
	6.7×10^{-1}		Katritzky et al. (1998)	Q	
	5.0×10^{-1}		Yaws et al. (1997)	Q	
	3.9×10^{-1}		Suzuki et al. (1992)	Q	232
	4.7×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	3.1×10^{-1}		Abraham et al. (1990)	?	
3-methyl-2-pentanol	5.0×10^{-1}		Plyasunov and Shock (2000)	L	
$C_6H_{14}O$	1.7×10^{-1}		Wang et al. (2017)	Q	80, 238
[565-60-6]	8.1×10^{-1}		Wang et al. (2017)	Q	80, 239
ZXNBBWHRUSXUFZ-UHFFFAOYSA-N	3.6×10^{-1}		Wang et al. (2017)	Q	80, 240
	4.0×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	2.8×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-2-pentanol	2.2×10^{-1}	7300	Brockbank (2013)	L	1
$C_6H_{14}O$	3.5×10^{-1}		Plyasunov and Shock (2000)	L	
[108-11-2]	2.1×10^{-1}		Meylan and Howard (1991)	V	
WVYWICLMDOOCFB-UHFFFAOYSA-N	2.2×10^{-1}		Hine and Mookerjee (1975)	V	
	2.1×10^{-1}		Keshavarz et al. (2022)	Q	
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	
	1.7×10^{-1}		Wang et al. (2017)	Q	80, 238
	5.6×10^{-1}		Wang et al. (2017)	Q	80, 239
	4.7×10^{-1}		Wang et al. (2017)	Q	80, 240
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245

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Table A3.2: Alcohols (ROH) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	2.6×10^{-1}		Hilal et al. (2008)	Q	
	2.8×10^{-1}		Modarresi et al. (2007)	Q	67
		7900	Kühne et al. (2005)	Q	
	2.3×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	5.3×10^{-1}		Katritzky et al. (1998)	Q	
	1.9×10^{-1}		Yaws et al. (1997)	Q	
	4.0×10^{-1}		Suzuki et al. (1992)	Q	232
	5.6×10^{-1}		Meylan and Howard (1991)	Q	
	4.8×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	2.2×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		8700	Kühne et al. (2005)	?	
	2.1×10^{-1}		Yaws (1999)	?	21, 402
	2.2×10^{-1}		Abraham et al. (1990)	?	
2-methyl-3-pentanol	2.9×10^{-1}		Hine and Mookerjee (1975)	V	
$C_6H_{14}O$	1.7×10^{-1}		Wang et al. (2017)	Q	80, 238
[565-67-3]	6.9×10^{-1}		Wang et al. (2017)	Q	80, 239
ISTJMQSHILQAEC-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	80, 240
	3.3×10^{-1}		Hilal et al. (2008)	Q	
	5.8×10^{-1}		Modarresi et al. (2007)	Q	67
	2.9×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	3.7×10^{-1}		English and Carroll (2001)	Q	230, 274
	3.7×10^{-1}		Yaws et al. (1997)	Q	
	4.2×10^{-1}		Suzuki et al. (1992)	Q	232
	5.2×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	2.9×10^{-1}		Abraham et al. (1990)	?	
3-methyl-3-pentanol	2.4×10^{-1}	7300	Brockbank (2013)	L	1
$C_6H_{14}O$	4.7×10^{-1}		Plyasunov and Shock (2000)	L	
[77-74-7]	4.8×10^{-1}		Merk and Riederer (1997)	M	
FRDAATYAJDYRNW-UHFFFAOYSA-N	5.6×10^{-1}		Duchowicz et al. (2020)	V	186
	2.4×10^{-1}		Duchowicz et al. (2020)	Q	
	1.0×10^{-1}		Wang et al. (2017)	Q	80, 238
	5.5×10^{-1}		Wang et al. (2017)	Q	80, 239
	2.8×10^{-1}		Wang et al. (2017)	Q	80, 240
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.1×10^{-1}		Hilal et al. (2008)	Q	
	3.3×10^{-1}		Modarresi et al. (2007)	Q	67
	2.9×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	5.6×10^{-1}		Katritzky et al. (1998)	Q	
	7.0×10^{-1}		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-ethyl-1-butanol	5.4×10^{-1}		Plyasunov and Shock (2000)	L	
$C_6H_{14}O$	1.9×10^{-1}		Duchowicz et al. (2020)	V	186
[97-95-0]	5.4×10^{-1}		Duchowicz et al. (2020)	Q	
TZYRSLHNPKPEFV-UHFFFAOYSA-N	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	4.7×10^{-1}		Hilal et al. (2008)	Q	
	5.5×10^{-1}		Modarresi et al. (2007)	Q	67
	3.5×10^{-1}		Yao et al. (2002)	Q	229
	2.0		Katritzky et al. (1998)	Q	
	4.8×10^{-1}		Yaws et al. (1997)	Q	
	4.8×10^{-1}		Yaws (1999)	?	21
2,2-dimethyl-1-butanol	1.0×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O$	5.4×10^{-1}		Wang et al. (2017)	Q	80, 239
[1185-33-7]	2.7×10^{-1}		Wang et al. (2017)	Q	80, 240
XRMVWAKMXZNZIL-UHFFFAOYSA-N	4.0×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	2.8×10^{-1}		Yaws et al. (1997)	Q	
2,3-dimethyl-1-butanol	1.7×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O$	9.1×10^{-1}		Wang et al. (2017)	Q	80, 239
[19550-30-2]	5.1×10^{-1}		Wang et al. (2017)	Q	80, 240
SXSWMAUXEHKFGX-UHFFFAOYSA-N	8.2×10^{-1}		Yaws et al. (1997)	Q	
	4.2×10^{-1}		Suzuki et al. (1992)	Q	403, 232
	4.7×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
2,3-dimethyl-2-butanol	3.8×10^{-1}		Plyasunov and Shock (2000)	L	
$C_6H_{14}O$	9.9×10^{-1}		Duchowicz et al. (2020)	V	186
[594-60-5]	3.0×10^{-1}		Hine and Mookerjee (1975)	V	404
IKECULIHBUCAKR-UHFFFAOYSA-N	9.3×10^{-2}		Duchowicz et al. (2020)	Q	
	1.2×10^{-1}		Wang et al. (2017)	Q	80, 238
	6.3×10^{-1}		Wang et al. (2017)	Q	80, 239
	3.0×10^{-1}		Wang et al. (2017)	Q	80, 240
	2.0×10^{-1}		Hilal et al. (2008)	Q	
	2.4×10^{-1}		Modarresi et al. (2007)	Q	67
	1.0		Yaffe et al. (2003)	Q	248, 249
	6.0×10^{-1}		Katritzky et al. (1998)	Q	
3,3-dimethyl-1-butanol	1.0×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O$	5.6×10^{-1}		Wang et al. (2017)	Q	80, 239
[624-95-3]	1.6		Wang et al. (2017)	Q	80, 240
DUXCSEISVMREAX-UHFFFAOYSA-N	2.4×10^{-1}		Gharagheizi et al. (2012)	Q	
3,3-dimethyl-2-butanol	1.2×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O$	5.3×10^{-1}		Wang et al. (2017)	Q	80, 239
[464-07-3]	2.0×10^{-1}		Wang et al. (2017)	Q	80, 240
DFOXKPDFWGNLJU-UHFFFAOYSA-N	5.6×10^{-1}		HSDB (2015)	Q	99
	4.0×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	4.9×10^{-1}		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
2,2-bis(hydroxymethyl)-1-butanol	1.2×10^{6}		Duchowicz et al. (2020)	V	186
$C_6H_{14}O_3$	8.8×10^{5}		Duchowicz et al. (2020)	Q	
[77-99-6]					
ZJCCRDAZUWHFQH-UHFFFAOYSA-N					
1-heptanol	5.3×10^{-1}	8200	Brockbank (2013)	L	1
$C_7H_{16}O$	5.4×10^{-1}	8600	Plyasunov and Shock (2000)	L	
[111-70-6]	3.8×10^{-1}	7200	Shunthirasingham et al. (2013)	M	
BBMCTIGTTCKYKF-UHFFFAOYSA-N	3.6×10^{-1}	6300	Lei et al. (2007)	M	395
	8.6×10^{-1}		Altschuh et al. (1999)	M	
	1.8×10^{-1}		Shiu and Mackay (1997)	M	
	6.2×10^{-1}		Mackay et al. (2006c)	V	
	6.2×10^{-1}		Shiu and Mackay (1997)	V	
	6.2×10^{-1}		Mackay et al. (1995)	V	
	4.6	5300	Djerki and Laub (1988)	V	
	4.9×10^{-1}	8700	Abraham (1984)	V	
	5.3×10^{-1}		Hine and Mookerjee (1975)	V	
	5.2×10^{-1}		Butler et al. (1935)	V	
	5.2×10^{-1}		Yaws (2003)	X	258
	4.6×10^{-1}		Dupeux et al. (2022)	Q	259
	2.8×10^{-1}		Keshavarz et al. (2022)	Q	
	1.4		Duchowicz et al. (2020)	Q	
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.0×10^{-1}		Hilal et al. (2008)	Q	
	7.3×10^{-1}		Modarresi et al. (2007)	Q	67
		8300	Kühne et al. (2005)	Q	
	1.9×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.9×10^{-1}		Yao et al. (2002)	Q	229
	5.0×10^{-1}		English and Carroll (2001)	Q	230, 231
	1.3		Katritzky et al. (1998)	Q	
	5.2×10^{-1}		Yaws et al. (1997)	Q	
	1.8×10^{-1}		Russell et al. (1992)	Q	279
	3.9×10^{-1}		Suzuki et al. (1992)	Q	232
	5.0×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	3.8×10^{-1}		Rumble (2021)	?	405
	5.2×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		9400	Kühne et al. (2005)	?	
	5.2×10^{-1}		Yaws (1999)	?	21
	8.5×10^{-1}		Yaws and Yang (1992)	?	21
	5.0×10^{-1}		Abraham et al. (1990)	?	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-heptanol	3.3×10^{-1}	8700	Brockbank (2013)	L	1
$C_7H_{16}O$	4.1×10^{-1}		Plyasunov and Shock (2000)	L	
[543-49-7]	1.8×10^{-1}		Duchowicz et al. (2020)	V	186
CETWDUZRCINIHU-UHFFFAOYSA-N	1.2×10^{-1}		Yaws (2003)	X	258
	1.2×10^{-1}		Yaws (2003)	X	237, 38
	5.8×10^{-1}		Dupeux et al. (2022)	Q	259
	5.5×10^{-1}		Duchowicz et al. (2020)	Q	
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-1}		Gharagheizi et al. (2010)	Q	246
	2.0×10^{-1}		Hilal et al. (2008)	Q	
	2.5×10^{-1}		Modarresi et al. (2007)	Q	67
	2.6×10^{-1}		Yao et al. (2002)	Q	229
	1.2×10^{-1}		Yaws et al. (1997)	Q	
	1.7×10^{-1}		Yaws (1999)	?	21, 38
3-heptanol	3.2×10^{-1}	9100	Brockbank (2013)	L	1
$C_7H_{16}O$	3.1×10^{-1}		Plyasunov and Shock (2000)	L	
[589-82-2]	3.5×10^{-1}		Duchowicz et al. (2020)	V	186
RZKSECIXORKHQS-UHFFFAOYSA-N	5.5×10^{-1}		Duchowicz et al. (2020)	Q	
	1.3×10^{-1}		Wang et al. (2017)	Q	80, 238
	4.1×10^{-1}		Wang et al. (2017)	Q	80, 239
	2.2×10^{-1}		Wang et al. (2017)	Q	80, 240
	1.9×10^{-1}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	4.0×10^{-1}		Modarresi et al. (2007)	Q	67
	3.7×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	5.3×10^{-1}		Katritzky et al. (1998)	Q	
	2.1×10^{-1}		Yaws et al. (1997)	Q	
4-heptanol	3.4×10^{-1}	9100	Plyasunov and Shock (2000)	L	
$C_7H_{16}O$	3.5×10^{-1}	9100	Cabani et al. (1975b)	T	
[589-55-9]	1.8×10^{-1}		Gharagheizi et al. (2012)	Q	
YVBCULSIZWMTFY-UHFFFAOYSA-N	2.2×10^{-1}		Yaws et al. (1997)	Q	
2-methyl-1-hexanol	6.9×10^{-1}	11000	Hiatt (2013)	M	
$C_7H_{16}O$	1.7×10^{-1}		Yaws et al. (1997)	Q	
[624-22-6]					
LCFKURIJYIJNRU-UHFFFAOYSA-N					
3-methyl-1-hexanol	1.3×10^{-1}		Yaws et al. (1997)	Q	
$C_7H_{16}O$					
[13231-81-7]					
YGZVAQICDGBHMD-UHFFFAOYSA-N					

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methyl-1-hexanol $C_7H_{16}O$ [818-49-5] YNPVNLWKVZZBTM-UHFFFAOYSA-N	1.3×10^{-1}		Yaws et al. (1997)	Q	
5-methyl-1-hexanol $C_7H_{16}O$ [627-98-5] ZVHAANQOQZVVFD-UHFFFAOYSA-N	2.8×10^{-1}		Yaws et al. (1997)	Q	
2-methyl-2-hexanol $C_7H_{16}O$ [625-23-0] KRIMXCDMVRMCTC-UHFFFAOYSA-N	9.1×10^{-2} 4.0×10^{-1} 3.8×10^{-1} 6.7×10^{-1} 6.4×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) Yaffe et al. (2003) Yaws et al. (1997)	Q Q Q Q Q	80, 238 80, 239 80, 240 248, 249
3-methyl-2-hexanol $C_7H_{16}O$ [2313-65-7] IRLSKJITMWPWNY-UHFFFAOYSA-N	1.5×10^{-1} 1.7×10^{-1} 1.2×10^{-1} 4.9×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	237 246
4-methyl-2-hexanol $C_7H_{16}O$ [2313-61-3] KZUBXUKRWLMPIO-UHFFFAOYSA-N	1.6×10^{-1} 5.1×10^{-1} 4.7×10^{-1} 5.0×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) Yaws et al. (1997)	Q Q Q Q	80, 238 80, 239 80, 240
5-methyl-2-hexanol $C_7H_{16}O$ [627-59-8] ZDVJGWXFXGJSIU-UHFFFAOYSA-N	1.6×10^{-1} 4.3×10^{-1} 5.9×10^{-1} 2.4×10^{-1} 4.2×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) Gharagheizi et al. (2012) Yaws et al. (1997)	Q Q Q Q Q	80, 238 80, 239 80, 240
2-methyl-3-hexanol $C_7H_{16}O$ [617-29-8] RGRUUTLDBCWYBL-UHFFFAOYSA-N	5.8×10^{-1}		Yaws et al. (1997)	Q	
3-methyl-3-hexanol $C_7H_{16}O$ [597-96-6] KYWJZCSJMOILIZ-UHFFFAOYSA-N	9.1×10^{-2} 4.7×10^{-1} 2.6×10^{-1} 9.2×10^{-1} 7.7×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) Yaffe et al. (2003) Yaws et al. (1997)	Q Q Q Q Q	80, 238 80, 239 80, 240 248, 272
4-methyl-3-hexanol $C_7H_{16}O$ [615-29-2] NZPGYIBESMMUFU-UHFFFAOYSA-N	1.1×10^{-1} 1.0×10^{-1} 1.3×10^{-1} 5.2×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	237 246

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5-methyl-3-hexanol	1.6×10^{-1}		Yaws (2003)	X	237
$C_7H_{16}O$	1.5×10^{-1}		Gharagheizi et al. (2012)	Q	
[623-55-2]	1.2×10^{-1}		Gharagheizi et al. (2010)	Q	246
RGCZULIFYUPTAR-UHFFFAOYSA-N	5.4×10^{-1}		Yaws et al. (1997)	Q	
2-ethyl-1-pentanol	1.0×10^{-1}		Yaws (2003)	X	237
$C_7H_{16}O$	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
[27522-11-8]	1.1×10^{-1}		Gharagheizi et al. (2010)	Q	246
UKFQWAVMIMCNEH-UHFFFAOYSA-N	3.4×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-1-pentanol	9.1×10^{-2}		Yaws (2003)	X	237
$C_7H_{16}O$	1.7×10^{-1}		Gharagheizi et al. (2012)	Q	
[66225-51-2]	1.2×10^{-1}		Gharagheizi et al. (2010)	Q	246
DVEFUHVVWJONKR-UHFFFAOYSA-N	3.4×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-2-pentanol	1.1×10^{-1}		Yaws (2003)	X	237
$C_7H_{16}O$	1.7×10^{-1}		Gharagheizi et al. (2012)	Q	
[609-27-8]	1.2×10^{-1}		Gharagheizi et al. (2010)	Q	246
NEHRITNOSGFGGS-UHFFFAOYSA-N	4.9×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-3-pentanol	3.0×10^{-1}		Plyasunov and Shock (2000)	L	
$C_7H_{16}O$	1.2		Yaffe et al. (2003)	Q	248, 249
[597-49-9]	1.1		Yaws et al. (1997)	Q	
XKIRHOWVQWCYBT-UHFFFAOYSA-N					
2,2-dimethyl-1-pentanol	9.6×10^{-2}		Yaws (2003)	X	237
$C_7H_{16}O$	5.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[2370-12-9]	1.1×10^{-1}		Gharagheizi et al. (2010)	Q	246
QTOMCRXZFDHJOL-UHFFFAOYSA-N	3.3×10^{-1}		Yaws et al. (1997)	Q	
2,3-dimethyl-1-pentanol	3.6×10^{-1}		Yaws et al. (1997)	Q	
$C_7H_{16}O$					
[10143-23-4]					
MIBBFRQOCRYDDB-UHFFFAOYSA-N					
2,4-dimethyl-1-pentanol	9.4×10^{-2}		Yaws (2003)	X	237
$C_7H_{16}O$	9.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[6305-71-1]	1.0×10^{-1}		Gharagheizi et al. (2010)	Q	246
OVOVDHYEOQJKMD-UHFFFAOYSA-N	3.3×10^{-1}		Yaws et al. (1997)	Q	
3,3-dimethyl-1-pentanol	3.5×10^{-1}		Yaws et al. (1997)	Q	
$C_7H_{16}O$					
[19264-94-9]					
IFDHMBHPLKHMOY-UHFFFAOYSA-N					
3,4-dimethyl-1-pentanol	1.6×10^{-1}		Yaws (2003)	X	237
$C_7H_{16}O$	1.6×10^{-1}		Gharagheizi et al. (2012)	Q	
[6570-87-2]	1.1×10^{-1}		Gharagheizi et al. (2010)	Q	246
SVJNECJVNWTYQG-UHFFFAOYSA-N	3.5×10^{-1}		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,4-dimethyl-1-pentanol $C_7H_{16}O$ [3121-79-7] OWCNPTHAWPMOJU-UHFFFAOYSA-N	8.5×10^{-2} 1.4×10^{-1} 1.1×10^{-1} 3.8×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	237 246
2,3-dimethyl-2-pentanol $C_7H_{16}O$ [4911-70-0] YRSIFCHKXFKNME-UHFFFAOYSA-N	9.2×10^{-1} 8.6×10^{-1}		Yaffe et al. (2003) Yaws et al. (1997)	Q Q	248, 249
2,4-dimethyl-2-pentanol $C_7H_{16}O$ [625-06-9] FMLSQAUAAGVTJO-UHFFFAOYSA-N	4.0×10^{-1} 5.7×10^{-1}		Yaffe et al. (2003) Yaws et al. (1997)	Q Q	248, 272
3,3-dimethyl-2-pentanol $C_7H_{16}O$ [19781-24-9] FCUOIGTWJDBTHR-UHFFFAOYSA-N	9.0×10^{-2} 1.0×10^{-1} 1.2×10^{-1} 5.5×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	237 246
3,4-dimethyl-2-pentanol $C_7H_{16}O$ [64502-86-9] SODKTKJZYBOMMT-UHFFFAOYSA-N	1.8×10^{-1} 4.7×10^{-1}		Gharagheizi et al. (2012) Yaws et al. (1997)	Q Q	
4,4-dimethyl-2-pentanol $C_7H_{16}O$ [6144-93-0] OIBKGNPMOMMSSI-UHFFFAOYSA-N	6.8×10^{-1}		Yaws et al. (1997)	Q	
2,2-dimethyl-3-pentanol $C_7H_{16}O$ [3970-62-5] HMSVXZJWPVIVIV-UHFFFAOYSA-N	4.0×10^{-1} 4.0×10^{-1}		Yaffe et al. (2003) Yaws et al. (1997)	Q Q	248, 249
2,3-dimethyl-3-pentanol $C_7H_{16}O$ [595-41-5] RFZHJHSNHYIRNE-UHFFFAOYSA-N	9.2×10^{-1} 9.2×10^{-1}		Yaffe et al. (2003) Yaws et al. (1997)	Q Q	248, 249
2,4-dimethyl-3-pentanol $C_7H_{16}O$ [600-36-2] BAYAKMPRFGNNFW-UHFFFAOYSA-N	4.0×10^{-1} 3.8×10^{-1}		Yaffe et al. (2003) Yaws et al. (1997)	Q Q	248, 249
2-ethyl-2-methyl-1-butanol $C_7H_{16}O$ [18371-13-6] KMWHQWJVSALJAW-UHFFFAOYSA-N	4.3×10^{-1}		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-ethyl-3-methyl-1-butanol $C_7H_{16}O$ [32444-34-1] OXFFPTMSBXBVLZ-UHFFFAOYSA-N	3.8×10^{-1}		Yaws et al. (1997)	Q	
2,2,3-trimethyl-1-butanol $C_7H_{16}O$ [55505-23-2] FAMOAJMEFGYSNY-UHFFFAOYSA-N	8.3×10^{-2} 6.2×10^{-2} 1.0×10^{-1} 4.3×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	237 246
2,3,3-trimethyl-1-butanol $C_7H_{16}O$ [36794-64-6] IWWVOLGZHKFWKK-UHFFFAOYSA-N	7.9×10^{-2} 1.0×10^{-1} 1.0×10^{-1} 4.0×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	237 246
2,3,3-trimethyl-2-butanol $C_7H_{16}O$ [594-83-2] OKXVARYIKDXAEO-UHFFFAOYSA-N	2.7×10^{-1}		Yaws et al. (1997)	Q	
1-octanol $C_8H_{18}O$ [111-87-5] KBPLFHHGFOOTCA-UHFFFAOYSA-N	3.4×10^{-1} 4.1×10^{-1} 1.7×10^{-1} 2.1×10^{-1} 1.9×10^{-1} 6.5×10^{-1} 2.7×10^{-1} 4.0×10^{-1} 3.8×10^{-1} 2.4×10^{-1} 4.1×10^{-1} 4.1×10^{-1} 3.9×10^{-1} 3.6×10^{-1} 3.8×10^{-1} 1.4 3.3×10^{-1} 4.1×10^{-1} 2.5×10^{-1} 2.0×10^{-1} 3.1×10^{-1} 2.5×10^{-1} 5.6×10^{-1} 3.2×10^{-1} 2.6×10^{-1} 4.0×10^{-1} 1.2	9000 8900 7000 6900 6000 8900 8600 	Brockbank (2013) Plyasunov and Shock (2000) Wu et al. (2022a) Shunthirasingham et al. (2013) Lei et al. (2007) Altschuh et al. (1999) Eger et al. (1999) Buttery et al. (1969) Mackay et al. (2006c) Mackay et al. (1995) Abraham (1984) Hine and Mookerjee (1975) Butler et al. (1935) Yaws (2003) Dupeux et al. (2022) Keshavarz et al. (2022) Duchowicz et al. (2020) Savary et al. (2014) Li et al. (2014) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Kühne et al. (2005) Yaffe et al. (2003) Yao et al. (2002) English and Carroll (2001) Katritzky et al. (1998)	L L M M M M M M V V V V V X Q Q Q Q Q Q Q Q Q Q Q Q Q Q Q Q	1 395 14 258 259 299 241 242, 243 244 245 67 248, 272 229 230, 260

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	3.9×10^{-1}		Yaws et al. (1997)	Q	
	3.0×10^{-1}		Suzuki et al. (1992)	Q	232
	3.9×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	4.0×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		7700	Kühne et al. (2005)	?	
	3.9×10^{-1}		Yaws (1999)	?	21
	6.2×10^{-1}		Yaws and Yang (1992)	?	21
	4.0×10^{-1}		Abraham et al. (1990)	?	
2-octanol $C_8H_{18}O$ [123-96-6] SJWFXCIHNDVPSH-UHFFFAOYSA-N	2.7×10^{-1}	9600	Brockbank (2013)	L	1
	3.5×10^{-1}		Plyasunov and Shock (2000)	L	
	2.7×10^{-1}		HSDB (2015)	V	
	2.7×10^{-1}		Meylan and Howard (1991)	V	
	9.6×10^{-1}		Yaws (2003)	X	258
	4.2×10^{-1}		Dupeux et al. (2022)	Q	259
	3.8×10^{-1}		Keshavarz et al. (2022)	Q	
	5.6×10^{-1}		Duchowicz et al. (2020)	Q	299
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.7×10^{-1}		Hilal et al. (2008)	Q	
	2.0×10^{-1}		Modarresi et al. (2007)	Q	67
	3.0×10^{-1}		Yaws et al. (1997)	Q	
	3.2×10^{-1}		Meylan and Howard (1991)	Q	
	8.0×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	9.6×10^{-1}		Yaws (1999)	?	21
3-octanol $C_8H_{18}O$ [589-98-0] NMRPBPVERJPACX-UHFFFAOYSA-N	3.2×10^{-1}		Plyasunov and Shock (2000)	L	
	1.2×10^{-1}	8300	Wu et al. (2022a)	M	
	1.3×10^{-1}		Yaws (2003)	X	237
	1.1×10^{-1}		Wang et al. (2017)	Q	80, 238
	3.2×10^{-1}		Wang et al. (2017)	Q	80, 239
	2.3×10^{-1}		Wang et al. (2017)	Q	80, 240
	1.2×10^{-1}		Gharagheizi et al. (2012)	Q	
	7.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
	3.1×10^{-1}		Yaws et al. (1997)	Q	
4-octanol $C_8H_{18}O$ [589-62-8] WOFPPJOZXUTRAU-UHFFFAOYSA-N	1.3×10^{-1}		Gharagheizi et al. (2012)	Q	
	2.9×10^{-1}		Yaws et al. (1997)	Q	
2-methyl-1-heptanol $C_8H_{18}O$ [60435-70-3] QZESEQBMSFFHRY-UHFFFAOYSA-N	9.1×10^{-2}		Yaws (2003)	X	237
	5.7×10^{-2}		Gharagheizi et al. (2012)	Q	
	7.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
	3.4×10^{-1}		Yaws et al. (1997)	Q	406

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-1-heptanol $C_8H_{18}O$ [1070-32-2] MUPPEBVXFKNMCI-UHFFFAOYSA-N	8.9×10^{-2} 7.5×10^{-2} 2.1×10^{-1}		Yaws (2003) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q	237 246
4-methyl-1-heptanol $C_8H_{18}O$ [817-91-4] LLUQZGDMUIMPTC-UHFFFAOYSA-N	9.3×10^{-2} 7.5×10^{-2} 2.3×10^{-1}		Yaws (2003) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q	237 246
5-methyl-1-heptanol $C_8H_{18}O$ [7212-53-5] KFARNLMRENFOHE-UHFFFAOYSA-N	1.1×10^{-1} 2.1×10^{-1}		Gharagheizi et al. (2012) Yaws et al. (1997)	Q Q	
6-methyl-1-heptanol $C_8H_{18}O$ [1653-40-3] BWDBEAQIHAEVLV-UHFFFAOYSA-N	1.1×10^{-1} 1.1×10^{-1} 5.6×10^{-1} 2.0×10^{-1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Yaws et al. (1997)	V V Q Q	186
2-methyl-2-heptanol $C_8H_{18}O$ [625-25-2] ACBMYYVZWKYLIP-UHFFFAOYSA-N	5.1×10^{-1}		Yaws et al. (1997)	Q	
3-methyl-2-heptanol $C_8H_{18}O$ [31367-46-1] SZERMVMTUUAYML-UHFFFAOYSA-N	7.8×10^{-2} 9.5×10^{-2} 7.9×10^{-2} 3.9×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	237 246
4-methyl-2-heptanol $C_8H_{18}O$ [56298-90-9] GUHWHNUGIGOSCN-UHFFFAOYSA-N	1.6×10^{-1} 3.4×10^{-1}		Gharagheizi et al. (2012) Yaws et al. (1997)	Q Q	
5-methyl-2-heptanol $C_8H_{18}O$ [54630-50-1] FYMBAYNKBWGEIK-UHFFFAOYSA-N	1.0×10^{-1} 1.7×10^{-1} 7.7×10^{-2} 3.3×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	237 246
6-methyl-2-heptanol $C_8H_{18}O$ [4730-22-7] FCOUHTHQYOMLJT-UHFFFAOYSA-N	1.6×10^{-1} 3.3×10^{-1}		Gharagheizi et al. (2012) Yaws et al. (1997)	Q Q	
2-methyl-3-heptanol $C_8H_{18}O$ [18720-62-2] QGVFLDUEHSIZIG-UHFFFAOYSA-N	3.8×10^{-1}		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-3-heptanol $C_8H_{18}O$ [5582-82-1] PQOSNJHBSNZITJ-UHFFFAOYSA-N	2.9×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-3-heptanol $C_8H_{18}O$ [14979-39-6] BKQICAFAUMRYLZ-UHFFFAOYSA-N	7.4×10^{-2} 4.7×10^{-2} 8.2×10^{-2} 5.3×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	237 246
5-methyl-3-heptanol $C_8H_{18}O$ [18720-65-5] SECKOSOTZOBWEI-UHFFFAOYSA-N	8.7×10^{-2} 6.6×10^{-2} 7.9×10^{-2} 5.6×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	237 246
6-methyl-3-heptanol $C_8H_{18}O$ [18720-66-6] MNBIBGDICHMQFN-UHFFFAOYSA-N	8.8×10^{-2} 7.9×10^{-2} 7.9×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2-methyl-4-heptanol $C_8H_{18}O$ [21570-35-4] QXPLZEKPCGUWEM-UHFFFAOYSA-N	3.9×10^{-1}		Yaws et al. (1997)	Q	
3-methyl-4-heptanol $C_8H_{18}O$ [1838-73-9] JMRDKKYZLXDPLN-UHFFFAOYSA-N	8.2×10^{-2} 6.2×10^{-2} 8.2×10^{-2} 4.1×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	237 246
4-methyl-4-heptanol $C_8H_{18}O$ [598-01-6] IQXKGRKRIRMQCQ-UHFFFAOYSA-N	4.5×10^{-1}		Yaws et al. (1997)	Q	
2-ethyl-1-hexanol $C_8H_{18}O$ [104-76-7] YIWUKEYIRIRTPP-UHFFFAOYSA-N	4.6×10^{-1} 1.5×10^{-1} 3.7×10^{-1} 3.8×10^{-1} 5.6×10^{-1} 7.0×10^{-2} 2.5×10^{-1} 3.1×10^{-1} 3.1×10^{-1} 3.1×10^{-1} 4.0×10^{-1} 1.1×10^{-1} 4.3×10^{-1} 4.2×10^{-2}	7200	Plyasunov and Shock (2000) Wu et al. (2022a) Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Gharagheizi et al. (2012) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Yao et al. (2002) Yaws et al. (1997) Yaws (1999)	L M V V Q Q Q Q Q Q Q Q Q ?	 186 271, 243 244 245 67 229, 267 21

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-1-hexanol	7.0×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	9.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[41065-95-6]	7.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
LWWJDXKGQVEZKT-UHFFFAOYSA-N					
4-ethyl-1-hexanol	7.0×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	9.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[66576-32-7]	7.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
RLGDVTUGYZAYIX-UHFFFAOYSA-N					
2,2-dimethyl-1-hexanol	4.9×10^{-1}		Yaws et al. (1997)	Q	
$C_8H_{18}O$					
[2370-13-0]					
GSSDZVRLQDXOPL-UHFFFAOYSA-N					
2,3-dimethyl-1-hexanol	7.0×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	5.5×10^{-2}		Gharagheizi et al. (2012)	Q	
HIYTVAULOHUDEC-UHFFFAOYSA-N	6.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
2,4-dimethyl-1-hexanol	6.9×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	5.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[3965-59-1]	6.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
GDRBQWCGBCJTLB-UHFFFAOYSA-N	4.6×10^{-1}		Yaws et al. (1997)	Q	
2,5-dimethyl-1-hexanol	6.5×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	6.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[6886-16-4]	6.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
OBOHUKJIPIBYTA-UHFFFAOYSA-N	4.1×10^{-1}		Yaws et al. (1997)	Q	
3,3-dimethyl-1-hexanol	5.7×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	1.0×10^{-1}		Gharagheizi et al. (2012)	Q	
[10524-70-6]	7.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
RAKYQWCHMSXUEG-UHFFFAOYSA-N					
3,4-dimethyl-1-hexanol	6.3×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	9.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[66576-57-6]	7.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
QVFKMROLPSPCIX-UHFFFAOYSA-N					
3,5-dimethyl-1-hexanol	6.1×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
[13501-73-0]	7.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
WETBJXIDTZXCBL-UHFFFAOYSA-N	3.6×10^{-1}		Yaws et al. (1997)	Q	
4,4-dimethyl-1-hexanol	5.6×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	1.0×10^{-1}		Gharagheizi et al. (2012)	Q	
[6481-95-4]	7.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
VZWIUKUDEGQHIO-UHFFFAOYSA-N					

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
4,5-dimethyl-1-hexanol	6.2×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	1.0×10^{-1}		Gharagheizi et al. (2012)	Q	
[60564-76-3]	7.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
QABJATQYUASJEM-UHFFFAOYSA-N					
5,5-dimethyl-1-hexanol	5.6×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	1.0×10^{-1}		Gharagheizi et al. (2012)	Q	
[2768-18-5]	7.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
QYFVEEMPFRRFNN-UHFFFAOYSA-N					
3-ethyl-2-hexanol	7.7×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	1.0×10^{-1}		Gharagheizi et al. (2012)	Q	
[24448-19-9]	7.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
YBQZSEZVMFENOM-UHFFFAOYSA-N	5.6×10^{-1}		Yaws et al. (1997)	Q	
4-ethyl-2-hexanol	7.7×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	1.5×10^{-1}		Gharagheizi et al. (2012)	Q	
ALAPJJMGVQNJIU-UHFFFAOYSA-N	7.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
2,3-dimethyl-2-hexanol	7.0×10^{-1}		Yaws et al. (1997)	Q	
$C_8H_{18}O$					
[19550-03-9]					
BFKOEFFCVFMWPF-UHFFFAOYSA-N					
2,4-dimethyl-2-hexanol	8.9×10^{-1}		Yaws et al. (1997)	Q	
$C_8H_{18}O$					
[42328-76-7]					
RTRZHEPXWQXCCI-UHFFFAOYSA-N					
2,5-dimethyl-2-hexanol	8.5×10^{-1}		Yaws et al. (1997)	Q	
$C_8H_{18}O$					
[3730-60-7]					
JPUIYNHIEXIFMV-UHFFFAOYSA-N					
3,3-dimethyl-2-hexanol	7.5×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	5.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[22025-20-3]	7.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
LTTHCWFPLXSQOD-UHFFFAOYSA-N					
3,4-dimethyl-2-hexanol	6.8×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
[19550-05-1]	7.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
LBJWJHMCZHKLQU-UHFFFAOYSA-N	5.2×10^{-1}		Yaws et al. (1997)	Q	
3,5-dimethyl-2-hexanol	8.1×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	8.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[66576-27-0]	7.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
VGGMROOHXNLMTP-UHFFFAOYSA-N	7.0×10^{-1}		Yaws et al. (1997)	Q	
4,4-dimethyl-2-hexanol	7.2×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	1.3×10^{-1}		Gharagheizi et al. (2012)	Q	
CJGWLHDFPXIKQX-UHFFFAOYSA-N	7.4×10^{-2}		Gharagheizi et al. (2010)	Q	246

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,5-dimethyl-2-hexanol	7.9×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	1.3×10^{-1}		Gharagheizi et al. (2012)	Q	
KHSOOQUMPPYGAW-UHFFFAOYSA-N	7.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
5,5-dimethyl-2-hexanol	6.7×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	1.4×10^{-1}		Gharagheizi et al. (2012)	Q	
[31841-77-7]	7.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
NMSUCVXVCHZTEH-UHFFFAOYSA-N	6.0×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-3-hexanol	7.2×10^{-1}		Yaws et al. (1997)	Q	
$C_8H_{18}O$					
[597-76-2]					
WNDLTOTUHMHNOC-UHFFFAOYSA-N					
4-ethyl-3-hexanol	1.3×10^{-1}		Yaws (2003)	X	237
$C_8H_{18}O$	8.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
[19780-44-0]	6.3×10^{-1}		Yaws et al. (1997)	Q	
BOJLCKCCKQMGKD-UHFFFAOYSA-N					
2,2-dimethyl-3-hexanol	6.2×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	3.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[4209-90-9]	8.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
PFHLGQKVKALLMD-UHFFFAOYSA-N	7.8×10^{-1}		Yaws et al. (1997)	Q	
2,3-dimethyl-3-hexanol	7.4×10^{-1}		Yaws et al. (1997)	Q	
$C_8H_{18}O$					
[4166-46-5]					
CGWJMIUMPDDHQC-UHFFFAOYSA-N					
2,4-dimethyl-3-hexanol	7.0×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	3.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[13432-25-2]	8.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
UCRQJBCLZKHOGX-UHFFFAOYSA-N	7.0×10^{-1}		Yaws et al. (1997)	Q	
2,5-dimethyl-3-hexanol	7.2×10^{-1}		Yaws et al. (1997)	Q	
$C_8H_{18}O$					
[19550-07-3]					
SNKTZHPOKPYBPT-UHFFFAOYSA-N					
3,4-dimethyl-3-hexanol	8.6×10^{-1}		Yaws et al. (1997)	Q	
$C_8H_{18}O$					
[19550-08-4]					
FJXOYCIYKQJAAF-UHFFFAOYSA-N					
3,5-dimethyl-3-hexanol	8.9×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	1.4×10^{-1}		Gharagheizi et al. (2012)	Q	
[4209-91-0]	7.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
INMGJWCKWKKMPN-UHFFFAOYSA-N	8.6×10^{-1}		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
4,4-dimethyl-3-hexanol $C_8H_{18}O$ [19550-09-5] BARKHVPKOOSMNW-UHFFFAOYSA-N	7.2×10^{-1}		Yaws et al. (1997)	Q	
4,5-dimethyl-3-hexanol $C_8H_{18}O$ UAVZZCGGBCLHIP-UHFFFAOYSA-N	8.7×10^{-2} 4.9×10^{-2} 7.9×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
5,5-dimethyl-3-hexanol $C_8H_{18}O$ [66576-31-6] NPZRPUOKIPAIEL-UHFFFAOYSA-N	8.4×10^{-1}		Yaws et al. (1997)	Q	
2-propyl-1-pentanol $C_8H_{18}O$ [58175-57-8] LASHFHLFDRTERB-UHFFFAOYSA-N	4.1×10^{-1}		Yaws et al. (1997)	Q	
2-ethyl-2-methyl-1-pentanol $C_8H_{18}O$ [5970-63-8] VZCOFGHOKLEMPL-UHFFFAOYSA-N	4.3×10^{-1}		Yaws et al. (1997)	Q	
2-ethyl-3-methyl-1-pentanol $C_8H_{18}O$ ALPFTHGDLMTYRM-UHFFFAOYSA-N	6.7×10^{-2} 6.0×10^{-2} 6.8×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2-ethyl-4-methyl-1-pentanol $C_8H_{18}O$ [106-67-2] QCHSJPKDWOFACC-UHFFFAOYSA-N	4.4×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-2-methyl-1-pentanol $C_8H_{18}O$ VWQDMMBTEFDWNM-UHFFFAOYSA-N	6.9×10^{-2} 5.7×10^{-2} 6.8×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
3-ethyl-3-methyl-1-pentanol $C_8H_{18}O$ [10524-71-7] XYUCPYMMHKJJSS-UHFFFAOYSA-N	6.3×10^{-2} 8.4×10^{-2} 7.2×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
3-ethyl-4-methyl-1-pentanol $C_8H_{18}O$ [38514-13-5] RWIFVESHBHTZEM-UHFFFAOYSA-N	6.9×10^{-2} 8.3×10^{-2} 7.0×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2,2,3-trimethyl-1-pentanol $C_8H_{18}O$ [57409-53-7] GBONVOIRPAJSLA-UHFFFAOYSA-N	4.7×10^{-1}		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,4-trimethyl-1-pentanol $C_8H_{18}O$ [123-44-4] CWPPDTVYIJETDF-UHFFFAOYSA-N	5.6×10^{-1}		Yaws et al. (1997)	Q	
2,3,3-trimethyl-1-pentanol $C_8H_{18}O$ LFRFDOWJBYDJGD-UHFFFAOYSA-N	5.7×10^{-2} 6.0×10^{-2} 6.7×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
2,3,4-trimethyl-1-pentanol $C_8H_{18}O$ [6570-88-3] PAZDSSMTPLLLIR-UHFFFAOYSA-N	5.5×10^{-2} 7.3×10^{-2} 6.3×10^{-2} 3.6×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	237 246
2,4,4-trimethyl-1-pentanol $C_8H_{18}O$ [16325-63-6] ZNRVRWHPZZOTIE-UHFFFAOYSA-N	5.2×10^{-2} 5.2×10^{-1}		Gharagheizi et al. (2012) Yaws et al. (1997)	Q Q	
3,3,4-trimethyl-1-pentanol $C_8H_{18}O$ OIPMJJVCOSACDS-UHFFFAOYSA-N	6.2×10^{-2} 7.6×10^{-2} 6.9×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
3,4,4-trimethyl-1-pentanol $C_8H_{18}O$ [16325-64-7] FQNYRSRCONKFCN-UHFFFAOYSA-N	6.2×10^{-2} 7.6×10^{-2} 6.9×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
3-ethyl-2-methyl-2-pentanol $C_8H_{18}O$ [19780-63-3] FRUMTAZIGSJVOJ-UHFFFAOYSA-N	7.4×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-4-methyl-2-pentanol $C_8H_{18}O$ [66576-23-6] PFRFNYYIOSQSDD-UHFFFAOYSA-N	7.6×10^{-2} 9.1×10^{-2} 7.7×10^{-2} 6.3×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	237 246
2,3,3-trimethyl-2-pentanol $C_8H_{18}O$ [23171-85-9] FBWWGYIEJGQWJP-UHFFFAOYSA-N	8.0×10^{-2} 1.2×10^{-1} 6.8×10^{-2} 7.0×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	237 246
2,3,4-trimethyl-2-pentanol $C_8H_{18}O$ [66576-26-9] FTPXXARYDFWPGE-UHFFFAOYSA-N	7.2×10^{-2} 1.7×10^{-1} 6.9×10^{-2} 7.4×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yaws et al. (1997)	X Q Q Q	237 246
2,4,4-trimethyl-2-pentanol $C_8H_{18}O$ [690-37-9] BSYJHYLAMMJNRC-UHFFFAOYSA-N	9.9×10^{-1}		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3,4-trimethyl-2-pentanol	6.3×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	6.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[19411-41-7]	7.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
BOBYQFFCQPQLOB-UHFFFAOYSA-N	6.1×10^{-1}		Yaws et al. (1997)	Q	
3,4,4-trimethyl-2-pentanol	7.4×10^{-1}		Yaws et al. (1997)	Q	
$C_8H_{18}O$					
[10575-56-1]					
MXDGSCZQIMQLII-UHFFFAOYSA-N					
3-ethyl-2-methyl-3-pentanol	7.5×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	8.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[597-05-7]	7.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
DMHIJUVUPKCGLJ-UHFFFAOYSA-N	7.0×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-3-methyl-2-pentanol	7.5×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	5.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[66576-22-5]	7.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
SLBLSROGXMXPPF-UHFFFAOYSA-N					
2,2,3-trimethyl-3-pentanol	1.2		Yaffe et al. (2003)	Q	248, 249
$C_8H_{18}O$	1.1		Yaws et al. (1997)	Q	
[7294-05-5]					
KLIHWYNSISMOMR-UHFFFAOYSA-N					
2,2,4-trimethyl-3-pentanol	8.9×10^{-1}		Yaws et al. (1997)	Q	
$C_8H_{18}O$					
[5162-48-1]					
AXINNNJHLJWMTC-UHFFFAOYSA-N					
2,3,4-trimethyl-3-pentanol	6.4×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	7.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[3054-92-0]	7.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
PLSMHHUFDLYURK-UHFFFAOYSA-N	7.6×10^{-1}		Yaws et al. (1997)	Q	
3-methyl-2-(1-methylethyl)-1-butanol	6.6×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	5.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[18593-92-5]	6.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
IDGDEUZERZKYHG-UHFFFAOYSA-N	4.9×10^{-1}		Yaws et al. (1997)	Q	
2,2,3,3-tetramethyl-1-butanol	5.0×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66576-24-7]	6.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
OCTRJUXIYWWVAR-UHFFFAOYSA-N					
2,2-diethyl-1-butanol	6.5×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	3.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[13023-60-4]	7.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
CBHXDVOSUKFRBE-UHFFFAOYSA-N					

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-dimethyl-2-ethyl-1-butanol	6.0×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	3.7×10^{-2}		Gharagheizi et al. (2012)	Q	
YPIJDMPDVZUWJO-UHFFFAOYSA-N	6.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
3,3-dimethyl-2-ethyl-1-butanol	6.0×10^{-2}		Yaws (2003)	X	237
$C_8H_{18}O$	5.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[66576-56-5]	6.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
WOVMYJCSCISMAU-UHFFFAOYSA-N					
2-(hexyloxy)-ethanol	3.2		Duchowicz et al. (2020)	V	186
$C_8H_{18}O_2$	8.4		Duchowicz et al. (2020)	Q	
[112-25-4]					
UPGSWASWQBLSKZ-UHFFFAOYSA-N					
1-nonanol	2.7×10^{-1}	9300	Brockbank (2013)	L	1
$C_9H_{20}O$	1.1×10^{-1}	6300	Shunthirasingham et al. (2013)	M	
[143-08-8]	1.4×10^{-1}	6200	Lei et al. (2007)	M	407, 395
ZWRUINPWMLAQRD-UHFFFAOYSA-N	3.2×10^{-1}		Duchowicz et al. (2020)	V	186
	3.2×10^{-1}		HSDB (2015)	V	
	2.8×10^{-1}		Abraham (1984)	V	
	3.8×10^{-1}		Yaws (2003)	X	258
	3.5×10^{-1}		Dupeux et al. (2022)	Q	259
	5.4×10^{-1}		Abney (2021)	Q	399
	1.4		Duchowicz et al. (2020)	Q	
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	5.1×10^{-1}		Modarresi et al. (2007)	Q	67
	3.2×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.4×10^{-1}		Yao et al. (2002)	Q	229
	1.0		Katritzky et al. (1998)	Q	
	3.1×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	3.2×10^{-1}		Yaws et al. (1997)	Q	
	3.0×10^{-1}		Yaws (1999)	?	21
	5.9×10^{-1}		Yaws and Yang (1992)	?	21
	2.9×10^{-1}		Abraham et al. (1990)	?	
2-nonanol	2.1×10^{-1}	11000	Brockbank (2013)	L	1
$C_9H_{20}O$	6.5×10^{-2}		van Ruth et al. (2002)	M	14
[628-99-9]	4.9×10^{-1}		van Ruth and Villeneuve (2002)	M	14, 361
NGDNVOAEIVQRFH-UHFFFAOYSA-N	6.9×10^{-2}		van Ruth et al. (2001)	M	14
	2.0×10^{-1}		Duchowicz et al. (2020)	V	186
	5.6×10^{-1}		Duchowicz et al. (2020)	Q	
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.2×10^{-1}		Modarresi et al. (2007)	Q	67
	2.1×10^{-1}		Yao et al. (2002)	Q	229

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Table A3.2: Alcohols (ROH) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.4×10^{-1}		Yaws et al. (1997)	Q	
	2.0×10^{-1}		Yaws (1999)	?	21, 80
3-nonanol	5.2×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	9.6×10^{-2}		Wang et al. (2017)	Q	80, 238
[624-51-1]	2.6×10^{-1}		Wang et al. (2017)	Q	80, 239
GYSCXPVAKHVAAY-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	80, 240
	8.4×10^{-2}		Gharagheizi et al. (2012)	Q	
	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
	3.0×10^{-1}		Yaws et al. (1997)	Q	
4-nonanol	5.4×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	8.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[5932-79-6]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
IXUOEGRSQCCEHB-UHFFFAOYSA-N	3.1×10^{-1}		Yaws et al. (1997)	Q	
5-nonanol	5.2×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	8.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[623-93-8]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
FCBBRODPXVPZAH-UHFFFAOYSA-N	2.9×10^{-1}		Yaws et al. (1997)	Q	
2-methyl-1-octanol	4.8×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[818-81-5]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
IGVGCQGTEINVOH-UHFFFAOYSA-N					
3-methyl-1-octanol	4.8×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	6.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[38514-02-2]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
CLFSZAMBOZSCOS-UHFFFAOYSA-N					
4-methyl-1-octanol	4.8×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	6.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[38514-03-3]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
MWWKESKJRHQWEF-UHFFFAOYSA-N					
5-methyl-1-octanol	4.8×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	6.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[38514-04-4]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
CGCDFYUPZXVGIX-UHFFFAOYSA-N					
6-methyl-1-octanol	4.3×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
[38514-05-5]	2.1×10^{-1}		Yaws et al. (1997)	Q	
WWRGKAMABZHMCN-UHFFFAOYSA-N					
7-methyl-1-octanol	4.3×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
[2430-22-0]	2.1×10^{-1}		Yaws et al. (1997)	Q	
QDTDKYHPHANITQ-UHFFFAOYSA-N					

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-2-octanol	5.7×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	1.7×10^{-1}		Gharagheizi et al. (2012)	Q	
[628-44-4]	5.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
KBCNUEXDHWDIFX-UHFFFAOYSA-N	4.8×10^{-1}		Yaws et al. (1997)	Q	
3-methyl-2-octanol	6.0×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[27644-49-1]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
WQADSKJNOTZWML-UHFFFAOYSA-N					
5-methyl-2-octanol	6.0×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	8.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-81-5]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
IWFICVXFFNDWOJ-UHFFFAOYSA-N					
7-methyl-2-octanol	6.0×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	8.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-83-7]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
NOEKZKTXHKNMAQ-UHFFFAOYSA-N					
2-methyl-3-octanol	5.7×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[26533-34-6]	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
DIVBBSLQUDHECU-UHFFFAOYSA-N	4.1×10^{-1}		Yaws et al. (1997)	Q	
3-methyl-3-octanol	5.4×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.8×10^{-2}		Yaws (2003)	X	237
[5340-36-3]	1.3×10^{-1}		Gharagheizi et al. (2012)	Q	
JEWXYDDSLPIBBO-UHFFFAOYSA-N	1.6×10^{-1}		Gharagheizi et al. (2012)	Q	
	5.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
	5.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
	3.6×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-3-octanol	5.6×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-80-4]	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
XPWBBDBJJRZCPW-UHFFFAOYSA-N					
6-methyl-3-octanol	5.6×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	6.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[40225-75-0]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
MFYHIHFYDULUQP-UHFFFAOYSA-N					
7-methyl-3-octanol	5.6×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	6.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-84-8]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
IDCFJIMYNKBKMB-UHFFFAOYSA-N					

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Table A3.2: Alcohols (ROH) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-4-octanol	5.7×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	6.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[40575-41-5]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
BIAVIOIDPRPYJK-UHFFFAOYSA-N	4.1×10^{-1}		Yaws et al. (1997)	Q	
3-methyl-4-octanol	6.1×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[26533-35-7]	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
MJOKZMZDONULOD-UHFFFAOYSA-N	4.6×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-4-octanol	5.5×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	1.2×10^{-1}		Gharagheizi et al. (2012)	Q	
[23418-37-3]	5.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
RXSIKQJQLQRQQY-UHFFFAOYSA-N	4.5×10^{-1}		Yaws et al. (1997)	Q	
5-methyl-4-octanol	5.9×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[59734-23-5]	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
YLTHHPQUTLMNIF-UHFFFAOYSA-N					
6-methyl-4-octanol	5.9×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-82-6]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
KFRCBGHGDZSOJV-UHFFFAOYSA-N					
7-methyl-4-octanol	5.9×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[33933-77-6]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
KJMBBHZOLRRVMV-UHFFFAOYSA-N					
2-ethyl-1-heptanol	4.9×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[817-60-7]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
QNJAZNNWHWYOEO-UHFFFAOYSA-N					
3-ethyl-1-heptanol	4.2×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
[3525-25-5]	2.0×10^{-1}		Yaws et al. (1997)	Q	
VRZRVMXNGMZLDB-UHFFFAOYSA-N					
5-ethyl-1-heptanol	4.9×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
[998-65-2]					
GOJBFVJUMYSMJJ-UHFFFAOYSA-N					
3-ethyl-2-heptanol	5.9×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	7.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[19780-39-3]	5.8×10^{-2}		Gharagheizi et al. (2012)	Q	
MMQDVLWWGWJSFS-UHFFFAOYSA-N	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	246

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-3-heptanol	5.4×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	8.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[19780-41-7]	5.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
XKRZDNKKANUBPV-UHFFFAOYSA-N	4.3×10^{-1}		Yaws et al. (1997)	Q	
4-ethyl-4-heptanol	5.7×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	7.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[597-90-0]	5.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
GNROHGFUVTWFNG-UHFFFAOYSA-N	4.7×10^{-1}		Yaws et al. (1997)	Q	
2,2-dimethyl-1-heptanol	4.5×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	2.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[14250-79-4]	4.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
WENIXZFPXMQPQQ-UHFFFAOYSA-N	3.2×10^{-1}		Yaws et al. (1997)	Q	
4,6-dimethyl-1-heptanol	5.9×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[820-05-3]	4.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
GCBXGQPBCBPHSP-UHFFFAOYSA-N					
6,6-dimethyl-1-heptanol	5.4×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[65769-10-0]	4.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
IOFUAVGBFVXDAO-UHFFFAOYSA-N					
2,3-dimethyl-2-heptanol	5.0×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	1.3×10^{-1}		Gharagheizi et al. (2012)	Q	
[66794-00-1]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
PQSMEVPHTJECDZ-UHFFFAOYSA-N					
2,4-dimethyl-2-heptanol	5.0×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
[65822-93-7]					
VORBOMMQBCSRQF-UHFFFAOYSA-N					
2,5-dimethyl-2-heptanol	5.0×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
[1561-18-8]					
LVIFBEPHIBJBEU-UHFFFAOYSA-N					
2,6-dimethyl-2-heptanol	5.9×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	1.4×10^{-1}		Gharagheizi et al. (2012)	Q	
[13254-34-7]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
HGDVHRITTGWMJK-UHFFFAOYSA-N	5.8×10^{-1}		Yaws et al. (1997)	Q	
4,6-dimethyl-2-heptanol	4.4×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	1.2×10^{-1}		Gharagheizi et al. (2012)	Q	
[51079-52-8]	4.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
YYUGBYFBCFRGNZ-UHFFFAOYSA-N	3.1×10^{-1}		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5,6-dimethyl-2-heptanol	4.6×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	1.2×10^{-1}		Gharagheizi et al. (2012)	Q	
[58795-24-7]	4.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
ONBXNGYZXZBRJA-UHFFFAOYSA-N	3.2×10^{-1}		Yaws et al. (1997)	Q	
2,2-dimethyl-3-heptanol	5.3×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	2.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[19549-70-3]	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
QENWAAAGDINHGE-UHFFFAOYSA-N					
2,3-dimethyl-3-heptanol	5.7×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	7.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[19549-71-4]	5.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
JIEGVNXCNNWVPH-UHFFFAOYSA-N	5.4×10^{-1}		Yaws et al. (1997)	Q	
2,6-dimethyl-3-heptanol	6.1×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	3.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[19549-73-6]	5.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
XZDMJRIWJSNEGC-UHFFFAOYSA-N	5.2×10^{-1}		Yaws et al. (1997)	Q	
3,5-dimethyl-3-heptanol	5.4×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
[19549-74-7]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
NOSOEGQGQOMHBF-UHFFFAOYSA-N					
2,2-dimethyl-4-heptanol	5.7×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-99-5]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
ZIKNXBYJTDTRQA-UHFFFAOYSA-N	5.4×10^{-1}		Yaws et al. (1997)	Q	
2,4-dimethyl-4-heptanol	5.9×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	9.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[19549-77-0]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
QKRRAXACNUNGCF-UHFFFAOYSA-N	5.7×10^{-1}		Yaws et al. (1997)	Q	
2,5-dimethyl-4-heptanol	1.6×10^{-1}		Yaws et al. (1997)	Q	
$C_9H_{20}O$					
NXLQTSHQSAVKJB-UHFFFAOYSA-N					
2,6-dimethyl-4-heptanol	1.0×10^{-1}	9300	Brockbank (2013)	L	1
$C_9H_{20}O$	7.7×10^{-2}		Duchowicz et al. (2020)	V	186
[108-82-7]	8.6×10^{-2}		Duchowicz et al. (2020)	Q	
HXQPUEQDBSPXTE-UHFFFAOYSA-N	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.7×10^{-1}		Hilal et al. (2008)	Q	
	3.7×10^{-1}		Modarresi et al. (2007)	Q	67
	1.6×10^{-1}		Katritzky et al. (1998)	Q	
	1.7×10^{-1}		Yaws et al. (1997)	Q	
	1.7×10^{-1}		Yaws (1999)	?	21

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3-dimethyl-4-heptanol	5.5×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	2.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[19549-78-1]	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
UGAZGYFCTFGQQH-UHFFFAOYSA-N	2.2×10^{-1}		Yaws et al. (1997)	Q	
3,5-dimethyl-4-heptanol	5.0×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	3.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[19549-79-2]	5.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
ZKXITRNXHWEQJU-UHFFFAOYSA-N					
3,6-dimethyl-3-heptanol	6.8×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	1.0×10^{-1}		Gharagheizi et al. (2012)	Q	
[1573-28-0]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
HVPGGLNDHUWMLS-UHFFFAOYSA-N					
2-ethyl-3-methyl-1-hexanol	4.9×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	3.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[66794-04-5]	4.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
DXXCMAAACWSRPE-UHFFFAOYSA-N					
2-ethyl-4-methyl-1-hexanol	4.7×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[66794-06-7]	4.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
NRZVENBFUFCASY-UHFFFAOYSA-N	1.2×10^{-1}		Yaws et al. (1997)	Q	
2-ethyl-5-methyl-1-hexanol	4.9×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	3.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[66794-07-8]	4.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
KVJOUCNJVQBRAO-UHFFFAOYSA-N					
3-ethyl-1-methyl-1-hexanol	5.0×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	1.2×10^{-1}		Gharagheizi et al. (2012)	Q	
YNZQSDTXBBBFQH-UHFFFAOYSA-N	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
3-ethyl-2-methyl-1-hexanol	1.3×10^{-1}		Yaws et al. (1997)	Q	
$C_9H_{20}O$					
[66794-01-2]					
UDZCUJOKBNABRS-UHFFFAOYSA-N					
3,3,5-trimethyl-1-hexanol	4.1×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[1484-87-3]	4.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
HRXNWQMMTLLJJQ-UHFFFAOYSA-N					
3,4,4-trimethyl-1-hexanol	4.2×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-73-5]	4.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
OLRPKAJSAOYYCY-UHFFFAOYSA-N	1.4×10^{-1}		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,5,5-trimethyl-1-hexanol	4.1×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[3452-97-9]	4.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
BODRLKRKPXBDBN-UHFFFAOYSA-N	1.3×10^{-1}		Yaws et al. (1997)	Q	
4,5,5-trimethyl-1-hexanol	3.4×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	7.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-75-7]	4.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
IECJUMYEWJOKHM-UHFFFAOYSA-N	9.4×10^{-2}		Yaws et al. (1997)	Q	
2-propyl-1-hexanol	5.8×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	3.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[817-46-9]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
JSUXZEJWGVYJJG-UHFFFAOYSA-N					
3-propyl-1-hexanol	5.8×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-85-9]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
MHJIVMDBOGBUHH-UHFFFAOYSA-N					
3-ethyl-2-methyl-2-hexanol	5.3×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	1.2×10^{-1}		Gharagheizi et al. (2012)	Q	
[66794-02-3]	5.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
HTOYXTGJEOUKPM-UHFFFAOYSA-N	2.1×10^{-1}		Yaws et al. (1997)	Q	
2,3,4-trimethyl-2-hexanol	3.7×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
[21102-13-6]					
JTOONBKGYWVPOY-UHFFFAOYSA-N					
2,4,4-trimethyl-2-hexanol	3.4×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66793-91-7]					
QMEHJTXRYVSFES-UHFFFAOYSA-N					
2,4,5-trimethyl-2-hexanol	3.7×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66793-93-9]					
CIVZBWYMPDUPSQ-UHFFFAOYSA-N					
2,5,5-trimethyl-2-hexanol	3.4×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66793-71-3]					
ASOCSFZHADJKFU-UHFFFAOYSA-N					
3-ethyl-2-methyl-3-hexanol	4.8×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	6.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[66794-03-4]	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
VUMFTWNZYFBYEB-UHFFFAOYSA-N	1.7×10^{-1}		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-ethyl-4-methyl-3-hexanol	5.2×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[51200-80-7]	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
YOCLWWFBEJQTBM-UHFFFAOYSA-N					
3-ethyl-5-methyl-3-hexanol	5.8×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	6.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[597-77-3]	5.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
RMBUNHOAKTUXTC-UHFFFAOYSA-N	2.5×10^{-1}		Yaws et al. (1997)	Q	
4-ethyl-2-methyl-3-hexanol	5.7×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	2.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[33943-21-4]	5.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
GBUYIUMHXYBONU-UHFFFAOYSA-N					
4-ethyl-3-methyl-3-hexanol	5.2×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	8.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[66794-05-6]	5.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
DUGZCTGTSJAPCV-UHFFFAOYSA-N					
2,2,3-trimethyl-3-hexanol	4.8×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[5340-41-0]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
DHNHHYWBZNQHGN-UHFFFAOYSA-N	2.4×10^{-1}		Yaws et al. (1997)	Q	
2,2,4-trimethyl-3-hexanol	5.7×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66793-89-3]	2.7×10^{-1}		Yaws et al. (1997)	Q	
YMBVVPXERVAJTB-UHFFFAOYSA-N					
2,2,5-trimethyl-3-hexanol	6.6×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
[3970-60-3]	3.4×10^{-1}		Yaws et al. (1997)	Q	
UCLXUUYVWJKXIK-UHFFFAOYSA-N					
2,3,4-trimethyl-3-hexanol	6.0×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66793-90-6]					
LTKHKGAPVGSECA-UHFFFAOYSA-N					
2,3,5-trimethyl-3-hexanol	6.0×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
[65927-60-8]					
ZVKQNIUBLJYSGN-UHFFFAOYSA-N					
2,4,4-trimethyl-3-hexanol	5.5×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66793-92-8]	2.5×10^{-1}		Yaws et al. (1997)	Q	
PDIVDRVTPZNRDZ-UHFFFAOYSA-N					

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Table A3.2: Alcohols (ROH) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,5,5-trimethyl-3-hexanol	5.7×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	2.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-72-4]	5.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
NPUIBFBNZSKEAP-UHFFFAOYSA-N					
3,4,4-trimethyl-3-hexanol	5.5×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66793-74-6]	2.9×10^{-1}		Yaws et al. (1997)	Q	
QWJDXMFJOMPTCV-UHFFFAOYSA-N					
3,5,5-trimethyl-3-hexanol	5.5×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66810-87-5]					
HGGJNDQMXCTKCR-UHFFFAOYSA-N					
4-methyl-2-propyl-1-pentanol	5.0×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[54004-41-0]	4.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
IGSWOIOCVJEQRH-UHFFFAOYSA-N	1.3×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-2-(1-methylethyl)-1-pentanol	5.0×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	3.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[55505-24-3]	4.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
CBHPZSADBWMIGE-UHFFFAOYSA-N	1.6×10^{-1}		Yaws et al. (1997)	Q	
2-ethyl-2,4-dimethyl-1-pentanol	4.4×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	2.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-98-4]	4.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
JIZZVMCXCCJUHI-UHFFFAOYSA-N	1.5×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-2,2-dimethyl-1-pentanol	4.5×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	2.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-95-1]	4.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
HEQYMZTUSVDQBW-UHFFFAOYSA-N					
2,3,3,4-tetramethyl-2-pentanol	3.9×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	8.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-86-0]	4.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
HLWCPAJEXXTJHY-UHFFFAOYSA-N					
2,3,4,4-tetramethyl-2-pentanol	3.9×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	1.3×10^{-1}		Gharagheizi et al. (2012)	Q	
[66793-87-1]	4.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
DBCCRNKDJIOKIO-UHFFFAOYSA-N					
3,3,4,4-tetramethyl-2-pentanol	3.9×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-88-2]	4.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
AIQOKYGLKGGWOI-UHFFFAOYSA-N	2.0×10^{-1}		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3-diethyl-2-pentanol	4.5×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-94-0]	5.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
IENXYHLNFHBNRR-UHFFFAOYSA-N					
2,3-dimethyl-3-ethyl-2-pentanol	3.7×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
[66793-97-3]	4.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
AVQHNUMJCWRCBA-UHFFFAOYSA-N					
4,4-dimethyl-3-ethyl-2-pentanol	4.1×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	7.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[21102-09-0]	4.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
YGQDLQQRBCOMKJ-UHFFFAOYSA-N					
3-ethyl-2,2-dimethyl-3-pentanol	4.8×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	3.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-96-2]	5.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
CFWIFHZJKFFDFU-UHFFFAOYSA-N	2.3×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-2,4-dimethyl-3-pentanol	4.9×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	4.8×10^{-2}		Yaws (2003)	X	237
[3970-59-0]	3.7×10^{-2}		Gharagheizi et al. (2012)	Q	
PZPYIRQFCOFLGJ-UHFFFAOYSA-N	3.6×10^{-2}		Gharagheizi et al. (2012)	Q	
	5.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
	5.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.1×10^{-1}		Yaws et al. (1997)	Q	
2,2,3,4-tetramethyl-3-pentanol	4.4×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	3.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[29772-39-2]	4.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
KNTFAYXQHRNXSM-UHFFFAOYSA-N	2.3×10^{-1}		Yaws et al. (1997)	Q	
2,2,4,4-tetramethyl-3-pentanol	5.0×10^{-2}		Yaws (2003)	X	237
$C_9H_{20}O$	5.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
[14609-79-1]	2.8×10^{-1}		Yaws et al. (1997)	Q	
WFJSIIHYYLHRHB-UHFFFAOYSA-N					
1-decanol	2.0×10^{-1}	9200	Brockbank (2013)	L	1, 408
$C_{10}H_{22}O$	7.6×10^{-2}	6600	Shunthirasingham et al. (2013)	M	
[112-30-1]	6.5×10^{-2}	5300	Lei et al. (2007)	M	395
MWKFXSUHUHTGQN-UHFFFAOYSA-N	3.1×10^{-1}		Altschuh et al. (1999)	M	
	1.9×10^{-1}		Abraham (1984)	V	
	2.1×10^{-1}		Yaws (2003)	X	258
	2.8×10^{-1}		Dupeux et al. (2022)	Q	259
	1.3×10^{-1}		Keshavarz et al. (2022)	Q	
	1.5		Duchowicz et al. (2020)	Q	
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-1}		Hilal et al. (2008)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.6×10^{-1}		Modarresi et al. (2007)	Q	67
	2.1×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.2×10^{-1}		Yao et al. (2002)	Q	229
	9.9×10^{-1}		Katritzky et al. (1998)	Q	
	2.4×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	2.1×10^{-1}		Yaws et al. (1997)	Q	
	3.1×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	4.4×10^{-2}		Maniere et al. (2011)	?	241, 165
	2.1×10^{-1}		Yaws (1999)	?	21
	3.7×10^{-1}		Yaws and Yang (1992)	?	21
	1.9×10^{-1}		Abraham et al. (1990)	?	
2-decanol $C_{10}H_{22}O$ [1120-06-5] ACUZDYFTRHEKOS-UHFFFAOYSA-N	5.4×10^{-1}		Yaws et al. (1997)	Q	
3-decanol	3.8×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	7.8×10^{-2}		Wang et al. (2017)	Q	80, 238
[1565-81-7]	2.1×10^{-1}		Wang et al. (2017)	Q	80, 239
ICEQLCZWZXUUIJ-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	80, 240
	7.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
4-decanol	3.8×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	7.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[2051-31-2]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
DTDMYWXTWWFLGJ-UHFFFAOYSA-N	5.3×10^{-1}		Yaws et al. (1997)	Q	
5-decanol	4.5×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	6.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[5205-34-5]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
SZMNDOUFZGODBR-UHFFFAOYSA-N	7.3×10^{-1}		Yaws et al. (1997)	Q	
2-methyl-1-nonanol	3.0×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
[40589-14-8]	3.4×10^{-1}		Yaws et al. (1997)	Q	
BEGNRPGEHZBNKK-UHFFFAOYSA-N					
2-methyl-2-nonanol	2.9×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
[10297-57-1]					
VREDNSVJXRJXRI-UHFFFAOYSA-N					
2-methyl-3-nonanol	3.6×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[26533-33-5]	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
OFIYMUXECPHIPZ-UHFFFAOYSA-N	5.7×10^{-1}		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-4-nonanol	3.6×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	5.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[26533-31-3]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
IBHHTADZYDLHPM-UHFFFAOYSA-N					
2-methyl-5-nonanol	3.6×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	5.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[29843-62-7]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
RLQVUGAVOCBRNQ-UHFFFAOYSA-N					
3-methyl-1-nonanol	3.5×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[22663-64-5]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
BXQPYGLPOMTAPU-UHFFFAOYSA-N					
3-methyl-2-nonanol	3.2×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	5.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[60671-32-1]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
QCBDLZKDRUKOFS-UHFFFAOYSA-N					
3-methyl-3-nonanol	3.2×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
[21078-72-8]	4.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
VZBFPIMCUSPDLS-UHFFFAOYSA-N					
3-methyl-5-nonanol	3.6×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	5.1×10^{-2}		Gharagheizi et al. (2012)	Q	
QRZAYHZIHWIJHD-UHFFFAOYSA-N	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
4-methyl-1-nonanol	3.1×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[1489-47-0]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
HECVGHIJHFNAIL-UHFFFAOYSA-N					
4-methyl-4-nonanol	3.2×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
[23418-38-4]	4.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
GDCOAKPWVJCNGI-UHFFFAOYSA-N					
5-methyl-1-nonanol	3.5×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[2768-16-3]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
DBJSFYCKLLBKGB-UHFFFAOYSA-N					
5-methyl-2-nonanol	3.2×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	8.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[66731-95-1]	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
KZTLXVUOEODDMR-UHFFFAOYSA-N					

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
5-methyl-3-nonanol	3.6×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	5.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-43-5]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
CCSZLOPBDJWYHV-UHFFFAOYSA-N					
5-methyl-4-nonanol	3.6×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-44-6]	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
BFYIAYZULSQBFQ-UHFFFAOYSA-N					
5-methyl-5-nonanol	4.9×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	9.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[33933-78-7]	4.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
AGSIGVZAVLOKLP-UHFFFAOYSA-N					
6-methyl-2-nonanol	3.2×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	8.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-60-8]	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
OYTRLQQQIHEJFE-UHFFFAOYSA-N					
7-methyl-1-nonanol	3.5×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[33234-93-4]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
BJKXZCGJAOWNTN-UHFFFAOYSA-N					
7-methyl-2-nonanol	3.2×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66256-61-9]					
GCOBJHFUTQUABB-UHFFFAOYSA-N					
7-methyl-4-nonanol	3.6×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	5.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[26981-98-6]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
KLZAWUYSXUGWGQ-UHFFFAOYSA-N					
8-methyl-1-nonanol	1.8×10^{-1}		HSDB (2015)	Q	99
$C_{10}H_{22}O$					
(isodecanol)					
[25339-17-7]					
PLLBRTOLHQQAQQ-UHFFFAOYSA-N					
8-methyl-2-nonanol	3.2×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	8.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[14779-92-1]	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
ZVZKLBCGIYWGOU-UHFFFAOYSA-N					
2,2-dimethyl-1-octanol	3.3×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	1.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[2370-14-1]	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
KEXGXAGJHHCTKD-UHFFFAOYSA-N	5.7×10^{-1}		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2-dimethyl-3-octanol	3.9×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	1.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[19841-72-6]	4.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
AZIWNYAWODSERA-UHFFFAOYSA-N					
2,2-dimethyl-4-octanol	4.2×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-52-6]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
IVLDCRDTRQCTIY-UHFFFAOYSA-N	1.0		Yaws et al. (1997)	Q	
2,3-dimethyl-3-octanol	4.2×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[19781-10-3]	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
AWHYRPPRRQITHX-UHFFFAOYSA-N	1.0		Yaws et al. (1997)	Q	
2,4-dimethyl-2-octanol	2.7×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
[18675-20-2]					
WHJCLXRXPLJSSV-UHFFFAOYSA-N					
2,4-dimethyl-4-octanol	4.1×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	6.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[33933-79-8]	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
VRFMFHBPJUSGFK-UHFFFAOYSA-N					
2,5-dimethyl-4-octanol	4.5×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	2.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-53-7]	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
VIHAZZPWGKHJQE-UHFFFAOYSA-N					
2,6-dimethyl-1-octanol	3.5×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	2.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[62417-08-7]	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
ZKWASVBZSAGDBI-UHFFFAOYSA-N					
2,6-dimethyl-2-octanol	2.7×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
[18479-57-7]					
WRFXXJKURVTLSY-UHFFFAOYSA-N					
2,6-dimethyl-4-octanol	3.5×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-54-8]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
ZFOGJEKQQNVCFB-UHFFFAOYSA-N					
2,7-dimethyl-2-octanol	2.7×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
[42007-73-8]					
JJZZVQICFJITMO-UHFFFAOYSA-N					

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Table A3.2: Alcohols (ROH) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,7-dimethyl-3-octanol	4.3×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	2.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-55-9]	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
VFUOFVONEDBLIJ-UHFFFAOYSA-N	9.0×10^{-1}		Yaws et al. (1997)	Q	
2,7-dimethyl-4-octanol	2.3×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[19781-11-4]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
FRJOBNOTOHIMIH-UHFFFAOYSA-N					
3,4-dimethyl-4-octanol	4.1×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-30-0]	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
JEBZCASOCDXENQ-UHFFFAOYSA-N					
3,5-dimethyl-3-octanol	4.0×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	7.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[56065-42-0]	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
DMIBTMSBSULJMT-UHFFFAOYSA-N					
3,6-dimethyl-3-octanol	4.0×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	6.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[151-19-9]	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
NPHCXUPGMINOPP-UHFFFAOYSA-N	9.6×10^{-1}		Yaws et al. (1997)	Q	
3,6-dimethyl-4-octanol	4.5×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	2.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-31-1]	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
XFUFFAQPWAGSDK-UHFFFAOYSA-N					
3,7-dimethyl-1-octanol	3.3×10^{-2}		Yaws (2003)	X	258
$C_{10}H_{22}O$	3.3×10^{-2}		Yaws (2003)	X	237
(pelargol)	3.7×10^{-1}		Dupeux et al. (2022)	Q	259
[106-21-8]	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
PRNCMAKCNVRZFX-UHFFFAOYSA-N	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
	5.0×10^{-1}		Yaws et al. (1997)	Q	
3,7-dimethyl-2-octanol	3.0×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	5.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[15340-96-2]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
XCWMPEYBKUYTLZ-UHFFFAOYSA-N					
3,7-dimethyl-3-octanol	3.7×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	7.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[78-69-3]	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
DLHQZZUEERVIGQ-UHFFFAOYSA-N	8.5×10^{-1}		Yaws et al. (1997)	Q	
4,5-dimethyl-1-octanol	3.3×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-32-2]	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
UQKHXPAWOMZBLN-UHFFFAOYSA-N					

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,6-dimethyl-1-octanol	3.3×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-33-3]	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
JOWDWXPTKVUHBV-UHFFFAOYSA-N					
4,6-dimethyl-4-octanol	4.1×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	6.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[56065-43-1]	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
QJVDAQVYZBSYCB-UHFFFAOYSA-N					
4,7-dimethyl-1-octanol	3.3×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-34-4]	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
UWAGZVFFZJGLJU-UHFFFAOYSA-N					
4,7-dimethyl-4-octanol	4.0×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	6.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[19781-13-6]	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
OTISWHNJCUMBFI-UHFFFAOYSA-N	9.6×10^{-1}		Yaws et al. (1997)	Q	
7,7-dimethyl-1-octanol	3.0×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-35-5]	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
RYFZXYQQFYLUHM-UHFFFAOYSA-N					
2-ethyl-1-octanol	3.9×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	2.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[20592-10-3]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
HTRVTKUOKQWGMO-UHFFFAOYSA-N					
3-ethyl-1-octanol	3.9×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-36-6]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
VXOCEIUJVCHLRR-UHFFFAOYSA-N					
3-ethyl-3-octanol	3.9×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	5.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[2051-32-3]	4.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
NPQPNSNHYJTUSA-UHFFFAOYSA-N	7.7×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-4-octanol	4.8×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	2.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[63126-48-7]	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
WXJDPIWUPZLVSF-UHFFFAOYSA-N					
4-ethyl-4-octanol	4.3×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[38395-42-5]	4.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
OYBUBRUQIKTRET-UHFFFAOYSA-N					

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
6-ethyl-3-octanol	4.3×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[19781-27-2]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
JWZFCOOWAQHCBP-UHFFFAOYSA-N					
2,2,3-trimethyl-3-heptanol	3.7×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	2.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[29772-40-5]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
GCLFPNQSLCWZAQ-UHFFFAOYSA-N	1.1		Yaws et al. (1997)	Q	
2,2,4-trimethyl-4-heptanol	4.1×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
[57233-31-5]	1.3		Yaws et al. (1997)	Q	
KNACVESXMPHLNM-UHFFFAOYSA-N					
2,2,5-trimethyl-4-heptanol	4.4×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66256-42-6]					
JHHGGYCQTXZCTL-UHFFFAOYSA-N					
2,2,6-trimethyl-3-heptanol	3.8×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	1.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-43-7]	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
AXUPPSSNJCYJOX-UHFFFAOYSA-N					
2,2,6-trimethyl-4-heptanol	4.4×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66256-44-8]					
ITTQYDBLGDGLMB-UHFFFAOYSA-N					
2,3,6-trimethyl-3-heptanol	3.8×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[58046-40-5]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
BAZNZYUOJWCTIQ-UHFFFAOYSA-N					
2,4,5-trimethyl-4-heptanol	4.4×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66256-46-0]					
RCSCLTAIPNDFGC-UHFFFAOYSA-N					
2,4,6-trimethyl-2-heptanol	3.6×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	1.0×10^{-1}		Gharagheizi et al. (2012)	Q	
[66256-47-1]	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
VUZHXHGZVRACMM-UHFFFAOYSA-N					
2,4,6-trimethyl-4-heptanol	4.4×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
[60836-07-9]	1.3		Yaws et al. (1997)	Q	
QSVYJSJPLCSACO-UHFFFAOYSA-N					

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,5,6-trimethyl-2-heptanol	3.6×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
[66256-48-2]	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
LQQYOLMGDBGEBC-UHFFFAOYSA-N	9.3×10^{-1}		Yaws et al. (1997)	Q	
3,3,6-trimethyl-4-heptanol	4.4×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
LTDMOZOPTDNTLG-UHFFFAOYSA-N					
3,5,5-trimethyl-3-heptanol	3.1×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	7.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-50-6]	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
WOUVARFKMJIYBY-UHFFFAOYSA-N	8.6×10^{-1}		Yaws et al. (1997)	Q	
4,6,6-trimethyl-2-heptanol	3.6×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[51079-79-9]	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
FHQUDZUTAZYJRH-UHFFFAOYSA-N					
3-(1-methylethyl)-1-heptanol	3.1×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[38514-15-7]	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
NTGBCQFKKOCODF-UHFFFAOYSA-N	4.4×10^{-1}		Yaws et al. (1997)	Q	
4-(1-methylethyl)-4-heptanol	4.2×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[51200-82-9]	4.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
OHSMKBPEDBXYDU-UHFFFAOYSA-N	1.0		Yaws et al. (1997)	Q	
3-ethyl-2-methyl-3-heptanol	4.0×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-37-7]	4.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
GYCRUUSYQLIIBA-UHFFFAOYSA-N	9.3×10^{-1}		Yaws et al. (1997)	Q	
3-ethyl-5-methyl-3-heptanol	4.0×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.8×10^{-2}		Gharagheizi et al. (2012)	Q	
FGJMKJVRSBVZPS-UHFFFAOYSA-N	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
5-ethyl-4-methyl-3-heptanol	4.4×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	2.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[66731-94-0]	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
XVSHXHABYNUHNI-UHFFFAOYSA-N					
2-propyl-1-heptanol	3.3×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[10042-59-8]	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
YLQLIQIAXYRMDL-UHFFFAOYSA-N	4.0×10^{-1}		Yaws et al. (1997)	Q	
4-propyl-4-heptanol	4.2×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[2198-72-3]	4.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
SJTPBRMACCDJPZ-UHFFFAOYSA-N	9.0×10^{-1}		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,3,4-tetramethyl-3-hexanol	3.1×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	2.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-63-1]	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
SAFMWGCEQYLRLS-UHFFFAOYSA-N	9.6×10^{-1}		Yaws et al. (1997)	Q	
2,2,4,4-tetramethyl-3-hexanol	3.2×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	6.7×10^{-3}		Gharagheizi et al. (2012)	Q	
[66256-65-3]	4.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
LKAPNEGVXBMYKE-UHFFFAOYSA-N	1.0		Yaws et al. (1997)	Q	
2,2,5,5-tetramethyl-3-hexanol	4.6×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
[55073-86-4]	1.7		Yaws et al. (1997)	Q	
CFEYPBVKHMZCFR-UHFFFAOYSA-N					
2,3,4,4-tetramethyl-2-hexanol	3.2×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	6.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-66-4]	3.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
IELWGTFQRBDDCZ-UHFFFAOYSA-N	1.0		Yaws et al. (1997)	Q	
2,3,4,4-tetramethyl-3-hexanol	2.5×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	2.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-67-5]	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
ZQFIWHOYWCJIHU-UHFFFAOYSA-N	7.3×10^{-1}		Yaws et al. (1997)	Q	
2,3,5,5-tetramethyl-3-hexanol	2.5×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	6.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[5396-09-8]	3.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
KTSYBVKVNWGHBC-UHFFFAOYSA-N					
2,4,4,5-tetramethyl-3-hexanol	2.8×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	1.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-68-6]	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
VVRHXTVKOHXZJX-UHFFFAOYSA-N					
3,3,5,5-tetramethyl-2-hexanol	3.2×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	2.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-69-7]	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
USWOQOMRDCYQMW-UHFFFAOYSA-N					
3,4,4,5-tetramethyl-3-hexanol	2.5×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-39-1]	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
UHJJSHWWLQIIOU-UHFFFAOYSA-N	7.0×10^{-1}		Yaws et al. (1997)	Q	
3,4,5,5-tetramethyl-3-hexanol	2.9×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	5.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-40-4]	3.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
LBLUJHQRJVUQJR-UHFFFAOYSA-N	8.8×10^{-1}		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4-dimethyl-4-ethyl-3-hexanol	4.0×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66719-48-0]					
NLGGBBOPZSANIC-UHFFFAOYSA-N					
2-butyl-1-hexanol	4.4×10^{-1}		Yaws et al. (1997)	Q	
$C_{10}H_{22}O$					
[2768-15-2]					
LAPPDPWPIZBBJY-UHFFFAOYSA-N					
4-ethyl-2,2-dimethyl-3-hexanol	4.0×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66719-47-9]	1.1		Yaws et al. (1997)	Q	
UOYRABPBVGDJLW-UHFFFAOYSA-N					
4-methyl-2-(1-methylethyl)-1-hexanol	3.7×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	1.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[66719-41-3]	3.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
VHGVOODVCUKVCL-UHFFFAOYSA-N	7.3×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-2-propyl-1-hexanol	3.6×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	2.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-62-0]	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
VZXWJVFQXZUFQS-UHFFFAOYSA-N	5.7×10^{-1}		Yaws et al. (1997)	Q	
5,5-dimethyl-2-ethyl-1-hexanol	2.7×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	2.7×10^{-2}		Gharagheizi et al. (2012)	Q	
DXDJMJLAABGHOH-UHFFFAOYSA-N	3.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
5,5-dimethyl-3-ethyl-3-hexanol	3.7×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	4.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[5340-62-5]	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
FVVBGHIXYRKNGT-UHFFFAOYSA-N					
5-methyl-2-(1-methylethyl)-1-hexanol	3.0×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	2.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[2051-33-4]	3.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
SFIQHFBITUEIBP-UHFFFAOYSA-N	4.8×10^{-1}		Yaws et al. (1997)	Q	
2-methyl-3-(1-methylethyl)-3-hexanol	4.3×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.7×10^{-2}		Yaws (2003)	X	237
(2,4-dimethyl-3-propyl-3-pentanol)	2.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[51200-81-8]	1.7×10^{-2}		Gharagheizi et al. (2012)	Q	
GGOIYPAZTVTJBE-UHFFFAOYSA-N	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
	9.6×10^{-1}		Yaws et al. (1997)	Q	
	1.2		Yaws et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,3,4,4-pentamethyl-3-pentanol	2.4×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	1.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[5857-69-2]	3.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
UYFZQUABCZILAI-UHFFFAOYSA-N	8.9×10^{-1}		Yaws et al. (1997)	Q	
2,3-dimethyl-2-*tert*-butyl-1-butanol	3.0×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[81931-81-9]	3.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
WQRJEFGWAMKEBO-UHFFFAOYSA-N					
2,4-dimethyl-3-(1-methylethyl)-3-pentanol	3.2×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	1.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[51200-83-0]	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
IFXNWIUSZUHIDG-UHFFFAOYSA-N	8.9×10^{-1}		Yaws et al. (1997)	Q	
3,4-dimethyl-3-isopropyl-2-pentanol	4.0×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66719-50-4]					
DNBJFVXHMLZKHP-UHFFFAOYSA-N					
4,4-dimethyl-3-isopropyl-1-pentanol	4.3×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	3.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66719-51-5]					
DQWFOEIWLQBIFY-UHFFFAOYSA-N					
3-ethyl-2,2,4-trimethyl-3-pentanol	3.1×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	1.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[66256-41-5]	3.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
CHZVHXPAKQDRSE-UHFFFAOYSA-N	9.9×10^{-1}		Yaws et al. (1997)	Q	
4-methyl-2-(2-methylpropyl)-1-pentanol	3.5×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{22}O$	2.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[22417-45-4]	3.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
FXXCTCCAZGTNNO-UHFFFAOYSA-N	6.6×10^{-1}		Yaws et al. (1997)	Q	
1-undecanol	1.4×10^{-1}		Brockbank (2013)	L	
$C_{11}H_{24}O$	2.2×10^{-1}		Yaws (2003)	X	258
[112-42-5]	2.1×10^{-1}		Dupeux et al. (2022)	Q	259
KJIOQYGWTQBHNH-UHFFFAOYSA-N	1.4×10^{-1}		HSDB (2015)	Q	99
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	1.7×10^{-1}		Yao et al. (2002)	Q	229
	2.2×10^{-1}		Yaws et al. (1997)	Q	
	3.0×10^{-1}		Yaws (1999)	?	21

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-undecanol	1.2×10^{-1}		Yaws (2003)	X	258
$C_{11}H_{24}O$	2.3×10^{-1}		Dupeux et al. (2022)	Q	259
[1653-30-1]					
XMUJIPOFTAHSOK-UHFFFAOYSA-N					
3-undecanol	6.0×10^{-2}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{24}O$	1.7×10^{-1}		Wang et al. (2017)	Q	80, 239
[6929-08-4]	1.6×10^{-1}		Wang et al. (2017)	Q	80, 240
HCARCYFXWDRVBZ-UHFFFAOYSA-N					
1-dodecanol	1.2×10^{-1}		Brockbank (2013)	L	
$C_{12}H_{26}O$	4.4×10^{-1}		Altschuh et al. (1999)	M	
[112-53-8]	1.4×10^{-1}	9800	Abraham (1984)	V	
LQZZUXJYWNFBMV-UHFFFAOYSA-N	1.9×10^{-1}		Yaws (2003)	X	258
	1.8×10^{-1}		Dupeux et al. (2022)	Q	259
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.5		Duchowicz et al. (2020)	Q	184
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.5×10^{-1}		Hilal et al. (2008)	Q	
	3.5×10^{-1}		Modarresi et al. (2007)	Q	67
	2.1×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	1.6×10^{-1}		Yao et al. (2002)	Q	229, 267
	1.9×10^{-1}		Yaws et al. (1997)	Q	
	4.4×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	1.9×10^{-1}		Yaws (1999)	?	21
	1.1×10^{-1}		Yaws and Yang (1992)	?	21
3-dodecanol	4.8×10^{-2}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{26}O$	1.5×10^{-1}		Wang et al. (2017)	Q	80, 239
[10203-30-2]	1.5×10^{-1}		Wang et al. (2017)	Q	80, 240
OKDGZLITBCRLLJ-UHFFFAOYSA-N					
2,6,8-trimethyl-4-nonanol	1.0×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_{12}H_{26}O$	1.1×10^{-1}		Zhang et al. (2010)	Q	287, 289
[123-17-1]	6.0×10^{-2}		Zhang et al. (2010)	Q	287, 290
LFEHSRSSAGQWNI-UHFFFAOYSA-N	2.6×10^{-2}		Zhang et al. (2010)	Q	287, 291
1-tridecanol	1.2×10^{-1}		Yaws (2003)	X	258
$C_{13}H_{28}O$	1.5×10^{-1}		Dupeux et al. (2022)	Q	259
[112-70-9]	7.6×10^{-2}		HSDB (2015)	Q	99
XFRVVPUIAFSTFO-UHFFFAOYSA-N	1.3×10^{-1}		Yao et al. (2002)	Q	229
	1.2×10^{-1}		Yaws et al. (1997)	Q	
	1.8×10^{-1}		Yaws (1999)	?	21

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-tetradecanol	6.2×10^{-2}		Duchowicz et al. (2020)	V	186
$C_{14}H_{30}O$	6.2×10^{-2}		HSDB (2015)	V	
[112-72-1]	2.2×10^{-1}		Abraham (1984)	R	
HLZKNKRTKFSKGZ-UHFFFAOYSA-N	9.4×10^{-2}		Yaws (2003)	X	258
	1.2×10^{-1}		Dupeux et al. (2022)	Q	259
	1.5		Duchowicz et al. (2020)	Q	
	6.2×10^{-2}		Hilal et al. (2008)	Q	
	2.7×10^{-1}		Modarresi et al. (2007)	Q	67
	9.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	6.6×10^{-2}		Yao et al. (2002)	Q	229
	9.5×10^{-2}		Yaws et al. (1997)	Q	
	9.5×10^{-2}		Yaws (1999)	?	21
	3.9×10^{3}		Yaws and Yang (1992)	?	21, 409
2-tetradecanol	1.7×10^{-1}		Gharagheizi et al. (2012)	Q	
$C_{14}H_{30}O$					
[4706-81-4]					
BRGJIIMZXMWMCC-UHFFFAOYSA-N					
1-pentadecanol	2.2×10^{-1}		Abraham (1984)	V	
$C_{15}H_{32}O$	2.5×10^{-2}		Yaws (2003)	X	237
[629-76-5]	8.9×10^{-2}		Gharagheizi et al. (2012)	Q	
REIUXOLGHVXAEO-UHFFFAOYSA-N	2.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.5×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.5×10^{-1}		Yaws et al. (1997)	Q	
	3.0×10^{3}		Yaws and Yang (1992)	?	21, 410
1-hexadecanol	2.1×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{16}H_{34}O$	2.1×10^{-1}		HSDB (2015)	V	
(cetyl alcohol)	3.5×10^{-1}		Abraham (1984)	R	
[124-29-8]	6.4×10^{-2}		Yaws (2003)	X	237
BXWNKGSJHAJOGX-UHFFFAOYSA-N	1.5		Duchowicz et al. (2020)	Q	
	7.4×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	67
	2.5×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	1.0×10^{-1}		Yaws et al. (1997)	Q	
	1.0×10^{-1}		Yaws (1999)	?	21
	5.9×10^{-1}		Yaws and Yang (1992)	?	21
2-hexadecanol	1.6×10^{-2}		Yaws (2003)	X	237
$C_{16}H_{34}O$	1.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
[14852-31-4]					
FVDRFBGMOWJEOR-UHFFFAOYSA-N					

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-heptadecanol	4.5×10^{-2}		Yaws (2003)	X	237
$C_{17}H_{36}O$	7.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[1454-85-9]	6.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
GOQYKNQRPGWPLP-UHFFFAOYSA-N	4.6×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	4.5×10^{-2}		Yaws et al. (1997)	Q	
	1.2×10^{1}		Yaws and Yang (1992)	?	21
2-heptadecanol	8.7×10^{-3}		Yaws (2003)	X	237
$C_{17}H_{36}O$	1.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
[16813-18-6]					
ZNYQHFLBAPNPRC-UHFFFAOYSA-N					
1-octadecanol	1.2×10^{-2}		Duchowicz et al. (2020)	V	186
$C_{18}H_{38}O$	1.2×10^{-2}		HSDB (2015)	V	
[112-92-5]	3.8×10^{-1}		Abraham (1984)	R	
GLDOVTGHNKAZLK-UHFFFAOYSA-N	1.5		Duchowicz et al. (2020)	Q	
	2.5×10^{-2}		Hilal et al. (2008)	Q	
	1.7×10^{-1}		Modarresi et al. (2007)	Q	67
	3.1×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	3.1×10^{-3}		Yaws et al. (1997)	Q	
	1.2×10^{-2}		Yaws (1999)	?	21, 411
	9.1×10^{-1}		Yaws and Yang (1992)	?	21, 411
1-nonadecanol	9.9×10^{-2}		Yaws et al. (1997)	Q	
$C_{19}H_{40}O$					
[1454-84-8]					
XGFDHKJUZCCPKQ-UHFFFAOYSA-N					
1-eicosanol	4.7×10^{-1}		HSDB (2015)	Q	99
$C_{20}H_{42}O$	5.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[629-96-9]	1.8×10^{-2}		Yaws et al. (1997)	Q	
BTFJIXJJCSYFAL-UHFFFAOYSA-N					
1-docosanol	6.2×10^{-3}		HSDB (2015)	Q	99
$C_{22}H_{46}O$					
(behenic alcohol)					
[661-19-8]					
NOPFSRXAKWQILS-UHFFFAOYSA-N					
1-tetracosanol	3.4×10^{-3}		HSDB (2015)	Q	99
$C_{24}H_{50}O$					
[506-51-4]					
TYWMIZZBOVGFOV-UHFFFAOYSA-N					
cyclopentanol	4.2	8200	Plyasunov and Shock (2000)	L	
C_5H_9OH	2.2	5900	Hovorka et al. (2002)	M	11
[96-41-3]	4.3	8000	Cabani et al. (1975b)	T	
XCIXKGXIYUWCLL-UHFFFAOYSA-N	3.8		HSDB (2015)	Q	99
	2.0		Hilal et al. (2008)	Q	
		7200	Kühne et al. (2005)	Q	
	4.4		Nirmalakhandan et al. (1997)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		7300	Kühne et al. (2005)	?	
	4.3		Abraham et al. (1990)	?	
cyclohexanol	4.3	7700	Brockbank (2013)	L	1
$C_6H_{11}OH$	4.4	8500	Plyasunov and Shock (2000)	L	
[108-93-0]	2.5		Chao et al. (2017)	M	
HPXRVTGHNJAIIH-UHFFFAOYSA-N	4.3	7700	Hovorka et al. (2002)	M	11
	2.2		Altschuh et al. (1999)	M	
	2.7		Chao et al. (2017)	V	
	4.5		Mackay et al. (2006c)	V	
	4.5		Mackay et al. (1995)	V	
	3.5		Meylan and Howard (1991)	V	
	1.7		Hine and Mookerjee (1975)	V	
	4.1	8500	Cabani et al. (1975b)	T	
	3.9		Yaws (2003)	X	258
	3.6		Howard (1993)	X	412
	6.2		Dupeux et al. (2022)	Q	259
	1.1		Keshavarz et al. (2022)	Q	
	4.1		Duchowicz et al. (2020)	Q	
	4.5×10^{-1}		Wang et al. (2017)	Q	80, 238
	4.5		Wang et al. (2017)	Q	80, 239
	6.3		Wang et al. (2017)	Q	80, 240
	1.6		Li et al. (2014)	Q	241
	2.0		Raventos-Duran et al. (2010)	Q	242, 243
	2.5		Raventos-Duran et al. (2010)	Q	244
	2.0		Raventos-Duran et al. (2010)	Q	245
	3.3		Hilal et al. (2008)	Q	
	2.3		Modarresi et al. (2007)	Q	67
		7500	Kühne et al. (2005)	Q	
	3.8		Yaffe et al. (2003)	Q	248, 249
	1.3		Yao et al. (2002)	Q	229
	4.1		English and Carroll (2001)	Q	230, 231
	2.3		Katritzky et al. (1998)	Q	
	2.7		Nirmalakhandan et al. (1997)	Q	
	3.6		Russell et al. (1992)	Q	279
	2.0		Suzuki et al. (1992)	Q	232
	2.0		Meylan and Howard (1991)	Q	
	3.4		Nirmalakhandan and Speece (1988)	Q	
	2.2		Duchowicz et al. (2020)	?	185, 21
		7500	Kühne et al. (2005)	?	
	3.9		Yaws (1999)	?	21
	4.1		Abraham et al. (1990)	?	
cycloheptanol	4.6	9000	Plyasunov and Shock (2000)	L	
$C_7H_{13}OH$	4.2	9000	Cabani et al. (1975b)	T	
[502-41-0]	1.0		Hilal et al. (2008)	Q	
QCRFMSUKWRQZEM-UHFFFAOYSA-N	3.7		English and Carroll (2001)	Q	230, 231
	4.2		Abraham et al. (1990)	?	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methylcyclohexanol $C_7H_{13}OH$ [589-91-3] MQWCXKGKQLNYQG-UHFFFAOYSA-N	2.5		Ebert et al. (2023)	?	318
2-methylcyclohexanol $C_7H_{14}O$ [583-59-5] NDVWOBYBJYUSMF-UHFFFAOYSA-N	1.4		Chao et al. (2017)	M	
	1.3		Altschuh et al. (1999)	M	
	5.9		Keshavarz et al. (2022)	Q	
	1.7		Duchowicz et al. (2020)	Q	184
	1.6		Raventos-Duran et al. (2010)	Q	242, 243
	1.6		Raventos-Duran et al. (2010)	Q	244
	1.6		Raventos-Duran et al. (2010)	Q	245
	1.3		Hilal et al. (2008)	Q	
	3.2		Modarresi et al. (2007)	Q	67
	1.3		Duchowicz et al. (2020)	?	185, 21
3-methylcyclohexanol $C_7H_{14}O$ [591-23-1] HTSABYAWKQAHBT-UHFFFAOYSA-N	2.9		Chao et al. (2017)	M	
	2.7		Altschuh et al. (1999)	M	
	5.9		Keshavarz et al. (2022)	Q	
	1.7		Duchowicz et al. (2020)	Q	299
	1.6		Raventos-Duran et al. (2010)	Q	242, 243
	1.6		Raventos-Duran et al. (2010)	Q	244
	1.6		Raventos-Duran et al. (2010)	Q	245
	1.7		Modarresi et al. (2007)	Q	67
	2.7		Duchowicz et al. (2020)	?	185, 21
MCM:C8BCOH $C_8H_{14}O$ CEOBYJRLFASWKF-UHFFFAOYSA-N	8.7×10^{-1}		Wang et al. (2017)	Q	80, 238
	2.4		Wang et al. (2017)	Q	80, 239
	1.5		Wang et al. (2017)	Q	80, 240
(4-methylcyclohexyl)methanol $C_8H_{16}O$ [34885-03-5] OSINZLLLLCUKJH-UHFFFAOYSA-N	1.5		HSDB (2015)	Q	99
borneol $C_{10}H_{18}O$ [507-70-0] DTGKSKDOIYIVQL-UHFFFAOYSA-N	4.4×10^{-1}		Ebert et al. (2023)	?	316
fenchol $C_{10}H_{18}O$ (fenchyl alcohol) [1632-73-1] IAIHUHQCLTYTSF-UHFFFAOYSA-N	3.5×10^{-1}		Ebert et al. (2023)	?	371
menthol $C_{10}H_{20}O$ [1490-04-6] NOOLISFMXDJSKH-UHFFFAOYSA-N	3.1×10^{-1}		Ebert et al. (2023)	?	318

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methylisoborneol $C_{11}H_{20}O$ [2371-42-8] LFYXNXGVLGKVCJ-BOBPJJCASA-N	8.9×10^{-2} 1.6	9800	Ömür-Özbek and Dietrich (2005) Wu et al. (2022a)	M Q	 413
geosmin $C_{12}H_{22}O$ [19700-21-1] JLPUXFOGCDVKGO-GRYCIOLGSA-N	8.1×10^{-2} 4.1	9800	Ömür-Özbek and Dietrich (2005) Wu et al. (2022a)	M Q	 413
cyclododecanol $C_{12}H_{24}O$ [1724-39-6] SFVWPXMPRCIVOK-UHFFFAOYSA-N	3.4 6.8 4.5 3.7×10^{-1} 3.4 8.0 5.3×10^{-2} 1.6 2.5×10^{-1} 3.4		Altschuh et al. (1999) Keshavarz et al. (2022) Duchowicz et al. (2020) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Duchowicz et al. (2020)	M Q Q Q Q Q Q Q Q ?	 287, 288 287, 289 287, 290 287, 291 67 185, 21
cedrol $C_{15}H_{26}O$ [77-53-2] SVURIXNDRWRAFU-OGMFBOKVSA-N	6.7		Dupeux et al. (2022)	Q	259
patchoulol $C_{15}H_{26}O$ [5986-55-0] GGHMUJBZYLPWFD-CUZKYEQNSA-N	1.3×10^{1}		Dupeux et al. (2022)	Q	259
perhydrobisphenol a $C_{15}H_{28}O_2$ [80-04-6] CDBAMNGURPMUTG-UHFFFAOYSA-N	9.7 6.1×10^{4} 3.4×10^{4} 1.8×10^{2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
3-(5,5,6-trimethyl-2-norbornyl)cyclohexanol $C_{16}H_{28}O$ [3407-42-9] BWVZAZPLUTUBKD-UHFFFAOYSA-N	6.1×10^{-1} 1.6×10^{1} 1.1×10^{1} 2.7×10^{-1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
4-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexan-1-ol $C_{16}H_{28}O$ [66068-84-6] PCFHYANYPQEMPU-UHFFFAOYSA-N	6.1×10^{-1} 1.8×10^{1} 4.4×10^{1} 2.7×10^{-1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-((1R,2R,4R)-born-2-yl)cyclohexanol	6.1×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_{16}H_{28}O$	9.9		Zhang et al. (2010)	Q	287, 289
[66072-32-0]	4.3×10^{1}		Zhang et al. (2010)	Q	287, 290
LFHQKYSBKVWWOS-UHFFFAOYSA-N	1.6×10^{-1}		Zhang et al. (2010)	Q	287, 291
ethenol	8.5×10^{-1}		Wang et al. (2017)	Q	80, 238
C_2H_4O	2.0		Wang et al. (2017)	Q	80, 239
(vinyl alcohol)	1.7		Wang et al. (2017)	Q	80, 240
[557-75-5]					
IMROMDMJAWUWLK-UHFFFAOYSA-N					
2-propen-1-ol		6500	Plyasunov and Shock (2000)	L	
C_3H_5OH	2.0		Lide and Frederikse (1995)	V	
(allyl alcohol)	1.6		Yaws (2003)	X	258
[107-18-6]	4.3	7200	Goldstein (1982)	X	298
XXROGKLTLUQVRX-UHFFFAOYSA-N	2.0		Pierotti et al. (1959)	X	414
	1.5		Dupeux et al. (2022)	Q	259
	9.0×10^{-1}		Keshavarz et al. (2022)	Q	
	4.0		Duchowicz et al. (2020)	Q	299
	6.9×10^{-1}		Wang et al. (2017)	Q	80, 238
	5.9		Wang et al. (2017)	Q	80, 239
	2.1		Wang et al. (2017)	Q	80, 240
	2.0		Li et al. (2014)	Q	241
	4.9		Raventos-Duran et al. (2010)	Q	242, 243
	3.9		Raventos-Duran et al. (2010)	Q	244
	1.6		Raventos-Duran et al. (2010)	Q	245
	2.8		Hilal et al. (2008)	Q	
	3.7		Modarresi et al. (2007)	Q	67
	2.0		Yaffe et al. (2003)	Q	248, 249
	3.8		Yao et al. (2002)	Q	229
	5.1		English and Carroll (2001)	Q	230, 231
	4.4		Katritzky et al. (1998)	Q	
	3.5		Nirmalakhandan et al. (1997)	Q	
	4.4		Suzuki et al. (1992)	Q	232
	3.4		Nirmalakhandan and Speece (1988)	Q	
	2.0		Duchowicz et al. (2020)	?	185, 21
	1.6		Yaws (1999)	?	21
	1.8		Yaws and Yang (1992)	?	21
	2.0		Abraham et al. (1990)	?	
2-propyn-1-ol	3.8	7400	Hiatt (2013)	M	
C_3H_4O	8.6		Duchowicz et al. (2020)	V	186
(propargyl alcohol)	9.0		HSDB (2015)	V	
[107-19-7]	7.0		Duchowicz et al. (2020)	Q	
TVDSBUOJIPERQY-UHFFFAOYSA-N	5.4		Hilal et al. (2008)	Q	
	7.0		Modarresi et al. (2007)	Q	67

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-buten-1-ol		6900	Plyasunov and Shock (2000)	L	
$CH_3CHCHCH_2OH$	3.1		Raventos-Duran et al. (2010)	Q	242, 243
[6117-91-5]	3.9		Raventos-Duran et al. (2010)	Q	244
WCASXYBKJHWFMY-UHFFFAOYSA-N	1.2		Raventos-Duran et al. (2010)	Q	245
	2.7		Hilal et al. (2008)	Q	
	3.0		Saxena and Hildemann (1996)	E	401
3-buten-1-ol		7000	Plyasunov and Shock (2000)	L	
C_4H_8O					
[627-27-0]					
ZSPTYLOMNJNZNG-UHFFFAOYSA-N					
4-penten-1-ol		7300	Plyasunov and Shock (2000)	L	
$C_5H_{10}O$					
[821-09-0]					
LQAVWYMTUMSFBE-UHFFFAOYSA-N					
3-pentyn-1-ol		7800	Plyasunov and Shock (2000)	L	
C_5H_8O					
[10229-10-4]					
IDYNOORNKYEHHO-UHFFFAOYSA-N					
2-methyl-3-buten-2-ol	6.4×10^{-1}		Iraci et al. (1999)	M	38
C_5H_9O	4.7×10^{-1}		Altschuh et al. (1999)	M	
[115-18-4]	1.6		Keshavarz et al. (2022)	Q	
HNVRRHSXBLFLIG-UHFFFAOYSA-N	7.9×10^{-1}		Duchowicz et al. (2020)	Q	299
	3.6×10^{-1}		Wang et al. (2017)	Q	80, 238
	1.2		Wang et al. (2017)	Q	80, 239
	7.3×10^{-1}		Wang et al. (2017)	Q	80, 240
	2.5		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	6.0×10^{-1}		Hilal et al. (2008)	Q	
	1.6		Modarresi et al. (2007)	Q	67
	4.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2-methyl-3-butyn-2-ol	2.5		Altschuh et al. (1999)	M	
C_5H_8O	1.6		Keshavarz et al. (2022)	Q	
[115-19-5]	1.5		Duchowicz et al. (2020)	Q	
CEBKHWWANWSNTI-UHFFFAOYSA-N	1.0		Hilal et al. (2008)	Q	
	8.3		Modarresi et al. (2007)	Q	67
	2.5		Duchowicz et al. (2020)	?	185, 21
3-methyl-1-pentyn-3-ol	9.9×10^{-1}		Hilal et al. (2008)	Q	
$C_6H_{10}O$	7.0		Modarresi et al. (2007)	Q	67
(meparfynol; methyl pentynol)	4.3		Katritzky et al. (1998)	Q	
[77-75-8]					
QXLPXWSKPNOQLE-UHFFFAOYSA-N					

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-cyclohexen-1-ol $C_6H_{10}O$ [822-67-3] PQANGXXSEABURG-UHFFFAOYSA-N		8500	Plyasunov and Shock (2000)	L	
bicyclo[2.2.1]heptan-2-ol $C_7H_{12}O$ (norborneol) [1632-68-4] ZQTYQMYDIHMKQB-UHFFFAOYSA-N	2.2	5000	van Roon et al. (2005)	V	
2-octen-1-ol $C_8H_{16}O$ [22104-78-5] AYQPVPFZWIQERS-UHFFFAOYSA-N	7.7×10^{-1}		Wu et al. (2022a)	Q	413
1-octen-3-ol $C_8H_{16}O$ [3391-86-4] VSMOENVRRABVKN-UHFFFAOYSA-N	1.9×10^{-1} 2.5×10^{-1} 1.3×10^{-1}	7900	Wu et al. (2022a) Druaux et al. (1998) Roberts and Pollien (1997)	M M M	
3,7-dimethyl-6-octen-1-ol $C_{10}H_{20}O$ (citronellol) [106-22-9] QMVPMAAFGQKVCJ-UHFFFAOYSA-N	5.2 4.9×10^{-1}		Martins et al. (2017) Dupeux et al. (2022)	V Q	315 259
3,7-dimethyl-1,6-octadien-3-ol $C_{10}H_{18}O$ (linalool) [78-70-6] CDOSHBSSFJOMGT-UHFFFAOYSA-N	2.0×10^{-1} 3.8×10^{-1} 4.6×10^{-1} 4.0×10^{-1} 4.8×10^{-1} 4.8×10^{-1} 2.1×10^{-1} 1.6 1.3×10^{-1} 3.3×10^{-1} 2.5×10^{-1} 2.5 6.2×10^{-1} 2.5×10^{-1} 6.9×10^{-1} 1.4 1.5×10^{-2} 4.6×10^{-1}	4400 14000 	Leng et al. (2013) Copolovici and Niinemets (2007) Altschuh et al. (1999) Martins et al. (2017) Copolovici and Niinemets (2005) Niinemets and Reichstein (2002) Li et al. (1998) Dupeux et al. (2022) Keshavarz et al. (2022) Duchowicz et al. (2020) Savary et al. (2014) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Hertel and Sommer (2006) Duchowicz et al. (2020)	M M M V V V V Q Q Q Q Q Q Q Q Q Q ?	 315 259 184 271, 243 244 245 67 415 185, 21
linalool oxide $C_{10}H_{18}O_2$ [1365-19-1] BXOURKNXQXLKRK-UHFFFAOYSA-N	3.0×10^{2}		Dupeux et al. (2022)	Q	259

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(*E*)-3,7-dimethyl-2,6-octadien-1-ol	3.1		Martins et al. (2017)	V	315
$C_{10}H_{18}O$	1.6		Dupeux et al. (2022)	Q	259
(geraniol)	1.7×10^{-1}		HSDB (2015)	Q	99
[106-24-1]					
GLZPCOQZEFWAFX-JXMROGBWSA-N					
(*Z*)-3,7-dimethyl-2,6-octadien-1-ol	8.6×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{10}H_{18}O$	2.1×10^{-1}		Duchowicz et al. (2020)	Q	
[106-25-2]					
GLZPCOQZEFWAFX-YFHOEESVSA-N					
tricyclo[3.3.1.1(3,7)]decan-1-ol	6.0	5300	van Roon et al. (2005)	V	
$C_{10}H_{16}O$					
(1-adamantanol)					
[768-95-6]					
VLLNJDMHDJRNFK-UHFFFAOYSA-N					
3,7,11-trimethyl-2,6,10-dodecatrien-1-ol	3.9×10^{-2}		HSDB (2015)	Q	99
$C_{15}H_{26}O$					
(farnesol)					
[4602-84-0]					
CRDAMVZIKSXKFV-YFVJMOTDSA-N					
(*Z*)-9-octadecen-1-ol	2.1×10^{-2}		HSDB (2015)	Q	99
$C_{18}H_{36}O$					
(oleyl alcohol)					
[143-28-2]					
ALSTYHKOOCGGFT-KTKRTIGZSA-N					
(3*E*,13*Z*)-octadeca-3,13-dien-1-ol	2.4×10^{-1}		Ebert et al. (2023)	?	318
$C_{18}H_{34}O$					
[66410-28-4]					
QBNCGBJHGBGHLS-IYUNJCAYSA-N					
dihydroabietyl alcohol	1.9×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_{20}H_{34}O$	2.4×10^{1}		Zhang et al. (2010)	Q	287, 289
[26266-77-3]	2.6×10^{1}		Zhang et al. (2010)	Q	287, 290
FLMIYUXOBAUKJM-UHFFFAOYSA-N	2.0×10^{-1}		Zhang et al. (2010)	Q	287, 291
ethylestrenol	4.3×10^{-1}		HSDB (2015)	Q	99
$C_{20}H_{32}O$					
[965-90-2]					
AOXRBFRFYPMWLR-UHFFFAOYSA-N					
trans-phytol	1.0×10^{-2}		Ebert et al. (2023)	?	365
$C_{20}H_{40}O$					
[150-86-7]					
BOTWFXYSPFMFNR-PYDDKJGSSA-N					

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hydroxybenzene	1.8×10^1	3000	Schwardt et al. (2021)	L	1
C_6H_5OH	2.2×10^1	8900	Brockbank (2013)	L	1
(phenol)	2.2×10^1	9800	Ji et al. (2008)	M	
[108-95-2]	2.8×10^1	2700	Guo and Brimblecombe (2007)	M	
ISWSIDIOOBJBQZ-UHFFFAOYSA-N	6.4	7700	Feigenbrugel et al. (2004b)	M	
	3.0×10^1	5900	Harrison et al. (2002)	M	
	1.9×10^1		Sheikheldin et al. (2001)	M	12
	>4.2		Altschuh et al. (1999)	M	
	8.1×10^1	7400	Tabai et al. (1997)	M	11
	4.2		Heal et al. (1995)	M	373
	1.6×10^1	6000	Dohnal and Fenclová (1995)	M	
	1.5×10^1		Tremp et al. (1993)	M	12
	1.7×10^1	6100	Abd-El-Bary et al. (1986)	M	
	7.6		Warner et al. (1980)	M	
	2.0×10^1		Mackay et al. (2006c)	V	
	2.5×10^1		Lide and Frederikse (1995)	V	
	1.9×10^1		Mackay et al. (1995)	V	
	1.9×10^1		Shiu et al. (1994)	V	
	3.4		Hwang et al. (1992)	V	
	1.1×10^1		Riederer (1990)	V	
	9.0×10^1		Leuenberger et al. (1985)	V	416
	4.8		Hine and Weimar (1965)	R	
	2.8×10^1	6800	Parsons et al. (1971)	T	417
	1.3×10^1		Yaws (2003)	X	258
	1.9	3600	Janini and Quaddora (1986)	X	298
	1.9×10^1	7300	Goldstein (1982)	X	298
	2.5×10^1		Howard (1989)	X	418
	3.0×10^1		Gaffney and Senum (1984)	X	389
	3.7×10^1		McCarty (1980)	X	368
	2.5×10^1		Schüürmann (2000)	C	21
	7.6		Shiu et al. (1994)	C	
	7.6		Smith et al. (1993)	C	
	2.1×10^1		Ryan et al. (1988)	C	
	7.6		Shen (1982)	C	
	1.8×10^1		Dupeux et al. (2022)	Q	259
	6.4×10^1		Keshavarz et al. (2022)	Q	
	4.2×10^1		Duchowicz et al. (2020)	Q	184
	6.3×10^1		Wang et al. (2017)	Q	80, 238
	1.1×10^1		Wang et al. (2017)	Q	80, 239
	3.6×10^1		Wang et al. (2017)	Q	80, 240
	2.5×10^1		Li et al. (2014)	Q	241
	9.9		Raventos-Duran et al. (2010)	Q	242, 243
	7.8		Raventos-Duran et al. (2010)	Q	244
	1.6×10^1		Raventos-Duran et al. (2010)	Q	245
	4.4		Hilal et al. (2008)	Q	
	1.8×10^1		Modarresi et al. (2007)	Q	67
		6200	Kühne et al. (2005)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.0×10^{1}		Yaffe et al. (2003)	Q	248, 249
	2.9×10^{1}		English and Carroll (2001)	Q	230, 231
	6.9		Katritzky et al. (1998)	Q	
	2.0×10^{1}		Russell et al. (1992)	Q	279
	2.0×10^{1}		Suzuki et al. (1992)	Q	232
	9.9		Nirmalakhandan and Speece (1988)	Q	
	3.0×10^{1}		Duchowicz et al. (2020)	?	185, 21
		5400	Kühne et al. (2005)	?	
	1.3×10^{1}		Yaws (1999)	?	21
	1.6×10^{1}		Abraham et al. (1990)	?	
(hydroxymethyl)-benzene	1.7×10^{1}		Chao et al. (2017)	M	
$C_6H_5CH_2OH$	$>3.7\times10^{1}$		Altschuh et al. (1999)	M	
(benzyl alcohol)	2.5×10^{1}		Chao et al. (2017)	V	
[100-51-6]	6.2×10^{-2}		Mackay et al. (2006c)	V	
WVDDGKGOMKODPV-UHFFFAOYSA-N	6.2×10^{-2}		Mackay et al. (1995)	V	
	2.9×10^{1}		Abraham et al. (1994a)	R	
	3.8×10^{1}		Yaws (2003)	X	258
	3.8×10^{1}		Yaws (2003)	X	237
	2.5×10^{1}		Howard (1993)	X	412
	1.6×10^{1}		Dupeux et al. (2022)	Q	259
	2.3×10^{1}		Keshavarz et al. (2022)	Q	
	2.3×10^{1}		Duchowicz et al. (2020)	Q	299
	3.8×10^{1}		Wang et al. (2017)	Q	80, 238
	4.9×10^{1}		Wang et al. (2017)	Q	80, 239
	3.8×10^{1}		Wang et al. (2017)	Q	80, 240
	8.6×10^{1}		Gharagheizi et al. (2012)	Q	
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	4.1×10^{1}		Gharagheizi et al. (2010)	Q	246
	2.2×10^{1}		Hilal et al. (2008)	Q	
	5.5×10^{1}		Modarresi et al. (2007)	Q	67
	1.1×10^{1}		Yao et al. (2002)	Q	229
	2.1×10^{1}		English and Carroll (2001)	Q	230, 231
	6.9×10^{1}		Nirmalakhandan et al. (1997)	Q	
	8.9×10^{1}		Saxena and Hildemann (1996)	E	401
	2.9×10^{1}		Duchowicz et al. (2020)	?	185, 21
	2.9×10^{1}		HSDB (2015)	?	419
	3.8×10^{1}		Yaws (1999)	?	21
	1.8×10^{1}		Abraham et al. (1990)	?	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-hydroxy-2-methylbenzene	6.7	7400	Brockbank (2013)	L	1
$HOC_6H_4CH_3$	6.5		Chao et al. (2017)	M	
(2-cresol; *o*-cresol)	4.2	8500	Feigenbrugel et al. (2004b)	M	
[95-48-7]	1.1×10^1	6700	Harrison et al. (2002)	M	
QWVGKYWNOKOFNN-UHFFFAOYSA-N	6.3		Altschuh et al. (1999)	M	
	5.6	5800	Dohnal and Fenclová (1995)	M	
	7.1		Tremp et al. (1993)	M	12
	8.2	7300	Parsons et al. (1972)	M	417
	5.8		Chao et al. (2017)	V	
			Mackay et al. (2006c)	V	420
	6.2		Lide and Frederikse (1995)	V	
	6.4		Mackay et al. (1995)	V	
	3.5×10^1		Leuenberger et al. (1985)	V	416
	8.8		Yaws (2003)	X	258
	2.6	4600	Janini and Quaddora (1986)	X	298
	6.2		Howard (1989)	X	418
	8.2		Gaffney and Senum (1984)	X	389
	8.3		Schüürmann (2000)	C	21
	8.4		Dupeux et al. (2022)	Q	259
	5.9		Keshavarz et al. (2022)	Q	
	2.3×10^1		Duchowicz et al. (2020)	Q	
	3.9×10^1		Wang et al. (2017)	Q	80, 238
	1.2×10^1		Wang et al. (2017)	Q	80, 239
	1.1×10^1		Wang et al. (2017)	Q	80, 240
	8.0		Li et al. (2014)	Q	241
	1.2×10^1		Gharagheizi et al. (2012)	Q	
	5.3		Hilal et al. (2008)	Q	
	6.2		Modarresi et al. (2007)	Q	67
		6500	Kühne et al. (2005)	Q	
	8.8		Yaffe et al. (2003)	Q	248, 249
	9.9		Yao et al. (2002)	Q	229, 267
	9.5		English and Carroll (2001)	Q	230, 231
	4.6		Katritzky et al. (1998)	Q	
	1.5×10^1		Suzuki et al. (1992)	Q	232
	7.2		Nirmalakhandan and Speece (1988)	Q	
	8.2		Duchowicz et al. (2020)	?	185, 21
		8100	Kühne et al. (2005)	?	
	5.8		Yaws (1999)	?	21, 12
	1.2×10^1		Yaws and Yang (1992)	?	21, 12
	8.0		Abraham et al. (1990)	?	
1-hydroxy-3-methylbenzene	1.2×10^1	6200	Brockbank (2013)	L	1
$HOC_6H_4CH_3$	7.9	9000	Feigenbrugel et al. (2004b)	M	
(3-cresol; *m*-cresol)	1.2×10^1		Altschuh et al. (1999)	M	
[108-39-4]	1.2×10^1	6000	Dohnal and Fenclová (1995)	M	
RLSSMJSEOOYNOY-UHFFFAOYSA-N	1.3×10^1		Mackay et al. (2006c)	V	
	1.2×10^1		Schüürmann (2000)	V	
	1.1×10^1		Lide and Frederikse (1995)	V	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^1		Mackay et al. (1995)	V	
	1.1×10^1		Meylan and Howard (1991)	V	
	4.9×10^1		Leuenberger et al. (1985)	V	416
	2.2×10^1		Yaws (2003)	X	258
	6.1	7700	Janini and Quaddora (1986)	X	298
	1.1×10^1		Howard (1989)	X	418
	1.8×10^1		Dupeux et al. (2022)	Q	259
	5.9		Keshavarz et al. (2022)	Q	
	2.3×10^1		Duchowicz et al. (2020)	Q	184
	1.2×10^1		Gharagheizi et al. (2012)	Q	
	3.9		Hilal et al. (2008)	Q	
	1.1×10^1		Modarresi et al. (2007)	Q	67
		6500	Kühne et al. (2005)	Q	
	1.2×10^1		Yaffe et al. (2003)	Q	248, 249
	1.0×10^1		Yao et al. (2002)	Q	229
	1.7×10^1		Katritzky et al. (1998)	Q	
	1.6×10^1		Meylan and Howard (1991)	Q	
	1.2×10^1		Duchowicz et al. (2020)	?	185, 21
		6500	Kühne et al. (2005)	?	
	1.4×10^1		Yaws (1999)	?	21, 12
	1.4×10^1		Yaws and Yang (1992)	?	21, 12
	4.3		Abraham et al. (1990)	?	
1-hydroxy-4-methylbenzene	1.3×10^1	6600	Brockbank (2013)	L	1
$HOC_6H_4CH_3$	1.0×10^1	9300	Feigenbrugel et al. (2004b)	M	
(4-cresol; *p*-cresol)	>2.9		Altschuh et al. (1999)	M	
[106-44-5]	1.3×10^1	6100	Dohnal and Fenclová (1995)	M	
IWDCLRJOBJJRNH-UHFFFAOYSA-N	1.3×10^1		Tremp et al. (1993)	M	12
	1.3×10^1	7200	Parsons et al. (1972)	M	417
	1.8×10^1		Mackay et al. (2006c)	V	
	1.0×10^1		Lide and Frederikse (1995)	V	
	1.5×10^1		Mackay et al. (1995)	V	
	4.5×10^1		Leuenberger et al. (1985)	V	416
	1.2		Smith and Bomberger (1980)	V	24
	2.2×10^1		Yaws (2003)	X	258
	5.2	4600	Janini and Quaddora (1986)	X	298
	1.0×10^1		Howard (1989)	X	418
	9.9		Gaffney and Senum (1984)	X	389
	1.3×10^1		Schüürmann (2000)	C	21
	1.6×10^1		Dupeux et al. (2022)	Q	259
	5.9		Keshavarz et al. (2022)	Q	
	2.3×10^1		Duchowicz et al. (2020)	Q	184
	1.8×10^1		Gharagheizi et al. (2012)	Q	
	4.2		Hilal et al. (2008)	Q	
	1.7×10^1		Modarresi et al. (2007)	Q	67
		6500	Kühne et al. (2005)	Q	
	8.8		Yaffe et al. (2003)	Q	248, 272
	1.5×10^1		Yao et al. (2002)	Q	229

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.7×10^{1}		English and Carroll (2001)	Q	230, 231
	1.5×10^{1}		Katritzky et al. (1998)	Q	
	1.4×10^{1}		Suzuki et al. (1992)	Q	232
	7.0		Nirmalakhandan and Speece (1988)	Q	
	9.9		Duchowicz et al. (2020)	?	185, 21
		6000	Kühne et al. (2005)	?	
	1.3×10^{1}		Yaws (1999)	?	21, 12
	2.5×10^{1}		Yaws and Yang (1992)	?	21, 12
	1.3×10^{1}		Abraham et al. (1990)	?	
1-hydroxy-2,3-dimethylbenzene	6.7	6100	Brockbank (2013)	L	1
$C_8H_{10}O$	9.3		Sheikheldin et al. (2001)	M	12
(2,3-xylenol; 2,3-dimethylphenol)	1.0×10^{1}	6800	Dohnal and Fenclová (1995)	M	
[526-75-0]	3.2		HSDB (2015)	V	
QWBBPBRQALCEIZ-UHFFFAOYSA-N	1.8×10^{1}		Mackay et al. (2006c)	V	
	1.9×10^{1}		Mackay et al. (1995)	V	
	4.9×10^{1}		Leuenberger et al. (1985)	V	416
	1.3×10^{1}		Abraham et al. (1994a)	R	
	7.9		Keshavarz et al. (2022)	Q	
	1.2×10^{1}		Duchowicz et al. (2020)	Q	184
	2.2×10^{1}		Wang et al. (2017)	Q	80, 238
	1.4×10^{1}		Wang et al. (2017)	Q	80, 239
	9.6		Wang et al. (2017)	Q	80, 240
	6.2		Raventos-Duran et al. (2010)	Q	242, 243
	7.8		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	245
	5.8		Hilal et al. (2008)	Q	
	5.2		Modarresi et al. (2007)	Q	67
	1.4×10^{1}		Yaffe et al. (2003)	Q	248, 249
	1.2×10^{1}		English and Carroll (2001)	Q	230, 231
	4.6×10^{1}		Nirmalakhandan et al. (1997)	Q	
	1.3×10^{1}		Duchowicz et al. (2020)	?	185, 21
1-hydroxy-2,4-dimethylbenzene	3.5	5500	Brockbank (2013)	L	1
$C_8H_{10}O$	6.6		Sheikheldin et al. (2001)	M	12
(2,4-xylenol; 2,4-dimethylphenol)	4.9	6100	Dohnal and Fenclová (1995)	M	
[105-67-9]	1.9×10^{-3}	-3200	Ashworth et al. (1988)	M	33, 278
KUFFULVDNCHOFZ-UHFFFAOYSA-N	5.5		Mackay et al. (2006c)	V	
	1.6×10^{1}		Lide and Frederikse (1995)	V	
	5.5		Mackay et al. (1995)	V	
	5.5×10^{-1}		Hwang et al. (1992)	V	
	4.9		Meylan and Howard (1991)	V	
	1.6×10^{1}		Leuenberger et al. (1985)	V	416
	1.0×10^{1}		Abraham et al. (1994a)	R	
	4.7		Yaws (2003)	X	258
	4.1	6600	Goldstein (1982)	X	298
	1.6×10^{1}		Howard (1989)	X	418
	5.8×10^{-1}		Smith et al. (1993)	C	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	5.4×10^{-1}		Ryan et al. (1988)	C	
	1.7×10^{1}		Petrasek et al. (1983)	C	
	6.7		Dupeux et al. (2022)	Q	259
	7.9		Keshavarz et al. (2022)	Q	
	1.2×10^{1}		Duchowicz et al. (2020)	Q	299
	2.2×10^{1}		Wang et al. (2017)	Q	80, 238
	1.2×10^{1}		Wang et al. (2017)	Q	80, 239
	8.7		Wang et al. (2017)	Q	80, 240
	4.6		Gharagheizi et al. (2012)	Q	
	6.2		Raventos-Duran et al. (2010)	Q	242, 243
	6.2		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	245
	5.1		Hilal et al. (2008)	Q	
	4.3		Modarresi et al. (2007)	Q	67
	1.1×10^{1}		Yaffe et al. (2003)	Q	248, 249
	1.6×10^{1}		English and Carroll (2001)	Q	230, 231
	6.7		Katritzky et al. (1998)	Q	
	4.6×10^{1}		Nirmalakhandan et al. (1997)	Q	
	1.4×10^{1}		Meylan and Howard (1991)	Q	
	1.0×10^{1}		Duchowicz et al. (2020)	?	185, 21
1-hydroxy-2,5-dimethylbenzene	8.2	8700	Brockbank (2013)	L	1
$C_8H_{10}O$	7.5	6800	Dohnal and Fenclová (1995)	M	
(2,5-xylenol; 2,5-dimethylphenol)	1.4		HSDB (2015)	V	
[95-87-4]	7.5		Mackay et al. (2006c)	V	
NKTOLZVEWDHZMU-UHFFFAOYSA-N	7.4		Mackay et al. (1995)	V	
	3.8×10^{1}		Leuenberger et al. (1985)	V	416
	8.8		Abraham et al. (1994a)	R	
	1.9		Yaws (2003)	X	258
	5.7		Dupeux et al. (2022)	Q	259
	7.9		Keshavarz et al. (2022)	Q	
	1.2×10^{1}		Duchowicz et al. (2020)	Q	299
	2.2×10^{1}		Wang et al. (2017)	Q	80, 238
	1.2×10^{1}		Wang et al. (2017)	Q	80, 239
	8.9		Wang et al. (2017)	Q	80, 240
	6.2		Raventos-Duran et al. (2010)	Q	242, 243
	6.2		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	245
	5.2		Hilal et al. (2008)	Q	
	4.8		Modarresi et al. (2007)	Q	67
	3.1		Yaffe et al. (2003)	Q	248, 272
	1.4×10^{1}		English and Carroll (2001)	Q	230, 274
	4.6×10^{1}		Nirmalakhandan et al. (1997)	Q	
	8.8		Duchowicz et al. (2020)	?	185, 21

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-hydroxy-2,6-dimethylbenzene	1.6	6300	Brockbank (2013)	L	1
$C_8H_{10}O$	2.3	6200	Dohnal and Fenclová (1995)	M	
(2,6-xylenol; 2,6-dimethylphenol)	1.3		Hawthorne et al. (1985)	M	
[576-26-1]	2.5		Mackay et al. (2006c)	V	
NXXYKOUNUYWIHA-UHFFFAOYSA-N	2.6		Mackay et al. (1995)	V	
	2.6		Shiu et al. (1994)	V	
	5.2		Leuenberger et al. (1985)	V	416
	2.9		Abraham et al. (1994a)	R	
	1.4		Yaws (2003)	X	258
	1.6		Dupeux et al. (2022)	Q	259
	7.9		Keshavarz et al. (2022)	Q	
	3.0		Duchowicz et al. (2020)	Q	299
	6.2		Raventos-Duran et al. (2010)	Q	242, 243
	3.9		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	245
	9.2		Hilal et al. (2008)	Q	
	1.8		Modarresi et al. (2007)	Q	67
	3.1		Yaffe et al. (2003)	Q	248, 249
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
	4.6×10^{1}		Nirmalakhandan et al. (1997)	Q	
	1.5		Duchowicz et al. (2020)	?	185, 21
	1.4		Yaws (1999)	?	21
1-hydroxy-3,4-dimethylbenzene	2.6×10^{1}	7200	Brockbank (2013)	L	1
$C_8H_{10}O$	2.4×10^{1}	7100	Dohnal and Fenclová (1995)	M	
(3,4-xylenol; 3,4-dimethylphenol)	8.2		HSDB (2015)	V	
[95-65-8]	4.6×10^{1}		Mackay et al. (2006c)	V	
YCOXTKKNXUZSKD-UHFFFAOYSA-N	4.7×10^{1}		Mackay et al. (1995)	V	
	4.7×10^{1}		Shiu et al. (1994)	V	
	1.1×10^{2}		Leuenberger et al. (1985)	V	416
	2.4×10^{1}		Abraham et al. (1994a)	R	
	1.1×10^{1}		Yaws (2003)	X	258
	1.8×10^{1}		Dupeux et al. (2022)	Q	259
	7.9		Keshavarz et al. (2022)	Q	
	1.2×10^{1}		Duchowicz et al. (2020)	Q	299
	1.1×10^{1}		Gharagheizi et al. (2012)	Q	
	6.2		Raventos-Duran et al. (2010)	Q	242, 243
	7.8		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	245
	4.4		Hilal et al. (2008)	Q	
	1.2×10^{1}		Modarresi et al. (2007)	Q	67
	2.4×10^{1}		Yaffe et al. (2003)	Q	248, 249
	2.1×10^{1}		English and Carroll (2001)	Q	230, 260
	4.6×10^{1}		Nirmalakhandan et al. (1997)	Q	
	2.4×10^{1}		Duchowicz et al. (2020)	?	185, 21

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-hydroxy-3,5-dimethylbenzene	1.5×10^1	7600	Brockbank (2013)	L	1
$C_8H_{10}O$	1.6×10^1	6900	Dohnal and Fenclová (1995)	M	
(3,5-xylenol; 3,5-dimethylphenol)	7.6		HSDB (2015)	V	
[108-68-9]	2.8×10^1		Mackay et al. (2006c)	V	
TUAMRELNJMMDMT-UHFFFAOYSA-N	3.1×10^1		Mackay et al. (1995)	V	
	2.5×10^1		Shiu et al. (1994)	V	
	6.2×10^1		Leuenberger et al. (1985)	V	416
	1.6×10^1		Abraham et al. (1994a)	R	
	7.3		Yaws (2003)	X	258
	1.2×10^1		Dupeux et al. (2022)	Q	259
	7.9		Keshavarz et al. (2022)	Q	
	1.2×10^1		Duchowicz et al. (2020)	Q	184
	6.2		Raventos-Duran et al. (2010)	Q	242, 243
	4.9		Raventos-Duran et al. (2010)	Q	244
	1.6×10^1		Raventos-Duran et al. (2010)	Q	245
	3.2		Hilal et al. (2008)	Q	
	1.1×10^1		Modarresi et al. (2007)	Q	67
	1.6×10^1		Yaffe et al. (2003)	Q	248, 249
	1.7×10^1		English and Carroll (2001)	Q	230, 231
	4.6×10^1		Nirmalakhandan et al. (1997)	Q	
	1.6×10^1		Duchowicz et al. (2020)	?	185, 21
2-methylbenzenemethanol	2.2×10^1		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O$	5.6×10^1		Wang et al. (2017)	Q	80, 239
[89-95-2]	1.7×10^1		Wang et al. (2017)	Q	80, 240
XPNGNIFUDRPBFJ-UHFFFAOYSA-N					
3-methylbenzenemethanol	2.2×10^1		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O$	4.5×10^1		Wang et al. (2017)	Q	80, 239
[587-03-1]	3.4×10^1		Wang et al. (2017)	Q	80, 240
JJCKHVUTVOPLBV-UHFFFAOYSA-N					
4-methylbenzenemethanol	9.0		HSDB (2015)	V	
$C_8H_{10}O$	2.2×10^1		Wang et al. (2017)	Q	80, 238
[589-18-4]	5.3×10^1		Wang et al. (2017)	Q	80, 239
KMTDMTZBNYGUNX-UHFFFAOYSA-N	4.6×10^1		Wang et al. (2017)	Q	80, 240
α-methylbenzyl alcohol	3.4×10^1		HSDB (2015)	Q	99
$C_8H_{10}O$					
[98-85-1]					
WAPNOHKVXSQRPX-UHFFFAOYSA-N					
1-hydroxy-2-ethylbenzene	2.1		Duchowicz et al. (2020)	V	186
$C_8H_{10}O$	2.1		HSDB (2015)	V	
(2-ethylphenol)	5.6		Mackay et al. (2006c)	V	
[90-00-6]	2.4×10^1		Duchowicz et al. (2020)	Q	
IXQGCWUGDFDQMF-UHFFFAOYSA-N	3.0×10^1		Wang et al. (2017)	Q	80, 238
	8.1		Wang et al. (2017)	Q	80, 239
	7.3		Wang et al. (2017)	Q	80, 240
	6.2		Raventos-Duran et al. (2010)	Q	242, 243

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.9		Raventos-Duran et al. (2010)	Q	244
	1.2×10^1		Raventos-Duran et al. (2010)	Q	245
	1.6		Modarresi et al. (2007)	Q	67
	2.2		Yaffe et al. (2003)	Q	248, 249
	3.1		Katritzky et al. (1998)	Q	
1-hydroxy-3-ethylbenzene	4.9		Karl et al. (2003)	M	
$C_8H_{10}O$	1.6×10^1		Abraham et al. (1994a)	R	
(3-ethylphenol)	7.9		Keshavarz et al. (2022)	Q	
[620-17-7]	2.4×10^1		Duchowicz et al. (2020)	Q	184
HMNKTRSOROOSPP-UHFFFAOYSA-N	9.0		HSDB (2015)	Q	99
	6.2		Raventos-Duran et al. (2010)	Q	242, 243
	4.9		Raventos-Duran et al. (2010)	Q	244
	1.2×10^1		Raventos-Duran et al. (2010)	Q	245
	3.4		Hilal et al. (2008)	Q	
	2.1×10^1		Modarresi et al. (2007)	Q	67
	1.5×10^1		Yaffe et al. (2003)	Q	248, 249
	1.8×10^1		English and Carroll (2001)	Q	230, 231
	5.4×10^1		Nirmalakhandan et al. (1997)	Q	
	1.6×10^1		Duchowicz et al. (2020)	?	185, 21
1-hydroxy-4-ethylbenzene	8.2		HSDB (2015)	V	
$C_8H_{10}O$	2.1×10^1		Mackay et al. (2006c)	V	
(4-ethylphenol)	1.3×10^1		Abraham et al. (1994a)	R	
[123-07-9]	7.9		Keshavarz et al. (2022)	Q	
HXDOZKJGKXYMEW-UHFFFAOYSA-N	2.4×10^1		Duchowicz et al. (2020)	Q	299
	6.2		Raventos-Duran et al. (2010)	Q	271, 243
	6.2		Raventos-Duran et al. (2010)	Q	244
	1.2×10^1		Raventos-Duran et al. (2010)	Q	245
	3.8		Hilal et al. (2008)	Q	
	9.4		Modarresi et al. (2007)	Q	67
	1.6×10^1		English and Carroll (2001)	Q	230, 231
	5.4×10^1		Nirmalakhandan et al. (1997)	Q	
	1.3×10^1		Duchowicz et al. (2020)	?	185, 21
2,3,4-trimethylphenol	1.3×10^1		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O$	1.8×10^1		Wang et al. (2017)	Q	80, 239
[526-85-2]	8.9		Wang et al. (2017)	Q	80, 240
XRUGBBIQLIVCSI-UHFFFAOYSA-N					
2,3,5-trimethylphenol	1.2×10^1		Mackay et al. (2006c)	V	
$C_9H_{12}O$	1.2×10^1		Mackay et al. (1995)	V	
[697-82-5]					
OGRAOKJKVGDSFR-UHFFFAOYSA-N					

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Table A3.2: Alcohols (ROH) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,6-trimethylphenol	2.5		Duchowicz et al. (2020)	V	186
$C_9H_{12}O$	2.5		HSDB (2015)	V	
[2416-94-6]	1.6		Duchowicz et al. (2020)	Q	
QQOMQLYQAXGHSU-UHFFFAOYSA-N	2.5		Wang et al. (2017)	Q	80, 238
	1.1×10^{1}		Wang et al. (2017)	Q	80, 239
	1.3		Wang et al. (2017)	Q	80, 240
	1.1×10^{1}		Hilal et al. (2008)	Q	
	4.1×10^{-1}		Modarresi et al. (2007)	Q	67
2,4,6-trimethylphenol	3.8		Duchowicz et al. (2020)	V	186
$C_9H_{12}O$	3.2		HSDB (2015)	V	
[527-60-6]	1.3		Mackay et al. (2006c)	V	
BPRYUXCVCCNUFE-UHFFFAOYSA-N	1.4		Mackay et al. (1995)	V	
	1.6		Duchowicz et al. (2020)	Q	
	2.5		Wang et al. (2017)	Q	80, 238
	8.9		Wang et al. (2017)	Q	80, 239
	1.2		Wang et al. (2017)	Q	80, 240
	4.9		Raventos-Duran et al. (2010)	Q	242, 243
	3.1		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	245
	9.2		Hilal et al. (2008)	Q	
	1.2		Modarresi et al. (2007)	Q	67
3,4,5-trimethylphenol	3.4×10^{1}		Mackay et al. (2006c)	V	
$C_9H_{12}O$	3.8×10^{1}		Mackay et al. (1995)	V	
[527-54-8]					
FDQQNNZKEJIHMS-UHFFFAOYSA-N					
1-hydroxy-4-propylbenzene	1.7		Mackay et al. (2006c)	V	
$C_9H_{12}O$	8.6		Abraham et al. (1994a)	R	
(4-propylphenol)	1.1×10^{1}		Keshavarz et al. (2022)	Q	
[645-56-7]	2.5×10^{1}		Duchowicz et al. (2020)	Q	
KLSLBUSXWBJMEC-UHFFFAOYSA-N	4.9		Raventos-Duran et al. (2010)	Q	271, 243
	3.9		Raventos-Duran et al. (2010)	Q	244
	9.9		Raventos-Duran et al. (2010)	Q	245
	3.1		Hilal et al. (2008)	Q	
	1.0×10^{1}		Modarresi et al. (2007)	Q	67
	8.8		Yaffe et al. (2003)	Q	248, 249
	1.2×10^{1}		English and Carroll (2001)	Q	230, 260
	4.3×10^{1}		Nirmalakhandan et al. (1997)	Q	
	8.7		Duchowicz et al. (2020)	?	185, 21
2-(1-methylethyl)-phenol	2.6		Mackay et al. (2006c)	V	
$C_9H_{12}O$	2.8×10^{1}		Wang et al. (2017)	Q	80, 238
[88-69-7]	3.9		Wang et al. (2017)	Q	80, 239
CRBJBYGJVIBWIY-UHFFFAOYSA-N	4.5		Wang et al. (2017)	Q	80, 240
	2.8		Hilal et al. (2008)	Q	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-phenylisopropanol	2.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O$	1.4×10^{1}		Wang et al. (2017)	Q	80, 239
[617-94-7]	1.2×10^{1}		Wang et al. (2017)	Q	80, 240
BDCFWIDZNLCTMF-UHFFFAOYSA-N	2.6×10^{1}		HSDB (2015)	Q	99
2-ethyl-3-methylphenol	1.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O$	8.9		Wang et al. (2017)	Q	80, 239
[6161-62-2]	5.8		Wang et al. (2017)	Q	80, 240
OCKYMBMCPOAFLL-UHFFFAOYSA-N					
2-ethyl-5-methylphenol	1.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O$	8.0		Wang et al. (2017)	Q	80, 239
[1687-61-2]	4.9		Wang et al. (2017)	Q	80, 240
LTRVUFFOMIUCPJ-UHFFFAOYSA-N					
2-ethyl-6-methylphenol	3.3		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O$	6.2		Wang et al. (2017)	Q	80, 239
[1687-64-5]	6.9×10^{-1}		Wang et al. (2017)	Q	80, 240
CIRRFAQIWQFQSS-UHFFFAOYSA-N					
5-ethyl-3-methylphenol	1.5×10^{1}		Duchowicz et al. (2020)	V	186
$C_9H_{12}O$	1.3×10^{1}		Duchowicz et al. (2020)	Q	
[698-71-5]	4.9		Raventos-Duran et al. (2010)	Q	242, 243
XTCHLXABLZQNNN-UHFFFAOYSA-N	3.9		Raventos-Duran et al. (2010)	Q	244
	9.9		Raventos-Duran et al. (2010)	Q	245
	2.9		Hilal et al. (2008)	Q	
	1.8×10^{1}		Modarresi et al. (2007)	Q	67
1-(2-methylphenyl)ethanol	2.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O$	2.9×10^{1}		Wang et al. (2017)	Q	80, 239
[7287-82-3]	1.6×10^{1}		Wang et al. (2017)	Q	80, 240
SDCBYRLJYGORNK-UHFFFAOYSA-N					
2-propylphenol	2.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O$	5.6		Wang et al. (2017)	Q	80, 239
[644-35-9]	5.0		Wang et al. (2017)	Q	80, 240
LCHYEKKJCUJAKN-UHFFFAOYSA-N					
1-phenyl-1-propanol	2.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O$	2.3×10^{1}		Wang et al. (2017)	Q	80, 239
[93-54-9]	9.8		Wang et al. (2017)	Q	80, 240
DYUQAZSOFZSPHD-UHFFFAOYSA-N					
2,3-dimethylbenzyl alcohol	1.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O$	7.4×10^{1}		Wang et al. (2017)	Q	80, 239
[13651-14-4]	2.3×10^{1}		Wang et al. (2017)	Q	80, 240
ZQQIVMXQYUZKIQ-UHFFFAOYSA-N					

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Table A3.2: Alcohols (ROH) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4-dimethylbenzyl alcohol	1.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O$	6.2×10^{1}		Wang et al. (2017)	Q	80, 239
[6966-10-5]	5.5×10^{1}		Wang et al. (2017)	Q	80, 240
OKGZCXPDJKKZAP-UHFFFAOYSA-N					
3,5-dimethylbenzyl alcohol	1.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O$	3.7×10^{1}		Wang et al. (2017)	Q	80, 239
[27129-87-9]	4.0×10^{1}		Wang et al. (2017)	Q	80, 240
IQWWTJDRVBWBEL-UHFFFAOYSA-N					
2-(1,1-dimethylethyl)-phenol	3.9×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{10}H_{14}O$	4.4		Duchowicz et al. (2020)	Q	
[88-18-6]	7.0		HSDB (2015)	Q	99
WJQOZHYUIDYNHM-UHFFFAOYSA-N					
3-(1,1-dimethylethyl)-phenol	5.1		Duchowicz et al. (2020)	V	186
$C_{10}H_{14}O$	4.4		Duchowicz et al. (2020)	Q	
[585-34-2]					
CYEKUDPFXBLGHH-UHFFFAOYSA-N					
2-(1-methylpropyl)phenol	4.7		HSDB (2015)	Q	99
$C_{10}H_{14}O$					
[89-72-5]					
NGFPWHGISWUQOI-UHFFFAOYSA-N					
4-(1-methylpropyl)-phenol	3.6		Mackay et al. (2006c)	V	
$C_{10}H_{14}O$	4.3		Mackay et al. (1995)	V	
(4-*sec*-butylphenol)					
[99-71-8]					
ZUTYZAFDFLLILI-UHFFFAOYSA-N					
4-*tert*-butylphenol	8.9	7700	Parsons et al. (1972)	M	417
$C_{10}H_{14}O$	1.6×10^{1}		Mackay et al. (2006c)	V	
[98-54-4]	2.1×10^{1}		Mackay et al. (1995)	V	
QHPQWRBYOIRBIT-UHFFFAOYSA-N	1.4×10^{1}		Keshavarz et al. (2022)	Q	
	4.4		Duchowicz et al. (2020)	Q	
	2.1		Hilal et al. (2008)	Q	
	4.8		Modarresi et al. (2007)	Q	67
	8.8		Yaffe et al. (2003)	Q	248, 249
	6.7		English and Carroll (2001)	Q	230, 231
	2.5×10^{1}		Katritzky et al. (1998)	Q	
	2.4×10^{1}		Nirmalakhandan et al. (1997)	Q	
	5.2		Suzuki et al. (1992)	Q	232
	2.7		Nirmalakhandan and Speece (1988)	Q	
	8.3		Duchowicz et al. (2020)	?	185, 21
	1.5×10^{-1}		Betterton (1992)	?	421
	8.8		Abraham et al. (1990)	?	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-5-(1-methylethyl)-phenol	1.5		Martins et al. (2017)	V	315
$C_{10}H_{14}O$	2.4	9300	van Roon et al. (2005)	V	
(carvacrol)					
[499-75-2]					
RECUKUPTGUEGMW-UHFFFAOYSA-N					
5-methyl-2-(1-methylethyl)-phenol	2.0×10^{1}		Duchowicz et al. (2020)	V	186
$C_{10}H_{14}O$	1.5		Martins et al. (2017)	V	315
(thymol)	3.0	9300	van Roon et al. (2005)	V	
[89-83-8]	5.1		Duchowicz et al. (2020)	Q	
MGSRCZKZVOBKFT-UHFFFAOYSA-N	3.1		Raventos-Duran et al. (2010)	Q	242, 243
	2.0		Raventos-Duran et al. (2010)	Q	244
	7.8		Raventos-Duran et al. (2010)	Q	245
	2.8		Hilal et al. (2008)	Q	
	7.1×10^{-1}		Modarresi et al. (2007)	Q	67
1-(3,5-dimethylphenyl)ethanol	1.2×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{14}O$	1.8×10^{1}		Wang et al. (2017)	Q	80, 239
[5379-18-0]	1.4×10^{1}		Wang et al. (2017)	Q	80, 240
RHBAJFPGUNNLFA-UHFFFAOYSA-N					
6-ethyl-2,4-xylenol	2.0		Wang et al. (2017)	Q	80, 238
$C_{10}H_{14}O$	5.8		Wang et al. (2017)	Q	80, 239
[2219-79-6]	6.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MXHAHSBTOVFDBK-UHFFFAOYSA-N					
2-(1,1-dimethylethyl)-4-methylphenol	6.6		HSDB (2015)	Q	99
$C_{11}H_{16}O$					
[2409-55-4]					
IKEHOXWJQXIQAG-UHFFFAOYSA-N					
4-(1,1-dimethylpropyl)phenol	4.9		HSDB (2015)	V	
$C_{11}H_{16}O$					
[80-46-6]					
NRZWYNLTFLDQQX-UHFFFAOYSA-N					
MCM:DE35TOH	1.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{16}O$	1.6×10^{1}		Wang et al. (2017)	Q	80, 239
OZZOZHVUMWFILP-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DEMPHOH	1.8		Wang et al. (2017)	Q	80, 238
$C_{11}H_{16}O$	3.8		Wang et al. (2017)	Q	80, 239
VUDWBUZLGAXSDX-UHFFFAOYSA-N	6.3×10^{-1}		Wang et al. (2017)	Q	80, 240
josenol	4.5×10^{1}		Dupeux et al. (2022)	Q	259
$C_{11}H_{14}O$					
(2-methyl-3-(4-methylphenyl)-2-propen-1-ol)					
[56138-10-4]					
WWHATUWNHYNMNW-UHFFFAOYSA-N					

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
lilyflore $C_{12}H_{16}O$ [285977-85-7] UWSPWQQZFOSTHS-UHFFFAOYSA-N	1.3×10^{1}		Dupeux et al. (2022)	Q	259
benzhydrol $C_{13}H_{12}O$ [91-01-0] QILSFLSDHQAZET-UHFFFAOYSA-N	3.8×10^{2}		Ebert et al. (2023)	?	318
1-hydroxy-4-octylbenzene $C_{14}H_{22}O$ (4-octylphenol) [1806-26-4] NTDQQZYCCIDJRK-UHFFFAOYSA-N	1.3 2.0		Mackay et al. (2006c) Mackay et al. (1995)	V V	
4-(1,1,3,3-tetramethylbutyl)-phenol $C_{14}H_{22}O$ (*p-tert*-octylphenol) [140-66-9] ISAVYTVYFVQUDY-UHFFFAOYSA-N	2.3 1.4 2.2 2.3 1.0×10^{1} 1.8	9000	Xie et al. (2004) HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	M Q Q Q Q Q	 99 287, 288 287, 289 287, 290 287, 291
1-hydroxy-4-nonylbenzene $C_{15}H_{24}O$ (4-nonylphenol) [104-40-5] IGFHQQFPSIBGKE-UHFFFAOYSA-N	2.9×10^{-1} 2.9×10^{-1} 3.6×10^{-1} 6.4×10^{-1} 2.8×10^{1}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006c) Mackay et al. (1995) Duchowicz et al. (2020)	V V V V Q	186
2,6-bis(1,1-dimethylethyl)-4-methylphenol $C_{15}H_{24}O$ (butylated hydroxytoluene; BHT) [128-37-0] NLZUEZXRPGMBCV-UHFFFAOYSA-N	2.9×10^{-3}		Yoshida et al. (1983)	V	
4-(3',5'-dimethyl-3'-heptyl)-phenol(+) $C_{15}H_{24}O$ RYIHVIPUIXFRNI-IUODEOHRSA-N	2.9	8700	Xie et al. (2004)	M	
4-(3',5'-dimethyl-3'-heptyl)-phenol(-) $C_{15}H_{24}O$ RYIHVIPUIXFRNI-SWLSCSKDSA-N	3.3	8600	Xie et al. (2004)	M	

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Table A3.2: Alcohols (ROH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-phenylethanol	1.7×10^{1}	7200	Brockbank (2013)	L	1
$C_8H_{10}O$	$>3.7\times10^{1}$		Altschuh et al. (1999)	M	
[60-12-8]	6.6×10^{1}		HSDB (2015)	V	
WRMNZCZEMHIOCP-UHFFFAOYSA-N	3.9×10^{1}		Abraham et al. (1994a)	R	
	3.5		Yaws (2003)	X	258
	1.6×10^{1}		Dupeux et al. (2022)	Q	259
	3.0×10^{1}		Keshavarz et al. (2022)	Q	
	2.0×10^{-3}		Abney (2021)	Q	399
	8.5		Duchowicz et al. (2020)	Q	184
	8.5		Wang et al. (2017)	Q	80, 238
	3.9×10^{1}		Wang et al. (2017)	Q	80, 239
	3.9×10^{1}		Wang et al. (2017)	Q	80, 240
	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	245
	1.9×10^{1}		Hilal et al. (2008)	Q	
	3.2×10^{1}		Modarresi et al. (2007)	Q	67
	2.4×10^{-1}		Emel'yanenko et al. (2007)	Q	415
	2.4×10^{-1}		Hertel and Sommer (2005)	Q	415
	3.9×10^{1}		Yaffe et al. (2003)	Q	248, 249
	1.0×10^{1}		Yao et al. (2002)	Q	229
	2.8×10^{1}		English and Carroll (2001)	Q	230, 274
	5.4×10^{1}		Katritzky et al. (1998)	Q	
	5.3×10^{1}		Nirmalakhandan et al. (1997)	Q	
	3.9×10^{1}		Duchowicz et al. (2020)	?	185, 21
	3.5		Yaws (1999)	?	21
3-phenyl-1-propanol	$>1.8\times10^{2}$		Altschuh et al. (1999)	M	
$C_9H_{12}O$	4.8×10^{1}		Abraham et al. (1994a)	R	
[122-97-4]	4.1×10^{1}		Keshavarz et al. (2022)	Q	
VAJVDSVGBWFCLW-UHFFFAOYSA-N	8.8		Duchowicz et al. (2020)	Q	299
	1.4×10^{1}		Hilal et al. (2008)	Q	
	2.0×10^{1}		Modarresi et al. (2007)	Q	67
	3.4×10^{1}		English and Carroll (2001)	Q	230, 231
	4.2×10^{1}		Nirmalakhandan et al. (1997)	Q	
	4.9×10^{1}		Duchowicz et al. (2020)	?	185, 21
4-phenyl-1-butanol	>6.7		Altschuh et al. (1999)	M	
$C_{10}H_{14}O$	1.2×10^{1}		Hilal et al. (2008)	Q	
[3360-41-6]					
LDZLXQFDGRCELX-UHFFFAOYSA-N					
1-naphthalenol	1.6×10^{2}		HSDB (2015)	V	
$C_{10}H_8O$	2.9×10^{1}		Mackay et al. (2006c)	V	
(1-naphthol)	1.7×10^{2}		Abraham et al. (1994a)	R	
[90-15-3]	2.1×10^{2}		Keshavarz et al. (2022)	Q	
KJCVRFUGPWSIIH-UHFFFAOYSA-N	1.7×10^{2}		Duchowicz et al. (2020)	Q	
	6.9×10^{1}		Hilal et al. (2008)	Q	
	8.4×10^{1}		Modarresi et al. (2007)	Q	67

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Table A3.2: Alcohols (ROH) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.5×10^{2}		English and Carroll (2001)	Q	230, 231
	1.5×10^{3}		Nirmalakhandan et al. (1997)	Q	
	1.6×10^{2}		Duchowicz et al. (2020)	?	185, 21
2-naphthalenol $C_{10}H_8O$ (2-naphthol) [135-19-3] JWAZRIHNYRIHIV-UHFFFAOYSA-N	1.1×10^{2}		Mackay et al. (2006c)	V	
	3.6×10^{2}		Abraham et al. (1994a)	R	
	2.1×10^{2}		Keshavarz et al. (2022)	Q	
	1.7×10^{2}		Duchowicz et al. (2020)	Q	
	2.1×10^{2}		HSDB (2015)	Q	99
	7.0×10^{1}		Hilal et al. (2008)	Q	
	2.7×10^{2}		Modarresi et al. (2007)	Q	67
		7400	Kühne et al. (2005)	Q	
	5.8×10^{2}		English and Carroll (2001)	Q	230, 231
	1.7×10^{3}		Nirmalakhandan et al. (1997)	Q	
	3.6×10^{2}		Duchowicz et al. (2020)	?	185, 21
		7200	Kühne et al. (2005)	?	
o-hydroxybiphenyl $C_{12}H_{10}O$ [90-43-7] LLEMOWNGBBNAJR-UHFFFAOYSA-N	9.4		Duchowicz et al. (2020)	V	186
	9.4		HSDB (2015)	V	
	2.9×10^{-1}		Mackay et al. (2006c)	V	
	2.1×10^{2}		Duchowicz et al. (2020)	Q	
	3.1×10^{1}		Hilal et al. (2008)	Q	
	1.1×10^{1}		Modarresi et al. (2007)	Q	67
p-hydroxybiphenyl $C_{12}H_{10}O$ [92-69-3] YXVFYQXJAXKLAK-UHFFFAOYSA-N	1.6×10^{-1}		Mackay et al. (2006c)	V	
	1.9×10^{2}		HSDB (2015)	Q	99
2,4,6-tris(1,1-dimethylethyl)phenol $C_{18}H_{30}O$ [732-26-3] PFEFOYRSMXVNEL-UHFFFAOYSA-N	1.0		Zhang et al. (2010)	Q	287, 288
	5.6×10^{-2}		Zhang et al. (2010)	Q	287, 289
	3.3×10^{-2}		Zhang et al. (2010)	Q	287, 290
	5.3×10^{-2}		Zhang et al. (2010)	Q	287, 291
dehydroabietol $C_{20}H_{30}O$ [3772-55-2] WSKGRAGZAQRSED-IOJLRTSASA-N	8.4		Zhang et al. (2010)	Q	287, 288
	1.8×10^{2}		Zhang et al. (2010)	Q	287, 289
	2.4×10^{1}		Zhang et al. (2010)	Q	287, 290
	7.2×10^{-1}		Zhang et al. (2010)	Q	287, 291
2,2'-methylenebis(6-(1,1-dimethylethyl)-4-methylphenol) $C_{23}H_{32}O_2$ [119-47-1] KGRVJHAUYBGFFP-UHFFFAOYSA-N	1.2×10^{6}		HSDB (2015)	Q	99
2,4-dinonylphenol $C_{24}H_{42}O$ [137-99-5] FDAJTLLBHNHECW-UHFFFAOYSA-N	1.5×10^{-1}		HSDB (2015)	Q	99
	1.6×10^{-1}		Zhang et al. (2010)	Q	287, 288
	3.8×10^{-1}		Zhang et al. (2010)	Q	287, 289
	7.0×10^{-1}		Zhang et al. (2010)	Q	287, 290
	2.5×10^{-1}		Zhang et al. (2010)	Q	287, 291

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A3.3 Polyols ($R(OH)_n$)

Table A3.3: Polyols ($R(OH)_n$)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
methanediol	9.9×10^1		Franco et al. (2021)	R	422
$HOCH_2OH$	4.0×10^3		Mansfield (2020)	T	423
[463-57-0]	7.1×10^2		Mansfield (2020)	T	423
CKFGINPQOCXMAZ-UHFFFAOYSA-N					
1,1-ethanediol	4.0×10^1		Mansfield (2020)	T	423
$CH_3CH_2(OH)_2$	1.4×10^1		Mansfield (2020)	T	423
[4433-56-1]					
AZHSSKPUVBVXLK-UHFFFAOYSA-N					
1,2-ethanediol	6.5×10^3		Burkholder et al. (2019)	L	
$HO(CH_2)_2OH$	6.5×10^3		Burkholder et al. (2015)	L	
(ethylene glycol)	4.0×10^3		Bone et al. (1983)	M	12
[107-21-1]	1.6×10^2		Butler and Ramchandani (1935)	M	424
LYCAIKOWRPUZTN-UHFFFAOYSA-N	4.7		HSDB (2015)	V	
	6.5×10^3	8800	Compernolle and Müller (2014b)	V	
	5.0×10^3		Hwang et al. (1992)	V	
	7.0×10^3		Yaws (2003)	X	258
	7.0×10^3		Yaws (2003)	X	237
	4.8×10^3		Dupeux et al. (2022)	Q	259
	2.9×10^2		Keshavarz et al. (2022)	Q	
	6.4×10^2		Duchowicz et al. (2020)	Q	184
	3.3×10^2		Wang et al. (2017)	Q	80, 238
	1.3×10^3		Wang et al. (2017)	Q	80, 239
	6.3×10^3		Wang et al. (2017)	Q	80, 240
	5.6×10^2		Olsen et al. (2016)	Q	425
	4.0×10^2		Olsen et al. (2016)	Q	426
	4.3×10^2		Olsen et al. (2016)	Q	427
	1.3×10^4		Gharagheizi et al. (2012)	Q	
	7.8×10^3		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^2		Raventos-Duran et al. (2010)	Q	244
	7.8×10^1		Raventos-Duran et al. (2010)	Q	245
	2.5×10^3		Gharagheizi et al. (2010)	Q	246
	7.2×10^2		Hilal et al. (2008)	Q	
	3.1×10^3		Modarresi et al. (2007)	Q	67
	6.9×10^3		Yao et al. (2002)	Q	229
	8.6×10^2		Katritzky et al. (1998)	Q	
	1.6×10^2		Duchowicz et al. (2020)	?	185, 21
	5.2×10^3		Yaws (1999)	?	21

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Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1,2-propanediol	2.7×10^3		Burkholder et al. (2019)	L	
$C_3H_8O_2$	2.7×10^3		Burkholder et al. (2015)	L	
(propylene glycol)	7.7×10^2		Duchowicz et al. (2020)	V	186
[57-55-6]	7.6×10^2		HSDB (2015)	V	
DNIAPMSPPWPWGF-UHFFFAOYSA-N	2.7×10^3	9500	Compernolle and Müller (2014b)	V	
	2.7×10^3		Yaws (2003)	X	258
	2.7×10^3		Yaws (2003)	X	237
	1.9×10^3		Dupeux et al. (2022)	Q	259
	3.5×10^2		Duchowicz et al. (2020)	Q	
	3.1×10^2		Wang et al. (2017)	Q	80, 238
	1.0×10^3		Wang et al. (2017)	Q	80, 239
	1.3×10^3		Wang et al. (2017)	Q	80, 240
	3.9×10^3		Gharagheizi et al. (2012)	Q	
	2.7×10^3		Gharagheizi et al. (2010)	Q	246
			Saxena and Hildemann (1996)	E	401, 428
1,3-propanediol	1.6×10^4		Burkholder et al. (2019)	L	
$C_3H_8O_2$	1.6×10^4		Burkholder et al. (2015)	L	
[504-63-2]	9.1×10^3		Bone et al. (1983)	M	12
YPFDHNVEDLHUCE-UHFFFAOYSA-N	1.6×10^4	9500	Compernolle and Müller (2014b)	V	
	7.4×10^2		Wang et al. (2017)	Q	80, 238
	6.3×10^3		Wang et al. (2017)	Q	80, 239
	4.8×10^3		Wang et al. (2017)	Q	80, 240
	3.1×10^3		Raventos-Duran et al. (2010)	Q	271, 243
	2.5×10^3		Raventos-Duran et al. (2010)	Q	244
	6.2×10^1		Raventos-Duran et al. (2010)	Q	245
	4.0×10^2		Hilal et al. (2008)	Q	
	2.0×10^3		Modarresi et al. (2007)	Q	67
1,2,3-propanetriol	4.7×10^6		Burkholder et al. (2019)	L	
$C_3H_8O_3$	4.7×10^6		Burkholder et al. (2015)	L	
(glycerol)	5.8×10^2		Butler and Ramchandani (1935)	M	424
[56-81-5]	4.7×10^6	11000	Compernolle and Müller (2014b)	V	
PEDCQBHIVMGVHV-UHFFFAOYSA-N	5.0×10^6		Hwang et al. (1992)	V	
	3.8×10^2		Keshavarz et al. (2022)	Q	
	1.7×10^5		Duchowicz et al. (2020)	Q	
			Saxena and Hildemann (1996)	E	401, 429
	5.7×10^2		Duchowicz et al. (2020)	?	185, 21
1,2-butanediol	2.1×10^3		Burkholder et al. (2019)	L	430
$C_4H_{10}O_2$	2.1×10^3		Burkholder et al. (2015)	L	431
[584-03-2]	$>3.4\times10^2$		Altschuh et al. (1999)	M	
BMRWNKZVCUKKSR-UHFFFAOYSA-N	1.7×10^3		Duchowicz et al. (2020)	V	186
	2.1×10^3	9900	Compernolle and Müller (2014b)	V	
	4.4×10^2		Duchowicz et al. (2020)	Q	
	2.9×10^2		Wang et al. (2017)	Q	80, 238
	7.6×10^2		Wang et al. (2017)	Q	80, 239
	4.8×10^2		Wang et al. (2017)	Q	80, 240

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Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1,3-butanediol	7.0×10^3		Burkholder et al. (2019)	L	
$C_4H_{10}O_2$	7.0×10^3		Burkholder et al. (2015)	L	
[107-88-0]	4.1×10^3		Duchowicz et al. (2020)	V	186
PUPZLCDOIYMWBV-UHFFFAOYSA-N	7.0×10^3	10000	Compernolle and Müller (2014b)	V	
	9.5×10^2		Duchowicz et al. (2020)	Q	
	6.9×10^2		Wang et al. (2017)	Q	80, 238
	4.0×10^3		Wang et al. (2017)	Q	80, 239
	2.5×10^3		Wang et al. (2017)	Q	80, 240
	4.9×10^4		Saxena and Hildemann (1996)	E	401
1,4-butanediol	3.5×10^4		Burkholder et al. (2019)	L	
$C_4H_{10}O_2$	3.5×10^4		Burkholder et al. (2015)	L	
[110-63-4]	$>9.0\times10^2$		Altschuh et al. (1999)	M	
WERYXYBDKMZEQL-UHFFFAOYSA-N	7.6×10^3		Duchowicz et al. (2020)	V	186
	7.6×10^3		HSDB (2015)	V	
	3.5×10^4	11000	Compernolle and Müller (2014b)	V	
	2.4×10^3		Duchowicz et al. (2020)	Q	
	6.0×10^2		Wang et al. (2017)	Q	80, 238
	7.6×10^3		Wang et al. (2017)	Q	80, 239
	9.6×10^3		Wang et al. (2017)	Q	80, 240
	3.1×10^4		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^3		Raventos-Duran et al. (2010)	Q	244
	3.9×10^1		Raventos-Duran et al. (2010)	Q	245
	8.0×10^3		Hilal et al. (2008)	Q	
	1.6×10^3		Modarresi et al. (2007)	Q	67
			Saxena and Hildemann (1996)	E	401, 432
	1.9×10^4		Yaws (1999)	?	21, 12
2,3-butanediol	1.1×10^3		Burkholder et al. (2019)	L	
$C_4H_{10}O_2$	1.1×10^3		Burkholder et al. (2015)	L	
[513-85-9]	3.4×10^2		Duchowicz et al. (2020)	V	186
OWBTYPJTUOEWEK-UHFFFAOYSA-N	3.4×10^2		HSDB (2015)	V	
	1.1×10^3	9900	Compernolle and Müller (2014b)	V	
	9.7×10^2		Yaws (2003)	X	237, 12
	1.7×10^2		Duchowicz et al. (2020)	Q	
	3.3×10^2		Wang et al. (2017)	Q	80, 238
	1.2×10^3		Wang et al. (2017)	Q	80, 239
	4.1×10^2		Wang et al. (2017)	Q	80, 240
	1.7×10^3		Gharagheizi et al. (2012)	Q	
	7.8×10^2		Gharagheizi et al. (2010)	Q	246
			Saxena and Hildemann (1996)	E	401, 433
meso-2,3-butanediol	2.2×10^2		Duchowicz et al. (2020)	V	186
$C_4H_{10}O_2$	6.8×10^2		Yaws (2003)	X	237, 12
[5341-95-7]	1.7×10^2		Duchowicz et al. (2020)	Q	
OWBTYPJTUOEWEK-ZXZARUISSA-N	1.6×10^3		Gharagheizi et al. (2012)	Q	
	7.8×10^2		Gharagheizi et al. (2010)	Q	246

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Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
2-methylpropane-1,2-diol	1.8×10^2		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_2$	5.1×10^2		Wang et al. (2017)	Q	80, 239
[558-43-0]	3.2×10^2		Wang et al. (2017)	Q	80, 240
BTVWZWFKMIUSGS-UHFFFAOYSA-N					
2-methylpropane-1,3-diol	6.9×10^2		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_2$	5.0×10^3		Wang et al. (2017)	Q	80, 239
[2163-42-0]	2.6×10^3		Wang et al. (2017)	Q	80, 240
QWGRWMMWNDWRQN-UHFFFAOYSA-N	4.3×10^1		HSDB (2015)	Q	99
1,2,3-butanetriol	3.0×10^9		Saxena and Hildemann (1996)	E	401
$C_4H_{10}O_3$					
[4435-50-1]					
YAXKTBLXMTYWDQ-UHFFFAOYSA-N					
1,2,4-butanetriol	7.1×10^5		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	1.9×10^6		Wang et al. (2017)	Q	80, 239
[3068-00-6]	3.2×10^5		Wang et al. (2017)	Q	80, 240
ARXKVVRQIIOZGF-UHFFFAOYSA-N	3.0×10^9		Saxena and Hildemann (1996)	E	401
1,2,3,4-butanetetrol	2.0×10^{14}		Saxena and Hildemann (1996)	E	401
$C_4H_{10}O_4$					
(1,2,3,4-tetrahydroxybutane; tetritol)					
[7541-59-5]					
UNXHWFMMPAWVPI-UHFFFAOYSA-N					
2(R),3(S)-1,2,3,4-butanetetrol	1.1×10^{10}		Burkholder et al. (2019)	L	
$C_4H_{10}O_4$	1.1×10^{10}		Burkholder et al. (2015)	L	
(erythritol)	2.5×10^9		Qin et al. (2021)	M	434
[149-32-6]	1.1×10^{10}	16000	Compernolle and Müller (2014b)	V	
UNXHWFMMPAWVPI-ZXZARUISSA-N	3.2×10^4		Qin et al. (2021)	Q	435
	4.1×10^8		Qin et al. (2021)	Q	436
	3.2×10^4		HSDB (2015)	Q	99
1,2-pentanediol	1.4×10^3		Compernolle and Müller (2014b)	V	
$C_5H_{12}O_2$	2.2×10^2		Wang et al. (2017)	Q	80, 238
[5343-92-0]	5.9×10^2		Wang et al. (2017)	Q	80, 239
WCVRQHFDJLLWFE-UHFFFAOYSA-N	4.2×10^2		Wang et al. (2017)	Q	80, 240
1,3-pentanediol	5.6×10^2		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	3.1×10^3		Wang et al. (2017)	Q	80, 239
[3174-67-2]	1.5×10^3		Wang et al. (2017)	Q	80, 240
RUOPINZRYMFPBF-UHFFFAOYSA-N					
1,4-pentanediol	2.3×10^4		Compernolle and Müller (2014b)	V	
$C_5H_{12}O_2$	5.6×10^2		Wang et al. (2017)	Q	80, 238
[626-95-9]	3.9×10^3		Wang et al. (2017)	Q	80, 239
GLOBUAZSRIOKLN-UHFFFAOYSA-N	4.8×10^3		Wang et al. (2017)	Q	80, 240

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Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1,5-pentanediol	7.0×10^4	12000	Compernolle and Müller (2014b)	V	
$C_5H_{12}O_2$	2.0×10^4		Raventos-Duran et al. (2010)	Q	242, 243
[111-29-5]	1.6×10^4		Raventos-Duran et al. (2010)	Q	244
ALQSHHUCVQOPAS-UHFFFAOYSA-N	3.1×10^1		Raventos-Duran et al. (2010)	Q	245
	7.7×10^3		Hilal et al. (2008)	Q	
	3.9×10^4		Saxena and Hildemann (1996)	E	401
2,3-pentanediol	2.6×10^2		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	1.2×10^3		Wang et al. (2017)	Q	80, 239
[42027-23-6]	1.7×10^2		Wang et al. (2017)	Q	80, 240
XLMFDCKSFJWJTP-UHFFFAOYSA-N	3.0×10^4		Saxena and Hildemann (1996)	E	401
2,4-pentanediol	3.8×10^3		Compernolle and Müller (2014b)	V	
$C_5H_{12}O_2$	6.5×10^2		Wang et al. (2017)	Q	80, 238
[625-69-4]	5.4×10^3		Wang et al. (2017)	Q	80, 239
GTCCGKPBSJZVRZ-UHFFFAOYSA-N	2.3×10^3		Wang et al. (2017)	Q	80, 240
	3.0×10^4		Saxena and Hildemann (1996)	E	401
3-methylbutane-1,2-diol	2.6×10^2		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	8.5×10^2		Wang et al. (2017)	Q	80, 239
[50468-22-9]	3.3×10^2		Wang et al. (2017)	Q	80, 240
HJJZIMFAIMUSBW-UHFFFAOYSA-N					
3-methylbutane-1,3-diol	4.0×10^2		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	2.6×10^3		Wang et al. (2017)	Q	80, 239
[2568-33-4]	2.1×10^3		Wang et al. (2017)	Q	80, 240
XPFCZYUVICHKDS-UHFFFAOYSA-N					
2-methylbutane-1,2-diol	1.6×10^2		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	4.3×10^2		Wang et al. (2017)	Q	80, 239
[41051-72-3]	1.1×10^2		Wang et al. (2017)	Q	80, 240
DOPZLYNWNJHAOS-UHFFFAOYSA-N					
2-methylbutane-1,3-diol	6.5×10^2		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	4.7×10^3		Wang et al. (2017)	Q	80, 239
[684-84-4]	2.0×10^3		Wang et al. (2017)	Q	80, 240
GNBPEYCZELNJMS-UHFFFAOYSA-N					
2-methylbutane-1,4-diol	5.6×10^2		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	6.0×10^3		Wang et al. (2017)	Q	80, 239
[2938-98-9]	6.2×10^3		Wang et al. (2017)	Q	80, 240
MWCBGWLCXSUTHK-UHFFFAOYSA-N					
2-methylbutane-2,3-diol	1.8×10^2		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	7.3×10^2		Wang et al. (2017)	Q	80, 239
[5396-58-7]	2.0×10^2		Wang et al. (2017)	Q	80, 240
IDEOPBXRUBNYBN-UHFFFAOYSA-N					

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Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
2,2-dimethylpropane-1,3-diol $C_5H_{12}O_2$ [126-30-7] SLCVBVWXLSEKPL-UHFFFAOYSA-N	4.0×10^2 3.1×10^3 6.8×10^2		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
2-(hydroxymethyl)-2-methyl-1,3-propanediol $C_5H_{12}O_3$ [77-85-0] QXJQHYBHAIHNGG-UHFFFAOYSA-N	9.0×10^2		HSDB (2015)	Q	99
2-methylbutane-1,2,4-triol $C_5H_{12}O_3$ [62875-07-4] XYHGSPUTABMVOC-UHFFFAOYSA-N	3.9×10^5 1.0×10^6 1.7×10^5		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:C56OH $C_5H_{12}O_3$ RXEJCNRKXVSXDJ-UHFFFAOYSA-N	6.6×10^5 2.0×10^6 8.1×10^4		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:HO124C5 $C_5H_{12}O_3$ MOIOWCZVZKHQIC-UHFFFAOYSA-N	6.6×10^5 1.3×10^6 1.5×10^5		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:HO134C5 $C_5H_{12}O_3$ ANUUQAHHEZMTAS-UHFFFAOYSA-N	6.6×10^5 3.2×10^6 1.4×10^5		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:MBOAOH $C_5H_{12}O_3$ QFZITDCVRJQLMZ-UHFFFAOYSA-N	3.0×10^5 1.1×10^6 5.4×10^3		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
2-pentene-2,4,5-triol $C_5H_{10}O_3$ (ME1TRIOL) MTMASQITBHTGFW-UHFFFAOYSA-N	4.8×10^7	11000	Wieser et al. (2023)	Q	437
2-methyl-3-butene-1,2,3-triol $C_5H_{10}O_3$ YXPJRFSYSVRDQI-UHFFFAOYSA-N	3.9×10^8 1.5×10^2 3.1×10^2		Qin et al. (2021) Qin et al. (2021) Qin et al. (2021)	M Q Q	434 435 436
(E)-2-methyl-1-butene-1,3,4-triol $C_5H_{10}O_3$ FVYHKVMWBMOFGS-DUXPYHPUSA-N	6.2×10^8 1.3×10^2 3.7×10^6		Qin et al. (2021) Qin et al. (2021) Qin et al. (2021)	M Q Q	434 435 436
(Z)-2-methyl-1-butene-1,3,4-triol $C_5H_{10}O_3$ FVYHKVMWBMOFGS-RQOWECAXSA-N	7.8×10^8 1.3×10^2 3.7×10^6		Qin et al. (2021) Qin et al. (2021) Qin et al. (2021)	M Q Q	434 435 436
2-methylthreitol $C_5H_{12}O_4$ HGVJFBSSLICXEM-WHFBIAKZSA-N	2.0×10^8 2.4×10^4 3.3×10^8		Qin et al. (2021) Qin et al. (2021) Qin et al. (2021)	M Q Q	434 435 436

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Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methylerythritol	3.1×10^{8}		Qin et al. (2021)	M	434
$C_5H_{12}O_4$	2.4×10^{4}		Qin et al. (2021)	Q	435
[93921-83-6]	3.3×10^{8}		Qin et al. (2021)	Q	436
HGVJFBSSLICXEM-CRCLSJGQSA-N	6.2×10^{10}		Isaacman-VanWertz et al. (2016)	Q	438, 439
	3.1×10^{8}		Isaacman-VanWertz et al. (2016)	Q	440, 441
	3.1×10^{4}		Isaacman-VanWertz et al. (2016)	Q	442
2-Methylbutane-1,2,3,4-tetrol	6.1×10^{10}	14000	Wieser et al. (2023)	Q	437
$C_5H_{12}O_4$					
(MeBuTETROL)					
[42933-13-1]					
HGVJFBSSLICXEM-UHFFFAOYSA-N					
2,2-bis(hydroxymethyl)1,3-propanediol	7.3×10^{10}		Burkholder et al. (2019)	L	
$C_5H_{12}O_4$	7.3×10^{10}		Burkholder et al. (2015)	L	
(pentaerythritol)	7.3×10^{10}	16000	Compernolle and Müller (2014b)	V	
[115-77-5]	1.5×10^{9}		Yaws (2003)	X	237, 12
WXZMFSXDPGVJKK-UHFFFAOYSA-N	2.4×10^{4}		HSDB (2015)	Q	99
	1.2×10^{8}		Gharagheizi et al. (2012)	Q	
	2.4×10^{9}		Gharagheizi et al. (2010)	Q	246
1,2,3,4,5-pentanepentol	8.9×10^{18}		Saxena and Hildemann (1996)	E	401
$C_5H_{12}O_5$					
[7643-75-6]					
HEBKCHPVOIAQTA-UHFFFAOYSA-N					
(2R,3R,4S)-pentane-1,2,3,4,5-pentol	4.9×10^{8}		Qin et al. (2021)	M	434
$C_5H_{12}O_5$	3.9×10^{11}	17000	Compernolle and Müller (2014b)	V	
(xylitol)	6.6×10^{5}		Qin et al. (2021)	Q	435
[87-99-0]	7.3×10^{11}		Qin et al. (2021)	Q	436
HEBKCHPVOIAQTA-SCDXWVJYSA-N	6.6×10^{5}		HSDB (2015)	Q	99
(2R,3S,4S)-pentane-1,2,3,4,5-pentol	4.6×10^{11}	18000	Compernolle and Müller (2014b)	V	
$C_5H_{12}O_5$					
(adonitol; ribitol)					
[488-81-3]					
HEBKCHPVOIAQTA-ZXFHETKHSA-N					
(2R,4R)-pentane-1,2,3,4,5-pentol	9.9×10^{9}		Qin et al. (2021)	M	434
$C_5H_{12}O_5$	6.7×10^{11}	18000	Compernolle and Müller (2014b)	V	
(arabitol; arabinitol)	6.6×10^{5}		Qin et al. (2021)	Q	435
[2152-56-9]	7.3×10^{11}		Qin et al. (2021)	Q	436
HEBKCHPVOIAQTA-QWWZWVQMSA-N					

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Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
levoglucosan	4.9×10^{10}		Qin et al. (2021)	M	434
$C_6H_{10}O_5$	6.9×10^{7}		Qin et al. (2021)	Q	435
[498-07-7]	4.3×10^{10}		Qin et al. (2021)	Q	436
TWNIBLMWSKIRAT-VFUOTHLCSA-N					
fructose	1.2×10^{9}		Qin et al. (2021)	M	434
$C_6H_{12}O_6$	1.0×10^{9}		Qin et al. (2021)	Q	435
[30237-26-4]	1.6×10^{14}		Qin et al. (2021)	Q	436
BJHIKXHVCXFQLS-UYFOZJQFSA-N					
mannose	1.2×10^{9}		Qin et al. (2021)	M	434
$C_6H_{12}O_6$	1.7×10^{5}		Qin et al. (2021)	Q	435
[3458-28-4]	1.4×10^{13}		Qin et al. (2021)	Q	436
GZCGUPFRVQAUEE-KVTDHHQDSA-N					
glucose	7.8×10^{8}		Qin et al. (2021)	M	434
$C_6H_{12}O_6$	1.0×10^{9}		Qin et al. (2021)	Q	435
[50-99-7]	1.8×10^{15}		Qin et al. (2021)	Q	436
GZCGUPFRVQAUEE-SLPGGIOYSA-N					
1,2-hexanediol	1.7×10^{3}		Compernolle and Müller (2014b)	V	
$C_6H_{14}O_2$	1.9×10^{2}		Wang et al. (2017)	Q	80, 238
[6920-22-5]	4.4×10^{2}		Wang et al. (2017)	Q	80, 239
FHKSXSQHXQEMOK-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	80, 240
1,4-hexanediol	4.5×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	3.3×10^{3}		Wang et al. (2017)	Q	80, 239
[16432-53-4]	1.6×10^{3}		Wang et al. (2017)	Q	80, 240
QVTWBMUAJHVAIJ-UHFFFAOYSA-N					
1,6-hexanediol	4.5×10^{4}		HSDB (2015)	Q	99
$C_6H_{14}O_2$	3.0×10^{4}		Saxena and Hildemann (1996)	E	401
[629-11-8]					
XXMIOPMDWAUFGU-UHFFFAOYSA-N					
2,3-hexanediol	2.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	8.7×10^{2}		Wang et al. (2017)	Q	80, 239
[617-30-1]	1.3×10^{2}		Wang et al. (2017)	Q	80, 240
QCIYAEYRVFUFAP-UHFFFAOYSA-N					
2,5-hexanediol	1.4×10^{4}		Compernolle and Müller (2014b)	V	
$C_6H_{14}O_2$	5.1×10^{2}		Wang et al. (2017)	Q	80, 238
[2935-44-6]	5.9×10^{3}		Wang et al. (2017)	Q	80, 239
OHMBHFSEKCCCBW-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
	2.0×10^{4}		Saxena and Hildemann (1996)	E	401
1,2-cyclohexanediol	6.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
[931-17-9]	1.3×10^{3}		Wang et al. (2017)	Q	80, 240
PFURGBBHAOXLIO-UHFFFAOYSA-N					

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Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-1,3-pentanediol $C_6H_{14}O_2$ [149-31-5] SPXWGAHNKXLXAP-UHFFFAOYSA-N	3.0×10^4		Saxena and Hildemann (1996)	E	401
2-methyl-1,4-pentanediol $C_6H_{14}O_2$ [6287-17-8] PNJNLCNHYSWUPT-UHFFFAOYSA-N	5.1×10^2 4.0×10^3 4.1×10^3		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
2-methyl-2,4-pentanediol $C_6H_{14}O_2$ [107-41-5] SVTBMSDMJJWYQN-UHFFFAOYSA-N	2.5×10^1 2.0×10^4		HSDB (2015) Saxena and Hildemann (1996)	Q E	99 401
3-methyl-1,3-pentanediol $C_6H_{14}O_2$ [33879-72-0] HIYKOZFIVZIBFO-UHFFFAOYSA-N	3.1×10^2 2.3×10^3 8.9×10^2		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
3-methyl-1,4-pentanediol $C_6H_{14}O_2$ [26787-63-3] WOHXXIWTEHLCQK-UHFFFAOYSA-N	5.1×10^2 5.8×10^3 2.6×10^3		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
4-methyl-1,4-pentanediol $C_6H_{14}O_2$ [1462-10-8] HAIVWDGLCRYQMC-UHFFFAOYSA-N	3.1×10^2 2.9×10^3 2.5×10^3		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
2,3-dimethyl-2,3-butanediol $C_6H_{14}O_2$ [76-09-5] IVDFJHOHABJVEH-UHFFFAOYSA-N	1.0×10^2 8.7×10^2 6.9×10^1		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
2,3-dimethyl-1,4-butanediol $C_6H_{14}O_2$ [57716-80-0] SKQUTIPQJKQFRA-UHFFFAOYSA-N	5.1×10^2 8.1×10^3 2.8×10^3		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
2,2-dimethyl-1,4-butanediol $C_6H_{14}O_2$ [32812-23-0] GQSZUUPRBBBHRI-UHFFFAOYSA-N	3.1×10^2 4.5×10^3 2.5×10^3		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
1,2,6-hexanetriol $C_6H_{14}O_3$ [106-69-4] ZWVMLYRJXORSEP-UHFFFAOYSA-N	2.0×10^9		Saxena and Hildemann (1996)	E	401

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Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:H134M3C5	3.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	2.4×10^{6}		Wang et al. (2017)	Q	80, 239
XPUHQLFLUQJINS-UHFFFAOYSA-N	8.3×10^{4}		Wang et al. (2017)	Q	80, 240
1,2,3,4,5,6-hexahydroxy hexane $C_6H_{14}O_6$ [45007-61-2] FBPFZTCFMRRESA-UHFFFAOYSA-N	3.9×10^{23}		Saxena and Hildemann (1996)	E	401
(2S,3R,4R,5R)-hexane-1,2,3,4,5,6-hexol	6.6×10^{14}	22000	Compernolle and Müller (2014b)	V	
$C_6H_{14}O_6$	1.4×10^{7}		HSDB (2015)	Q	99
(sorbitol) [50-70-4] FBPFZTCFMRRESA-JGWLITMVSA-N					
(2R,3R,4R,5R)-hexane-1,2,3,4,5,6-hexol	3.1×10^{9}		Qin et al. (2021)	M	434
$C_6H_{14}O_6$	1.8×10^{15}	22000	Compernolle and Müller (2014b)	V	
(mannitol)	1.4×10^{7}		Qin et al. (2021)	Q	435
[69-65-8]	1.0×10^{15}		Qin et al. (2021)	Q	436
FBPFZTCFMRRESA-KVTDHHQDSA-N	1.4×10^{7}		HSDB (2015)	Q	99
(2R,3S,4R,5S)-hexane-1,2,3,4,5,6-hexol $C_6H_{14}O_6$ (dulcitol; galactitol) [608-66-2] FBPFZTCFMRRESA-GUCUJZIJSA-N	9.0×10^{14}	22000	Compernolle and Müller (2014b)	V	
1,2,4,5-cyclohexanetetrol $C_6H_{12}O_4$ (1,2,4,5-tetrahydroxycyclohexane) [35652-37-0] RDIDGZFQASQXBU-UHFFFAOYSA-N	3.9×10^{14}		Saxena and Hildemann (1996)	E	401
1,2,3,4,5,6-hexahydroxycyclohexane $C_6H_{12}O_6$ [87-89-8] CDAISMWEOUEBRE-UHFFFAOYSA-N	9.9×10^{23}		Saxena and Hildemann (1996)	E	401
1,7-heptanediol			Compernolle and Müller (2014b)	V	443
$C_7H_{16}O_2$	2.0×10^{4}		Saxena and Hildemann (1996)	E	401
[629-30-1] SXCBDZAEHILGLM-UHFFFAOYSA-N					
2,4-heptanediol $C_7H_{16}O_2$ [20748-86-1] XVEOUOTUJBYHNL-UHFFFAOYSA-N	2.0×10^{4}		Saxena and Hildemann (1996)	E	401

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Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
2,5-heptanediol $C_7H_{16}O_2$ [70444-25-6] XTVHTJKQKUOEQA-UHFFFAOYSA-N	4.2×10^2 4.7×10^3 7.3×10^2		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
4-methyl-1,4-hexanediol $C_7H_{16}O_2$ [40646-08-0] ZRCYHJNCCBSTSZ-UHFFFAOYSA-N	2.5×10^2 2.6×10^3 1.2×10^3		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
2-methyl-2,5-hexanediol $C_7H_{16}O_2$ [29044-06-2] KZWQVDXGMOSSNY-UHFFFAOYSA-N	2.9×10^2 4.1×10^3 1.2×10^3		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
3-methyl-2,5-hexanediol $C_7H_{16}O_2$ PMORVUNYTOZCSE-UHFFFAOYSA-N	4.8×10^2 7.6×10^3 2.2×10^3		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
2,2-diethyl-1,3-propanediol $C_7H_{16}O_2$ [115-76-4] XRVCFZPJAHWYTB-UHFFFAOYSA-N	2.0×10^4		Saxena and Hildemann (1996)	E	401
1,2,3,4,5-pentahydroxyheptane $C_7H_{16}O_5$ HUYORHVLGRMTGF-UHFFFAOYSA-N	4.9×10^{18}		Saxena and Hildemann (1996)	E	401
1,2,3,4,6-pentahydroxyheptane $C_7H_{16}O_5$ HBKKLPCMKBGRJH-UHFFFAOYSA-N	3.9×10^{18}		Saxena and Hildemann (1996)	E	401
1,2,3,5,7-pentahydroxyheptane $C_7H_{16}O_5$ NSOOVWLSFZLKQX-UHFFFAOYSA-N	4.9×10^{18}		Saxena and Hildemann (1996)	E	401
1,2,3,4,5,6-hexahydroxyheptane $C_7H_{16}O_6$ (1-deoxy-heptitol) [688007-16-1] YMEXGEAJNZRQEH-VIFPVBQESA-N	3.0×10^{23}		Saxena and Hildemann (1996)	E	401
3,6-octanediol $C_8H_{18}O_2$ [24434-09-1] BCKOQWWRTRBSGR-UHFFFAOYSA-N	3.7×10^2 4.1×10^3 2.1×10^2		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
1,4-cyclohexanedimethanol $C_8H_{16}O_2$ [105-08-8] YIMQCDZDWXUDCA-UHFFFAOYSA-N	1.5×10^5		HSDB (2015)	V	

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Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
2-ethyl-1,3-hexanediol	7.2×10^2		Duchowicz et al. (2020)	V	186
$C_8H_{18}O_2$	5.4×10^2		Duchowicz et al. (2020)	Q	
[94-96-2]	7.8×10^2		Raventos-Duran et al. (2010)	Q	242, 243
RWLALWYNXFYRGW-UHFFFAOYSA-N	7.8×10^2		Raventos-Duran et al. (2010)	Q	244
	1.6×10^1		Raventos-Duran et al. (2010)	Q	245
	1.1×10^2		Hilal et al. (2008)	Q	
	7.5×10^2		Modarresi et al. (2007)	Q	67
	2.0×10^4		Saxena and Hildemann (1996)	E	401
2,2,4-trimethyl-1,3-pentanediol	2.2×10^2		Duchowicz et al. (2020)	V	186
$C_8H_{18}O_2$	9.2×10^1		Duchowicz et al. (2020)	Q	
[144-19-4]	1.4×10^1		HSDB (2015)	Q	99
JCTXKRPTIMZBJT-UHFFFAOYSA-N					
2,5-dimethyl-2,5-hexanediol	1.4×10^1		Zhang et al. (2010)	Q	287, 288
$C_8H_{18}O_2$	1.9×10^3		Zhang et al. (2010)	Q	287, 289
[110-03-2]	7.9×10^2		Zhang et al. (2010)	Q	287, 290
ZWNMRZQYWRLGMM-UHFFFAOYSA-N	4.7×10^1		Zhang et al. (2010)	Q	287, 291
1,9-nonanediol			Compernolle and Müller (2014b)	V	444
$C_9H_{20}O_2$					
[3937-56-2]					
ALVZNPYWJMLXKV-UHFFFAOYSA-N					
3,6-nonanediol	3.0×10^2		Wang et al. (2017)	Q	80, 238
$C_9H_{20}O_2$	3.2×10^3		Wang et al. (2017)	Q	80, 239
[4469-85-6]	1.8×10^2		Wang et al. (2017)	Q	80, 240
YKEWIFGQPMVBEF-UHFFFAOYSA-N					
1,10-decanediol			Compernolle and Müller (2014b)	V	445
$C_{10}H_{22}O_2$					
[112-47-0]					
FOTKYAAJKYLFFN-UHFFFAOYSA-N					
3,6-decanediol	2.4×10^2		Wang et al. (2017)	Q	80, 238
$C_{10}H_{22}O_2$	2.6×10^3		Wang et al. (2017)	Q	80, 239
RBFBEPALGOYNGK-UHFFFAOYSA-N	2.8×10^2		Wang et al. (2017)	Q	80, 240
MCM:APINBOH	5.5×10^2		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_2$	3.2×10^3		Wang et al. (2017)	Q	80, 239
MOILFCKRQFQVFS-UHFFFAOYSA-N	6.5×10^3		Wang et al. (2017)	Q	80, 240
MCM:APINCOH	1.8×10^3		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_2$	2.0×10^5		Wang et al. (2017)	Q	80, 239
OMDMTHRBGUBUCO-UHFFFAOYSA-N	3.0×10^4		Wang et al. (2017)	Q	80, 240
MCM:BPINAOH	5.5×10^2		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_2$	7.4×10^2		Wang et al. (2017)	Q	80, 239
VXXAKGMRLUXFQH-UHFFFAOYSA-N	1.0×10^3		Wang et al. (2017)	Q	80, 240

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Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:BPINCOH	1.6×10^3		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_2$	3.5×10^5		Wang et al. (2017)	Q	80, 239
XYKGEKWHBMLSGS-UHFFFAOYSA-N	5.5×10^4		Wang et al. (2017)	Q	80, 240
MCM:HO36C11	2.2×10^2		Wang et al. (2017)	Q	80, 238
$C_{11}H_{24}O_2$	2.0×10^3		Wang et al. (2017)	Q	80, 239
VCLRIEYYOZNUNU-UHFFFAOYSA-N	2.2×10^2		Wang et al. (2017)	Q	80, 240
MCM:HO36C12	1.7×10^2		Wang et al. (2017)	Q	80, 238
$C_{12}H_{26}O_2$	1.6×10^3		Wang et al. (2017)	Q	80, 239
CLQOYXKLYNGAHW-UHFFFAOYSA-N	1.5×10^2		Wang et al. (2017)	Q	80, 240
2-butene-1,4-diol	$>3.4\times10^2$		Altschuh et al. (1999)	M	
$C_4H_8O_2$	2.5×10^3		Wang et al. (2017)	Q	80, 238
[110-64-5]	1.2×10^5		Wang et al. (2017)	Q	80, 239
ORTVZLZNOYNASJ-UHFFFAOYSA-N	3.4×10^4		Wang et al. (2017)	Q	80, 240
3-butene-1,2-diol	7.8×10^2		Wang et al. (2017)	Q	80, 238
$C_4H_8O_2$	8.5×10^2		Wang et al. (2017)	Q	80, 239
[497-06-3]	3.0×10^2		Wang et al. (2017)	Q	80, 240
ITMIAZBRRZANGB-UHFFFAOYSA-N					
2-butyne-1,4-diol	$>2.0\times10^3$		Altschuh et al. (1999)	M	
$C_4H_6O_2$	5.8×10^5		HSDB (2015)	V	
(1,4-dihydroxy-2-butyne)					
[110-65-6]					
DLDJFQGPPSQZKI-UHFFFAOYSA-N					
MCM:C524OH	1.3×10^6		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	6.5×10^4		Wang et al. (2017)	Q	80, 239
PGARYUHLQUORKU-UHFFFAOYSA-N	6.0×10^4		Wang et al. (2017)	Q	80, 240
MCM:ISOPAOH	1.6×10^3		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	7.4×10^4		Wang et al. (2017)	Q	80, 239
FLXLJBCLEUWWCG-UHFFFAOYSA-N	3.4×10^4		Wang et al. (2017)	Q	80, 240
MCM:ISOPBOH	4.5×10^2		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	5.4×10^2		Wang et al. (2017)	Q	80, 239
XZRGYMKUQMPDQH-UHFFFAOYSA-N	7.1×10^1		Wang et al. (2017)	Q	80, 240
MCM:ISOPDOH	5.3×10^2		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	7.4×10^2		Wang et al. (2017)	Q	80, 239
HBHXLSPUXXXICF-UHFFFAOYSA-N	2.1×10^2		Wang et al. (2017)	Q	80, 240
MCM:C622OH	1.0×10^3		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	4.3×10^3		Wang et al. (2017)	Q	80, 239
VCGCHTQYUUAIGQ-UHFFFAOYSA-N	7.6×10^2		Wang et al. (2017)	Q	80, 240
MCM:C624OH	1.0×10^3		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	3.6×10^3		Wang et al. (2017)	Q	80, 239
BZQZWOYZOVQJLT-UHFFFAOYSA-N	8.7×10^2		Wang et al. (2017)	Q	80, 240

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Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:C720OH	4.5×10^3		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_2$	8.7×10^4		Wang et al. (2017)	Q	80, 239
JRLLENLHZCUEBJ-UHFFFAOYSA-N	7.6×10^4		Wang et al. (2017)	Q	80, 240
MCM:LIMAOH	5.1×10^2		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_2$	5.5×10^3		Wang et al. (2017)	Q	80, 239
WKZWTZTZWGWEGE-UHFFFAOYSA-N	1.9×10^3		Wang et al. (2017)	Q	80, 240
MCM:LIMCOH	6.9×10^2		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_2$	4.3×10^3		Wang et al. (2017)	Q	80, 239
ZJALAEQNHJQSTN-UHFFFAOYSA-N	1.2×10^3		Wang et al. (2017)	Q	80, 240
(*E*,*E*)-8,10-dodecadien-1-ol $C_{12}H_{22}O$ (codlemone) [33956-49-9] CSWBSLXBXRFNST-MQQKCMAXSA-N	1.7		Ebert et al. (2023)	?	316
MCM:BCAOH	5.4×10^2		Wang et al. (2017)	Q	80, 238
$C_{15}H_{26}O_2$	1.2×10^4		Wang et al. (2017)	Q	80, 239
XZTGVWRBZDBQLP-UHFFFAOYSA-N	1.1×10^4		Wang et al. (2017)	Q	80, 240
MCM:BCCOH	6.8×10^2		Wang et al. (2017)	Q	80, 238
$C_{15}H_{26}O_2$	1.8×10^4		Wang et al. (2017)	Q	80, 239
ALNVAIGKARRJOT-UHFFFAOYSA-N	5.9×10^3		Wang et al. (2017)	Q	80, 240
1,2-dihydroxybenzene	8.2×10^3		Duchowicz et al. (2020)	V	186
$C_6H_4(OH)_2$	8.2×10^3		HSDB (2015)	V	
(pyrocatechol)	1.8×10^3		Mackay et al. (2006c)	V	
[120-80-9]	1.6×10^2		Schüürmann (2000)	V	
YCIMNLLNPGFGHC-UHFFFAOYSA-N	4.5×10^1		Mackay et al. (1995)	V	
	2.6×10^3		Duchowicz et al. (2020)	Q	
	1.4×10^4		Wang et al. (2017)	Q	80, 238
	5.4×10^3		Wang et al. (2017)	Q	80, 239
	4.4×10^3		Wang et al. (2017)	Q	80, 240
	7.8×10^3		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^3		Raventos-Duran et al. (2010)	Q	244
	1.6×10^5		Raventos-Duran et al. (2010)	Q	245
	1.2×10^3		Hilal et al. (2008)	Q	
	7.9×10^2		Modarresi et al. (2007)	Q	67
		8300	Kühne et al. (2005)	Q	
		7400	Kühne et al. (2005)	?	
1,3-dihydroxybenzene	1.0×10^5		Duchowicz et al. (2020)	V	186
$C_6H_4(OH)_2$	1.0×10^5		HSDB (2015)	V	
(resorcinol)	8.5×10^4		Mackay et al. (2006c)	V	
[108-46-3]	5.0×10^3		Schüürmann (2000)	V	
GHMLBKRAJCXXBS-UHFFFAOYSA-N	6.4×10^4		Goldstein (1982)	X	446
	8.1×10^4	6300	Goldstein (1982)	X	298
	1.4×10^5		Duchowicz et al. (2020)	Q	
	2.4×10^4		Gharagheizi et al. (2012)	Q	

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Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	5.3×10^4		Hilal et al. (2008)	Q	
1,4-dihydroxybenzene	2.1×10^5		Duchowicz et al. (2020)	V	186
$C_6H_4(OH)_2$	2.6×10^5		HSDB (2015)	V	
(hydroquinone)	2.5×10^5		Mackay et al. (2006c)	V	
[123-31-9]	3.2×10^4		Schüürmann (2000)	V	
QIGBRXMKCJKVMJ-UHFFFAOYSA-N	2.5×10^5		Mackay et al. (1995)	V	
	2.6×10^5		Meylan and Howard (1991)	V	
	7.6×10^3		Yaws (2003)	X	258
	2.3×10^5		Dupeux et al. (2022)	Q	259
	1.3×10^5		Duchowicz et al. (2020)	Q	
	3.1×10^4		Raventos-Duran et al. (2010)	Q	271, 243
	1.2×10^5		Raventos-Duran et al. (2010)	Q	244
	1.6×10^5		Raventos-Duran et al. (2010)	Q	245
	3.7×10^4		Hilal et al. (2008)	Q	
		8300	Kühne et al. (2005)	Q	
	1.7×10^5		Meylan and Howard (1991)	Q	
		7700	Kühne et al. (2005)	?	
1,2,3-benzenetriol	6.3×10^4		HSDB (2015)	V	
$C_6H_6O_3$	5.1×10^6		Gharagheizi et al. (2012)	Q	
(pyrogallic acid)					
[87-66-1]					
WQGWDDDVZFFDIG-UHFFFAOYSA-N					
1,2-dihydroxy-3-methylbenzene	8.1×10^3		Wang et al. (2017)	Q	80, 238
$C_7H_8O_2$	3.7×10^3		Wang et al. (2017)	Q	80, 239
[488-17-5]	7.4×10^2		Wang et al. (2017)	Q	80, 240
PGSWEKYNAOWQDF-UHFFFAOYSA-N					
MCM:ECATECHOL	7.4×10^3		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_2$	2.3×10^3		Wang et al. (2017)	Q	80, 239
UUCQGNWZASKXNN-UHFFFAOYSA-N	3.8×10^2		Wang et al. (2017)	Q	80, 240
MCM:MXYCATECH	4.8×10^3		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_2$	2.9×10^3		Wang et al. (2017)	Q	80, 239
YGLVLWAMIJMBPF-UHFFFAOYSA-N	6.0×10^2		Wang et al. (2017)	Q	80, 240
MCM:OXYCATECH	4.8×10^3		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_2$	3.6×10^3		Wang et al. (2017)	Q	80, 239
RYHGQTREHREIBC-UHFFFAOYSA-N	3.1×10^2		Wang et al. (2017)	Q	80, 240
MCM:PXYCATECH	4.8×10^3		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_2$	3.9×10^3		Wang et al. (2017)	Q	80, 239
RGUZWBOJHNWZOK-UHFFFAOYSA-N	7.8×10^1		Wang et al. (2017)	Q	80, 240
MCM:IPCATECHOL	6.8×10^3		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	1.1×10^3		Wang et al. (2017)	Q	80, 239
XLZHGKDRKSKCAU-UHFFFAOYSA-N	2.9×10^2		Wang et al. (2017)	Q	80, 240

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Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:METCATECH	4.4×10^3		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	1.9×10^3		Wang et al. (2017)	Q	80, 239
IFERDVOUSBGAOD-UHFFFAOYSA-N	3.3×10^2		Wang et al. (2017)	Q	80, 240
MCM:OETCATECH	4.4×10^3		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	2.2×10^3		Wang et al. (2017)	Q	80, 239
QTXIMHKRKLVXRS-UHFFFAOYSA-N	3.4×10^2		Wang et al. (2017)	Q	80, 240
MCM:PCATECHOL	5.9×10^3		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	1.5×10^3		Wang et al. (2017)	Q	80, 239
GOZVFLWHGAXTPA-UHFFFAOYSA-N	3.6×10^2		Wang et al. (2017)	Q	80, 240
MCM:PETCATECH	4.4×10^3		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	2.5×10^3		Wang et al. (2017)	Q	80, 239
WVRWBYUJPWRFQO-UHFFFAOYSA-N	4.3×10^1		Wang et al. (2017)	Q	80, 240
MCM:T123CATECH	2.9×10^3		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	4.6×10^3		Wang et al. (2017)	Q	80, 239
DEIKGXRMQUHZJD-UHFFFAOYSA-N	5.1×10^2		Wang et al. (2017)	Q	80, 240
MCM:T124CATECH	2.9×10^3		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	4.9×10^3		Wang et al. (2017)	Q	80, 239
NZEZVJPYSAXNTR-UHFFFAOYSA-N	4.8×10^1		Wang et al. (2017)	Q	80, 240
2,3-dihydroxynaphthalene $C_{10}H_8O_2$ [92-44-4] JRNGUTKWMSBIBF-UHFFFAOYSA-N	2.0×10^5		Ebert et al. (2023)	?	316
hexylresorcinol $C_{12}H_{18}O_2$ [136-77-6] WFJIVOKAWHGMBH-UHFFFAOYSA-N	3.8×10^4		HSDB (2015)	Q	99
2,6-bis(1,1-dimethylethyl)phenol $C_{14}H_{22}O$ [128-39-2] DKCPKDPYUFEZCP-UHFFFAOYSA-N	3.1		HSDB (2015)	Q	99
4-(1-methyl-1-phenylethyl)phenol $C_{15}H_{16}O$ [599-64-4] QBDSZLJBMIMQRS-UHFFFAOYSA-N	1.1×10^2		HSDB (2015)	Q	447
2,2',3,3'-tetrahydro-3,3,3',3'-tetramethyl-1,1'-spirobi(1H-indene)-6,6'-diol	1.5×10^6		Zhang et al. (2010)	Q	287, 288
$C_{21}H_{24}O_2$	1.0×10^6		Zhang et al. (2010)	Q	287, 289
[1568-80-5]	2.2×10^6		Zhang et al. (2010)	Q	287, 290
SICLLPHPVFCNTJ-UHFFFAOYSA-N	8.2×10^5		Zhang et al. (2010)	Q	287, 291

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Table A3.3: Polyols ($R(OH)_n$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,4'-(3,3,5-trimethylcyclohexane-1,1-diyl)diphenol	4.4×10^{5}		Zhang et al. (2010)	Q	287, 288
$C_{21}H_{26}O_2$	3.2×10^{5}		Zhang et al. (2010)	Q	287, 289
[129188-99-4]	2.7×10^{6}		Zhang et al. (2010)	Q	287, 290
UMPGNGRIGSEMTC-UHFFFAOYSA-N	7.9×10^{5}		Zhang et al. (2010)	Q	287, 291
3,3,3',3'-tetramethyl-1,1'-spirobi(indan)-5,5',6,6'-tetrol	1.4×10^{14}		Zhang et al. (2010)	Q	287, 288
$C_{21}H_{24}O_4$	1.6×10^{10}		Zhang et al. (2010)	Q	287, 289
[77-08-7]	2.0×10^{11}		Zhang et al. (2010)	Q	287, 290
POFMQEVZKZVAPQ-UHFFFAOYSA-N	2.7×10^{10}		Zhang et al. (2010)	Q	287, 291
9,9-bis(4-hydroxyphenyl)fluorene	8.4×10^{8}		Zhang et al. (2010)	Q	287, 288
$C_{25}H_{18}O_2$	6.2×10^{7}		Zhang et al. (2010)	Q	287, 289
[3236-71-3]	2.1×10^{8}		Zhang et al. (2010)	Q	287, 290
YWFPGFJLYRKYJZ-UHFFFAOYSA-N	3.1×10^{9}		Zhang et al. (2010)	Q	287, 291

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A3.4 Peroxides (ROOH) and peroxy radicals (ROO)

Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl hydroperoxide	3.0	5300	Burkholder et al. (2019)	L	
CH_3OOH	3.0	5300	Burkholder et al. (2015)	L	
(methyl peroxide)	3.0	5200	Brockbank (2013)	L	1
[3031-73-0]	2.9	5200	Warneck and Williams (2012)	L	
MEUKEBNAABNAEX-UHFFFAOYSA-N	3.0	5300	Sander et al. (2011)	L	
	3.0	5300	Sander et al. (2006)	L	
	3.1	5300	Staudinger and Roberts (2001)	L	
	2.5	4400	Li et al. (2004)	M	
	>6.9		Magi et al. (1997)	M	448
	1.2×10^{1}		Sauer (1997)	M	449
	3.1	5200	O'Sullivan et al. (1996)	M	
	3.0	5300	Lind and Kok (1994)	M	52
	1.0×10^{1}		Wang et al. (2017)	Q	80, 238
	1.0×10^{1}		Wang et al. (2017)	Q	80, 239
	6.2		Wang et al. (2017)	Q	80, 240
	4.9		Raventos-Duran et al. (2010)	Q	271, 243
	1.2		Raventos-Duran et al. (2010)	Q	244
	1.6		Raventos-Duran et al. (2010)	Q	245
	9.0×10^{-1}		Hilal et al. (2008)	Q	
	1.3×10^{1}		Modarresi et al. (2007)	Q	67
		6200	Kühne et al. (2005)	Q	
		5200	Kühne et al. (2005)	?	
ethyl hydroperoxide	3.3	6000	Burkholder et al. (2019)	L	
C_2H_5OOH	3.3	6000	Burkholder et al. (2015)	L	
(ethyl peroxide)	3.3	6000	Brockbank (2013)	L	1
[3031-74-1]	3.3	6000	Sander et al. (2011)	L	
ILHIHKRJJMKBEE-UHFFFAOYSA-N	1.1×10^{1}		Sauer (1997)	M	449
	3.3	6000	O'Sullivan et al. (1996)	M	
	5.0		Keshavarz et al. (2022)	Q	
	1.0×10^{1}		Duchowicz et al. (2020)	Q	184
	8.1		Wang et al. (2017)	Q	80, 238
	8.0		Wang et al. (2017)	Q	80, 239
	5.5		Wang et al. (2017)	Q	80, 240
	3.9		Raventos-Duran et al. (2010)	Q	271, 243
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	5.8×10^{-1}		Hilal et al. (2008)	Q	
		6600	Kühne et al. (2005)	Q	
	3.4		Duchowicz et al. (2020)	?	185, 21
		6000	Kühne et al. (2005)	?	

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hydroxymethyl hydroperoxide	1.7×10^{4}	9900	Burkholder et al. (2019)	L	
$HOCH_2OOH$	1.7×10^{4}	9900	Burkholder et al. (2015)	L	
(HMHP; HMP)	1.7×10^{4}	9900	Sander et al. (2011)	L	
[15932-89-5]	1.7×10^{4}	9900	Sander et al. (2006)	L	
NEZWFWIACBUQMN-UHFFFAOYSA-N	1.6×10^{4}	10000	Staudinger and Roberts (2001)	L	
	1.6×10^{4}	9700	O'Sullivan et al. (1996)	M	
	1.6×10^{4}	10000	Staffelbach and Kok (1993)	M	
	4.7×10^{3}	1500	Zhou and Lee (1992)	M	
	1.6×10^{4}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{4}		Raventos-Duran et al. (2010)	Q	245
		8600	Kühne et al. (2005)	Q	
		10000	Kühne et al. (2005)	?	
bis-(hydroxymethyl)-peroxide	$>9.9\times10^{4}$		Staffelbach and Kok (1993)	M	
$HOCH_2OOCH_2OH$	4.4×10^{3}	8400	Zhou and Lee (1992)	M	
(BHMP)		9400	Kühne et al. (2005)	Q	
[17088-73-2]		8500	Kühne et al. (2005)	?	
JLJXMZMKMRQOLN-UHFFFAOYSA-N					
tert-butyl hydroperoxide	4.2		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_2$	1.4		Wang et al. (2017)	Q	80, 239
[75-91-2]	3.6		Wang et al. (2017)	Q	80, 240
CIHOLLKRGTVIJN-UHFFFAOYSA-N	6.2×10^{-1}		HSDB (2015)	Q	99
di-*tert*-butylperoxide	8.2×10^{-4}		HSDB (2015)	Q	99
$C_8H_{18}O_2$	1.2×10^{-4}		Hilal et al. (2008)	Q	
[110-05-4]	1.6×10^{-2}		Modarresi et al. (2007)	Q	67
LSXWFXONGKSEMY-UHFFFAOYSA-N					
1-methyl-1- phenylethylhydroperoxide	2.1×10^{2}		Duchowicz et al. (2020)	V	186
$C_9H_{12}O_2$	2.1×10^{2}		HSDB (2015)	V	
[80-15-9]	2.3×10^{1}		Duchowicz et al. (2020)	Q	
YQHLDYVWEZKEOX-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	80, 238
	2.3×10^{1}		Wang et al. (2017)	Q	80, 239
	2.3×10^{1}		Wang et al. (2017)	Q	80, 240
	2.3		Hilal et al. (2008)	Q	
	7.3×10^{1}		Modarresi et al. (2007)	Q	67
dicumyl peroxide	2.2×10^{-1}		HSDB (2015)	Q	99
$C_{18}H_{22}O_2$					
[80-43-3]					
XMNIXWIUMCBBBL-UHFFFAOYSA-N					
methylperoxy radical	1.5×10^{-1}	3700	Leriche et al. (2000)	E	450
CH_3OO			Lelieveld and Crutzen (1991)	E	451
[2143-58-0]	5.9×10^{-2}	5600	Jacob (1986)	E	452
WTFNSXYULBQCQV-UHFFFAOYSA-N					

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hydroxymethylperoxy radical $HOCH_2OO$ [27828-51-9] OLHGCLQZCFQBGO-UHFFFAOYSA-N	7.9×10^{2}	8200	Leriche et al. (2000)	E	450
peroxyacetyl radical $CH_3C(O)O_2$ [36709-10-1] ZBQKPDHUDKSCRS-UHFFFAOYSA-N	$<9.9\times10^{-4}$ $<9.9\times10^{-4}$ $<9.9\times10^{-4}$ $<9.9\times10^{-4}$ $<9.9\times10^{-4}$		Burkholder et al. (2019) Burkholder et al. (2015) Sander et al. (2011) Sander et al. (2006) Villalta et al. (1996)	L L L L M	
MCM:ACO3H $C_3H_4O_3$ AZIQALWHRUQPHV-UHFFFAOYSA-N	2.7×10^{2} 1.4×10^{1} 2.0×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:IC3H7OOH $C_3H_8O_2$ SGJUFIMCHSLMRJ-UHFFFAOYSA-N	7.6 3.9 4.4		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:NC3H7OOH $C_3H_8O_2$ TURGQPDWYFJEDY-UHFFFAOYSA-N	6.8 4.7 3.0		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:PERPROACID $C_3H_6O_3$ CZPZWMPYEINMCF-UHFFFAOYSA-N	9.8×10^{1} 5.3 6.3×10^{-2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:C3DBCO3H $C_4H_6O_3$ TXNBRZBEFMJQMW-UHFFFAOYSA-N	3.2×10^{2} 1.0×10^{1} 5.4×10^{-2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:IC4H9OOH $C_4H_{10}O_2$ FUHWWEDRJKHMKK-UHFFFAOYSA-N	6.0 3.6 2.2		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:MACO3H $C_4H_6O_3$ OELQSSWXRGADDE-UHFFFAOYSA-N	1.8×10^{2} 8.7 1.6×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
IEPOX1CO3H $C_4H_6O_5$ DJPWYFXNRMHUNU-UHFFFAOYSA-N	9.0×10^{2}	14000	Wieser et al. (2023)	Q	437
MCM:NC4H9OOH $C_4H_{10}O_2$ AKUNSTOMHUXJOZ-UHFFFAOYSA-N	5.3 3.4 3.2		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:PERBUACID $C_4H_8O_3$ LBAYFEDWGHXMSM-UHFFFAOYSA-N	7.8×10^{1} 2.8 4.1×10^{-2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PERIBUACID	8.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	3.2		Wang et al. (2017)	Q	80, 239
LVQKOPBJHBWELS-UHFFFAOYSA-N	2.4×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:SC4H9OOH	6.0		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_2$	2.4		Wang et al. (2017)	Q	80, 239
SPQMVUPFYWDFCB-UHFFFAOYSA-N	2.4		Wang et al. (2017)	Q	80, 240
MCM:BUT2CO3H	7.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	2.0		Wang et al. (2017)	Q	80, 239
LWBFPIVRZGBOFS-UHFFFAOYSA-N	1.8×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C3ME3CO3H	7.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	2.3		Wang et al. (2017)	Q	80, 239
GTLLKMCVRPVGBK-UHFFFAOYSA-N	2.8×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:IPEAOOH	5.5		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	2.6		Wang et al. (2017)	Q	80, 239
HIHRAMNMOMKJDG-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	80, 240
MCM:IPEBOOH	5.6		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	2.1		Wang et al. (2017)	Q	80, 239
VIUWCQFVAFABHL-UHFFFAOYSA-N	2.1		Wang et al. (2017)	Q	80, 240
MCM:IPECOOH	3.4		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	9.8×10^{-1}		Wang et al. (2017)	Q	80, 239
XRXANEMIFVRKLN-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	80, 240
MCM:NEOPOOH	3.4		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	2.1		Wang et al. (2017)	Q	80, 239
UEQURRFROJBOLG-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	80, 240
MCM:PEAOOH	4.7		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	2.6		Wang et al. (2017)	Q	80, 239
KCHNMIKAMRQBHD-UHFFFAOYSA-N	2.3		Wang et al. (2017)	Q	80, 240
MCM:PEBOOH	5.5		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	1.8		Wang et al. (2017)	Q	80, 239
XRIRVAYMWUMXBR-UHFFFAOYSA-N	2.4		Wang et al. (2017)	Q	80, 240
MCM:PECOOH	5.5		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	1.7		Wang et al. (2017)	Q	80, 239
RLBQWRSRDVXRTJ-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	80, 240
MCM:PERPENACID	6.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	1.9		Wang et al. (2017)	Q	80, 239
UQGPCEVQKLOLLM-UHFFFAOYSA-N	2.8×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:TBUTCO3H	5.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	1.8		Wang et al. (2017)	Q	80, 239
YVAACGXAZGGQSM-UHFFFAOYSA-N	1.6×10^{-2}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
C520OOH $C_5H_{10}O_7$ GRPDYNZWDDUILX-UHFFFAOYSA-N	5.3×10^{11}	22000	Wieser et al. (2023)	Q	437
C518OOH $C_5H_8O_4$ PQEISBQMLHJHJQ-UHFFFAOYSA-N	4.1×10^{4}	14000	Wieser et al. (2023)	Q	437
MCM:C54CO3H $C_6H_{12}O_3$ JTSRVXQXWWOTER-UHFFFAOYSA-N	5.6×10^{1} 1.4 1.4×10^{-2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:C5H11CO3H $C_6H_{12}O_3$ NQUPKCJGWCPODR-UHFFFAOYSA-N	5.6×10^{1} 1.4 2.5×10^{-2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
ROO6R7OOH $C_6H_{12}O_4$ UPAWKBDHGPWUCG-UHFFFAOYSA-N	3.3×10^{7}	14000	Wieser et al. (2023)	Q	437
ROO6R6OOH $C_6H_{12}O_5$ QZPUZDFJKAEVLL-UHFFFAOYSA-N	2.6×10^{8}	14000	Wieser et al. (2023)	Q	437
C624OOH $C_6H_{12}O_6$ FUTSLQULSAKEJA-UHFFFAOYSA-N	1.2×10^{13}	20000	Wieser et al. (2023)	Q	437
MCM:CHEXOOH $C_6H_{12}O_2$ FGGJBCRKSVGDPO-UHFFFAOYSA-N	1.2×10^{1} 1.4×10^{1} 3.0×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:HEXAOOH $C_6H_{14}O_2$ RZICEOJUAFHYFO-UHFFFAOYSA-N	3.8 2.1 2.2		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:HEXBOOH $C_6H_{14}O_2$ XWXUHAUZCICPHE-UHFFFAOYSA-N	9.9×10^{-1} 4.4 1.4 1.8	7300	Wieser et al. (2023) Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q Q	437 80, 238 80, 239 80, 240
MCM:HEXCOOH $C_6H_{14}O_2$ NMNOLZYZNVYLRJ-UHFFFAOYSA-N	4.4 1.4 1.1		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:M22C3CO3H $C_6H_{12}O_3$ RQLGMECUXRQENU-UHFFFAOYSA-N	4.0×10^{1} 1.5 2.1×10^{-2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:M22C43OOH $C_6H_{14}O_2$ XDWQBMWWYOVNSC-UHFFFAOYSA-N	3.2 1.4 1.4		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:M22C4OOH	3.0		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	2.0		Wang et al. (2017)	Q	80, 239
VWOCCXGIWJLCIT-UHFFFAOYSA-N	3.6		Wang et al. (2017)	Q	80, 240
MCM:M23C43OOH	3.2		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	1.1		Wang et al. (2017)	Q	80, 239
UPTQBPSUWRBZRD-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	80, 240
MCM:M23C4OOH	5.1		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	2.6		Wang et al. (2017)	Q	80, 239
MCTQHWIBGOKRHO-UHFFFAOYSA-N	1.6		Wang et al. (2017)	Q	80, 240
MCM:M2C43CO3H	6.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.8		Wang et al. (2017)	Q	80, 239
KGAQRBNLHLEGET-UHFFFAOYSA-N	1.9×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:M2PEAOOH	4.4		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	2.1		Wang et al. (2017)	Q	80, 239
OTKKOLXSCMINFN-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	80, 240
MCM:M2PEBOOH	5.1		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	1.4		Wang et al. (2017)	Q	80, 239
XHHITPKXZQXJIC-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	80, 240
MCM:M2PECOOH	5.1		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	1.5		Wang et al. (2017)	Q	80, 239
JBJSMFBSVBRLAK-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	80, 240
MCM:M2PEDOOH	3.0		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	8.0×10^{-1}		Wang et al. (2017)	Q	80, 239
BZGMEGUFFDTCNP-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	80, 240
MCM:M33C3CO3H	4.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.2		Wang et al. (2017)	Q	80, 239
IHLWWYDUPGXTHJ-UHFFFAOYSA-N	8.9×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:M33C4OOH	3.0		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	1.7		Wang et al. (2017)	Q	80, 239
OUMLJDCULPJYHU-UHFFFAOYSA-N	1.8		Wang et al. (2017)	Q	80, 240
MCM:M3C4CO3H	5.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.7		Wang et al. (2017)	Q	80, 239
CHSVHHKRTQKZCN-UHFFFAOYSA-N	2.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:M3PEAOOH	4.4		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	2.5		Wang et al. (2017)	Q	80, 239
AOZFMIRWQXSLHO-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	80, 240
MCM:M3PEBOOH	5.1		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	1.9		Wang et al. (2017)	Q	80, 239
XCSSHHOKPSJZJS-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:M3PECOOH	3.0		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	7.8×10^{-1}		Wang et al. (2017)	Q	80, 239
BWMWVYKKWYNWMF-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
ROO6R5OOH	4.6×10^{7}	16000	Wieser et al. (2023)	Q	437
$C_7H_{12}O_6$					
RAASFOSVQCCDRJ-UHFFFAOYSA-N					
MCM:C6H13CO3H	4.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_3$	1.1		Wang et al. (2017)	Q	80, 239
GLAYRDYYNSCSPO-UHFFFAOYSA-N	2.2×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:HEPTOOH	3.6		Wang et al. (2017)	Q	80, 238
$C_7H_{16}O_2$	1.1		Wang et al. (2017)	Q	80, 239
RCPMMXGHMBPBLI-UHFFFAOYSA-N	9.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:M2HEXAOOH	4.1		Wang et al. (2017)	Q	80, 238
$C_7H_{16}O_2$	1.2		Wang et al. (2017)	Q	80, 239
MZRXBNCEXTUOSL-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	80, 240
MCM:M2HEXBOOH	2.5		Wang et al. (2017)	Q	80, 238
$C_7H_{16}O_2$	6.6×10^{-1}		Wang et al. (2017)	Q	80, 239
VERXWMXNIBWXFV-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:M3HEXAOOH	4.1		Wang et al. (2017)	Q	80, 238
$C_7H_{16}O_2$	1.4		Wang et al. (2017)	Q	80, 239
SLXXGGKZGKGOKQ-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	80, 240
MCM:M3HEXBOOH	2.5		Wang et al. (2017)	Q	80, 238
$C_7H_{16}O_2$	6.8×10^{-1}		Wang et al. (2017)	Q	80, 239
YDBMAIVJCSJSKQ-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
1-methylhexyl hydroperoxide	7.7×10^{-1}	7600	Wieser et al. (2023)	Q	437
$C_7H_{16}O_2$					
(C7H15O2H)					
[762-46-9]					
FWELUXZVATZEMI-UHFFFAOYSA-N					
C7OHOOH	4.1×10^{3}	12000	Wieser et al. (2023)	Q	437
$C_7H_{16}O_3$					
KHWIBANUCNWWGW-UHFFFAOYSA-N					
MCM:C8BCOOH	2.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_2$	7.4		Wang et al. (2017)	Q	80, 239
TWXDGALDAWYAQL-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:OCTOOH	2.8		Wang et al. (2017)	Q	80, 238
$C_8H_{18}O_2$	9.8×10^{-1}		Wang et al. (2017)	Q	80, 239
PXUMFRDGKQLDGL-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-methylheptl hydroperoxide $C_8H_{18}O_2$ (C8H17O2H) NAXZMRYIZGEALQ-UHFFFAOYSA-N	5.8×10^{-1}	8000	Wieser et al. (2023)	Q	437
C8OHOOH $C_8H_{18}O_3$ QQTSMKQYSKGCOU-UHFFFAOYSA-N	3.2×10^{3}	12000	Wieser et al. (2023)	Q	437
MCM:NONOOH $C_9H_{20}O_2$ BXPIMWLPPYUCSQ-UHFFFAOYSA-N	2.6 8.3×10^{-1} 9.6×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:DECOOH $C_{10}H_{22}O_2$ MPMVWDJTKHXCAN-UHFFFAOYSA-N	2.0 7.3×10^{-1} 1.2		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
C5H11O2H $C_{10}H_{22}O_4$ AXIHYONNAPPFSO-UHFFFAOYSA-N	1.4	7000	Wieser et al. (2023)	Q	437
LIMAB15OOH2 $C_{10}H_{20}O_6$ IRUZCTPAAZATQM-UHFFFAOYSA-N	2.3×10^{12}	20000	Wieser et al. (2023)	Q	437
RO5R1O2H $C_{10}H_{18}O_4$ NSOHXIGSWKLSHV-UHFFFAOYSA-N	9.9×10^{5}	17000	Wieser et al. (2023)	Q	437
RO5R2O2H $C_{10}H_{18}O_5$ MFXJOKCSTDMZRM-UHFFFAOYSA-N	1.8×10^{7}	19000	Wieser et al. (2023)	Q	437
ROO6R1OOH $C_{10}H_{18}O_5$ GBBPAXKBVMQHIG-UHFFFAOYSA-N	6.8×10^{4}	16000	Wieser et al. (2023)	Q	437
RO5R3O2H $C_{10}H_{18}O_6$ IEPFJXDIWPQIRC-UHFFFAOYSA-N	7.7×10^{7}	22000	Wieser et al. (2023)	Q	437
MCM:UDECOOH $C_{11}H_{24}O_2$ PPEGYVQDERYKNI-UHFFFAOYSA-N	1.6 6.5×10^{-1} 9.6×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:DDECOOH $C_{12}H_{26}O_2$ ONWAGJMEBPWHEG-UHFFFAOYSA-N	1.5 5.8×10^{-1} 8.3×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:C6H5OOH $C_6H_6O_2$ JYINMLPNDRBKKZ-UHFFFAOYSA-N	3.2×10^{2} 8.9×10^{1} 3.0×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C6H5CH2OOH	2.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_2$	9.1×10^{1}		Wang et al. (2017)	Q	80, 239
YVJRCWCFDJYONJ-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C6H5CO3H	3.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_6O_3$	6.2×10^{1}		Wang et al. (2017)	Q	80, 239
XCRBXWCUXJNEFX-UHFFFAOYSA-N	2.4		Wang et al. (2017)	Q	80, 240
MCM:MXYL1OOH	1.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_2$	7.8×10^{1}		Wang et al. (2017)	Q	80, 239
VCTGBWYTEXZDNM-UHFFFAOYSA-N	3.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:OXYL1OOH	1.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_2$	1.0×10^{2}		Wang et al. (2017)	Q	80, 239
OCSKWYCRTWOMLG-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PXYL1OOH	1.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_2$	9.1×10^{1}		Wang et al. (2017)	Q	80, 239
ZCUUEQJCOSBJOR-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C6H5C2CO3H	3.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_8O_3$	6.3×10^{1}		Wang et al. (2017)	Q	80, 239
BXGXGTXWGGOFSP-UHFFFAOYSA-N	2.7		Wang et al. (2017)	Q	80, 240
MCM:C6H5C2OOH	2.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_2$	6.9×10^{1}		Wang et al. (2017)	Q	80, 239
VZQOBPXGQJXYGY-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DM123OOH	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_2$	1.3×10^{2}		Wang et al. (2017)	Q	80, 239
FPXURWFXMHYDGM-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DM124OOH	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_2$	1.0×10^{2}		Wang et al. (2017)	Q	80, 239
UQJVEYMRRMOLPI-UHFFFAOYSA-N	3.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DMPHOOH	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_2$	6.5×10^{1}		Wang et al. (2017)	Q	80, 239
AGQLZSPEKWKXRP-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:EBENZOOH	1.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_2$	6.3×10^{1}		Wang et al. (2017)	Q	80, 239
SULLUHFYVRLICT-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MXY1OOH	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_2$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
LDNGPDBEDBLXJS-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MXYLCO3H	2.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_8O_3$	5.0×10^{1}		Wang et al. (2017)	Q	80, 239
INFFZTZRGNVBOC-UHFFFAOYSA-N	2.7×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MXYLOOH	1.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_2$	8.3×10^{1}		Wang et al. (2017)	Q	80, 239
UTKFWOZXPFIBPQ-UHFFFAOYSA-N	7.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:OXYLCO3H	2.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_8O_3$	6.2×10^{1}		Wang et al. (2017)	Q	80, 239
DNEXRQSSNZPAJJ-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:OXYLOOH	1.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_2$	9.3×10^{1}		Wang et al. (2017)	Q	80, 239
JTJQZHCBMBJJMV-UHFFFAOYSA-N	6.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PXY1OOH	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_2$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
QBGYVNGBYXOUAG-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PXYLCO3H	2.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_8O_3$	5.6×10^{1}		Wang et al. (2017)	Q	80, 239
IFDPVSBDNAQBRQ-UHFFFAOYSA-N	7.1×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:PXYLOOH	1.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_2$	9.8×10^{1}		Wang et al. (2017)	Q	80, 239
VCEHMDXCOGIOJJ-UHFFFAOYSA-N	8.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:EMPHOOH	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	4.0×10^{1}		Wang et al. (2017)	Q	80, 239
MKWUSWBHCPKVBI-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ETOLOOH	1.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	5.0×10^{1}		Wang et al. (2017)	Q	80, 239
DWPOLKIWKCGPAM-UHFFFAOYSA-N	4.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:IPBENZOOH	1.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	5.0×10^{1}		Wang et al. (2017)	Q	80, 239
CZNJIWCDRJWKLG-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MET1OOH	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	6.5×10^{1}		Wang et al. (2017)	Q	80, 239
HUAUUZDXRNWOSS-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:OET1OOH	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	7.4×10^{1}		Wang et al. (2017)	Q	80, 239
KVZSMDLRNLVTLK-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PBENZOOH	1.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	4.9×10^{1}		Wang et al. (2017)	Q	80, 239
BFUPNGCSYHWOOH-UHFFFAOYSA-N	1.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PET1OOH	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	6.6×10^{1}		Wang et al. (2017)	Q	80, 239
IKLGQZOVXYBNEV-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PHC3OOH	2.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	3.6×10^{1}		Wang et al. (2017)	Q	80, 239
JYLUDNGUBXOJPX-UHFFFAOYSA-N	5.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:TM123BCO3H	1.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_3$	7.3×10^{1}		Wang et al. (2017)	Q	80, 239
NQSDUJYDMWXHMR-UHFFFAOYSA-N	3.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:TM123BOOH	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	1.2×10^{2}		Wang et al. (2017)	Q	80, 239
HSKYDUVZGAHSEO-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:TM123OOH	6.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	1.6×10^{2}		Wang et al. (2017)	Q	80, 239
QIIZMGNSXSJCNA-UHFFFAOYSA-N	5.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:TM124BCO3H	1.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_3$	6.0×10^{1}		Wang et al. (2017)	Q	80, 239
HPLBJCPAWPQKDU-UHFFFAOYSA-N	4.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:TM124BOOH	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
ZUEBLWOBXMLPMV-UHFFFAOYSA-N	7.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:TM124OOH	6.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	1.3×10^{2}		Wang et al. (2017)	Q	80, 239
DSGKIBNJTLHQCN-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:TMBCO3H	1.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_3$	3.9×10^{1}		Wang et al. (2017)	Q	80, 239
APDYULOMODUXLL-UHFFFAOYSA-N	2.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:TMBOOH	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	6.9×10^{1}		Wang et al. (2017)	Q	80, 239
GOKTXPLVCSLYGI-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DM35EBOOH	9.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{14}O_2$	3.6×10^{1}		Wang et al. (2017)	Q	80, 239
NSJZLSFVHPJVDL-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:EMPHCO3H	1.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{12}O_3$	2.3×10^{1}		Wang et al. (2017)	Q	80, 239
GYXFVTDASBFNQD-UHFFFAOYSA-N	2.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:DE35TOOH	7.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{16}O_2$	2.4×10^{1}		Wang et al. (2017)	Q	80, 239
HPTJZRKCFIXEOP-UHFFFAOYSA-N	3.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HOCH2CO3H	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_2H_4O_4$	1.9×10^{2}		Wang et al. (2017)	Q	80, 239
IUEZWLCUORJBDZ-UHFFFAOYSA-N	8.5×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HYETHO2H	2.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_2H_6O_3$	2.9×10^{3}		Wang et al. (2017)	Q	80, 239
FKPAKAOEHCFKLE-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C2OHOCOOH	1.8×10^{7}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_5$	2.2×10^{5}		Wang et al. (2017)	Q	80, 239
GTTVGDRVLZEEEW-UHFFFAOYSA-N	3.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C3DIOLOOH	2.8×10^{7}		Wang et al. (2017)	Q	80, 238
$C_3H_8O_4$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
XSLBWJPPWWFTQY-UHFFFAOYSA-N	3.5×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:HO1C3OOH	2.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_3H_8O_3$	2.1×10^{3}		Wang et al. (2017)	Q	80, 239
LTKFKDLZMYUGKU-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HOC2H4CO3H	2.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_4$	8.9×10^{4}		Wang et al. (2017)	Q	80, 239
HPIZQAHZLDXVRM-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HYPROPO2H	2.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_3H_8O_3$	3.0×10^{3}		Wang et al. (2017)	Q	80, 239
CGHALRGHFXEMJB-UHFFFAOYSA-N	4.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:IPROPOLO2H	2.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_3H_8O_3$	2.1×10^{3}		Wang et al. (2017)	Q	80, 239
LGTUXDWECPSIQO-UHFFFAOYSA-N	4.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:IPROPOLPER	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_4$	1.5×10^{2}		Wang et al. (2017)	Q	80, 239
LLWVBKQQPPRNEX-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:BUT2OLOOH	2.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	1.5×10^{3}		Wang et al. (2017)	Q	80, 239
VRQPOZSYDWHVQK-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:BUTDAOOH	6.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	2.5×10^{5}		Wang et al. (2017)	Q	80, 239
ATNKTSDVMCPWQK-UHFFFAOYSA-N	1.6×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:BUTDBOOH	5.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	2.3×10^{3}		Wang et al. (2017)	Q	80, 239
VQGAWAMXUXLZCZ-UHFFFAOYSA-N	2.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:BUTDCOOH	5.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	1.9×10^{3}		Wang et al. (2017)	Q	80, 239
TVUDLONEIXNOQY-UHFFFAOYSA-N	3.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HC3CCO3H	3.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_4$	2.2×10^{2}		Wang et al. (2017)	Q	80, 239
ZSVMRAYUVFDTKB-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HC3CO3H	9.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_4$	1.9×10^{5}		Wang et al. (2017)	Q	80, 239
AVWVUWGQXKTDKD-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HMACO3H	4.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_4$	2.0×10^{4}		Wang et al. (2017)	Q	80, 239
IZGOVIKWSGSSGB-UHFFFAOYSA-N	9.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HO13C3CO3H	3.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_5$	9.8×10^{5}		Wang et al. (2017)	Q	80, 239
SAVJJQFYFPVKTL-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HO13C4OOH	5.9×10^{7}		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_4$	7.3×10^{6}		Wang et al. (2017)	Q	80, 239
WTIWPVYZJGYFOG-UHFFFAOYSA-N	1.2×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:HO1C4OOH	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	6.9×10^{4}		Wang et al. (2017)	Q	80, 239
RCPPCOTVBKCJGX-UHFFFAOYSA-N	3.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO2C3CO3H	2.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	1.0×10^{5}		Wang et al. (2017)	Q	80, 239
WSXMRWGMMYXEOT-UHFFFAOYSA-N	4.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HO2C4OOH	1.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	9.1×10^{2}		Wang et al. (2017)	Q	80, 239
VJLLYXNZUMWUFH-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HO3C3CO3H	1.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	8.9×10^{1}		Wang et al. (2017)	Q	80, 239
BPXTXQLLUZFFNC-UHFFFAOYSA-N	1.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HO3C4OOH	2.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
RMYCTZOJULYKEL-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HOC3H6CO3H	2.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	8.9×10^{4}		Wang et al. (2017)	Q	80, 239
CAGKPIQTEWLESW-UHFFFAOYSA-N	3.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HOIPRCO3H	2.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	9.8×10^{4}		Wang et al. (2017)	Q	80, 239
XMJMNOOOSJCSST-UHFFFAOYSA-N	6.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:IBUTOLBO2H	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	1.3×10^{3}		Wang et al. (2017)	Q	80, 239
NCECNUIKMRTTTQ-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:IBUTOLCO2H	1.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	1.5×10^{3}		Wang et al. (2017)	Q	80, 239
IYIYQILWOLBTBM-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:IPRHOCO3H	8.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	3.2×10^{1}		Wang et al. (2017)	Q	80, 239
VAHIZEUROSIQMC-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	80, 240
MCM:NBUTOLAOOH	2.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	2.1×10^{3}		Wang et al. (2017)	Q	80, 239
KPUCJKMFRKKADT-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NBUTOLBOOH	1.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
UKXKMFPUVLQYHV-UHFFFAOYSA-N	2.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:TBUTOLOOH	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	8.0×10^{2}		Wang et al. (2017)	Q	80, 239
OLMJQPVPWWPTBW-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C3M3OHCO3H	1.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	7.6×10^{1}		Wang et al. (2017)	Q	80, 239
OPXDDGDNASPZKO-UHFFFAOYSA-N	8.1		Wang et al. (2017)	Q	80, 240
MCM:C42CO3H	3.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_5$	1.2×10^{6}		Wang et al. (2017)	Q	80, 239
ZMIMRJOKAFWNST-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C46CO3H	4.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	1.4×10^{5}		Wang et al. (2017)	Q	80, 239
VWNMYJVYTYSNQP-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C4OH2CO3H	9.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_5$	2.0×10^{5}		Wang et al. (2017)	Q	80, 239
WQUIEUVQOLAPHC-UHFFFAOYSA-N	9.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C4OHCO3H	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	5.5×10^{1}		Wang et al. (2017)	Q	80, 239
OQVSVCDIVLTQNI-UHFFFAOYSA-N	6.8		Wang et al. (2017)	Q	80, 240
MCM:C51OH2OOH	1.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	1.7×10^{3}		Wang et al. (2017)	Q	80, 239
YEVLRKKUVOPQLT-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C524OOH	1.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	1.2×10^{7}		Wang et al. (2017)	Q	80, 239
CMYVSBWTXHBCDK-UHFFFAOYSA-N	8.5×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C52OH1OOH	1.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	1.0×10^{3}		Wang et al. (2017)	Q	80, 239
UCQFCLCUMHUGLJ-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C52OH3OOH	1.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	1.7×10^{3}		Wang et al. (2017)	Q	80, 239
HJJMDLGJAJYCSL-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C52OOH	1.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	5.1×10^{4}		Wang et al. (2017)	Q	80, 239
ZPHQYWRKWRKGNS-UHFFFAOYSA-N	3.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C53OH2OOH	1.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	1.0×10^{3}		Wang et al. (2017)	Q	80, 239
AJVYEIIRONFKES-UHFFFAOYSA-N	8.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C54OOH	3.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_4$	5.9×10^{6}		Wang et al. (2017)	Q	80, 239
YUSGXJKDHCBGQE-UHFFFAOYSA-N	6.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C56OOH	5.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_4$	7.6×10^{6}		Wang et al. (2017)	Q	80, 239
ZJCLGCDNIIJGCW-UHFFFAOYSA-N	7.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:H13C43CO3H	1.9×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_5$	4.1×10^{5}		Wang et al. (2017)	Q	80, 239
AHAADFOLDXPWKJ-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:H2M2C3CO3H	1.4×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	5.9×10^{4}		Wang et al. (2017)	Q	80, 239
WNBRWGLXVYJADJ-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:H2M3C4OOH	1.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	8.5×10^{2}		Wang et al. (2017)	Q	80, 239
ZUPZYIDTDVLJQO-UHFFFAOYSA-N	6.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HC4ACO3H	6.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	2.0×10^{5}		Wang et al. (2017)	Q	80, 239
RKJIARBOZVRICG-UHFFFAOYSA-N	8.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HC4CCO3H	6.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	1.9×10^{5}		Wang et al. (2017)	Q	80, 239
BKBSBVFBLVOVGK-UHFFFAOYSA-N	7.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HM22C3OOH	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	9.8×10^{2}		Wang et al. (2017)	Q	80, 239
YTVLHPDOOITGNI-UHFFFAOYSA-N	2.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HM22CO3H	1.4×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	5.4×10^{4}		Wang et al. (2017)	Q	80, 239
JLDURWTXWMLEQQ-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HM2C43OOH	1.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	1.6×10^{3}		Wang et al. (2017)	Q	80, 239
HSLVQIVCJSWUOZ-UHFFFAOYSA-N	8.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HM33C3OOH	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	7.3×10^{2}		Wang et al. (2017)	Q	80, 239
WHBWUNCJQHRHKD-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HO13C5OOH	5.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_4$	7.6×10^{6}		Wang et al. (2017)	Q	80, 239
MPQCFHWMMIVYQV-UHFFFAOYSA-N	1.3×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:HO1C5OOH	1.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	4.8×10^{4}		Wang et al. (2017)	Q	80, 239
NOIFGIIKGVCIDM-UHFFFAOYSA-N	2.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO24C4CO3H	3.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_5$	7.6×10^{5}		Wang et al. (2017)	Q	80, 239
BPXJXZFDALRNCD-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HO24C5OOH	5.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_4$	3.4×10^{6}		Wang et al. (2017)	Q	80, 239
LXCUFKDAZLTFBK-UHFFFAOYSA-N	7.6×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:HO2C43CO3H	2.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	7.3×10^{4}		Wang et al. (2017)	Q	80, 239
JJSNUFSNLCXQDD-UHFFFAOYSA-N	3.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HO2C4CO3H	2.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	6.3×10^{4}		Wang et al. (2017)	Q	80, 239
WEYKGJBTAJHRDZ-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO2C54OOH	1.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	5.4×10^{2}		Wang et al. (2017)	Q	80, 239
NQEGDBNDYHCERX-UHFFFAOYSA-N	6.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO2C5OOH	7.1×10^{3}	11000	Wieser et al. (2023)	Q	437
$C_5H_{12}O_3$	1.5×10^{4}		Wang et al. (2017)	Q	80, 238
GSRFGQMXWRCOMF-UHFFFAOYSA-N	5.4×10^{4}		Wang et al. (2017)	Q	80, 239
	1.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO2M2C4OOH	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	5.4×10^{2}		Wang et al. (2017)	Q	80, 239
BPHNXEOBBWBBGO-UHFFFAOYSA-N	4.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO3C4CO3H	2.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	5.6×10^{4}		Wang et al. (2017)	Q	80, 239
OFXAQZFPCOWEPU-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HO3C5OOH	1.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	6.9×10^{2}		Wang et al. (2017)	Q	80, 239
AMTQAQGRUCFWLQ-UHFFFAOYSA-N	5.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HOBUT2CO3H	2.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	5.8×10^{4}		Wang et al. (2017)	Q	80, 239
HHXRGEGWJUDFIW-UHFFFAOYSA-N	1.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HOIBUTCO3H	2.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	5.6×10^{4}		Wang et al. (2017)	Q	80, 239
JVGUWDNKCJEDLO-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:ISOPAOOH	4.4×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	1.7×10^5		Wang et al. (2017)	Q	80, 239
PEJOQVDRQFVMLE-UHFFFAOYSA-N	8.5×10^4		Wang et al. (2017)	Q	80, 240
MCM:ISOPBOOH	1.2×10^3	9900	Rivera-Rios (2018)	M	
$C_5H_{10}O_3$	9.9×10^2		Rivera-Rios (2018)	Q	453
QTGGFXPTAQEODO-UHFFFAOYSA-N	1.3×10^4		Rivera-Rios (2018)	Q	454
	3.3×10^4		Wang et al. (2017)	Q	80, 238
	1.4×10^3		Wang et al. (2017)	Q	80, 239
	4.2×10^2		Wang et al. (2017)	Q	80, 240
MCM:ISOPCOOH	4.4×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	2.0×10^5		Wang et al. (2017)	Q	80, 239
FCLDANRCFPUKED-UHFFFAOYSA-N	1.0×10^5		Wang et al. (2017)	Q	80, 240
MCM:ISOPDOOH	1.2×10^2	7500	Rivera-Rios (2018)	M	
$C_5H_{10}O_3$	2.6×10^4		Rivera-Rios (2018)	Q	453
HYHMYONEYJINON-UHFFFAOYSA-N	1.3×10^4		Rivera-Rios (2018)	Q	454
	4.0×10^4		Wang et al. (2017)	Q	80, 238
	1.8×10^3		Wang et al. (2017)	Q	80, 239
	8.1×10^2		Wang et al. (2017)	Q	80, 240
MCM:M2BU2OLOOH	1.4×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	1.1×10^3		Wang et al. (2017)	Q	80, 239
YWZMEYHQKKHRJF-UHFFFAOYSA-N	2.1×10^3		Wang et al. (2017)	Q	80, 240
MCM:M2BUOL2OOH	1.2×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	1.1×10^3		Wang et al. (2017)	Q	80, 239
KLOVYRXVQOACLZ-UHFFFAOYSA-N	6.6×10^2		Wang et al. (2017)	Q	80, 240
MCM:M3BU2OLOOH	1.9×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	1.1×10^3		Wang et al. (2017)	Q	80, 239
AFEDOYRLNKBWPZ-UHFFFAOYSA-N	8.7×10^2		Wang et al. (2017)	Q	80, 240
MCM:MBOAOOH	4.1×10^7		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_4$	4.5×10^6		Wang et al. (2017)	Q	80, 239
VJEOLZUQMDEVMO-UHFFFAOYSA-N	6.8×10^3		Wang et al. (2017)	Q	80, 240
MCM:MBOBOOH	1.4×10^7		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_4$	6.3×10^5		Wang et al. (2017)	Q	80, 239
GXJWPCHTRDIVHR-UHFFFAOYSA-N	5.1×10^3		Wang et al. (2017)	Q	80, 240
MCM:ME2BUOLOOH	1.4×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	6.9×10^2		Wang et al. (2017)	Q	80, 239
SAXHQAUHEBEDAO-UHFFFAOYSA-N	9.3×10^2		Wang et al. (2017)	Q	80, 240
MCM:ME3BUOLOOH	1.9×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	2.3×10^3		Wang et al. (2017)	Q	80, 239
MUYQYONVNPPJGI-UHFFFAOYSA-N	9.8×10^2		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PROL11MOOH	1.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	5.6×10^{2}		Wang et al. (2017)	Q	80, 239
UVDGWSPEOVCOFS-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:PROL1MCO3H	6.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	2.1×10^{1}		Wang et al. (2017)	Q	80, 239
KTQROZYFUGXCGA-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	80, 240
MCM:BZBIPER2OH	3.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	1.9×10^{6}		Wang et al. (2017)	Q	80, 239
BVNIDXNYDXJAFS-UHFFFAOYSA-N	8.5×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:BZBIPEROOH	7.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	9.3×10^{6}		Wang et al. (2017)	Q	80, 239
MXPMOVDECINDPN-UHFFFAOYSA-N	2.3×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C4ME2OHOOH	7.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	3.8×10^{2}		Wang et al. (2017)	Q	80, 239
HOGFDWYRBLIMGM-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C518CO3H	4.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	5.6×10^{4}		Wang et al. (2017)	Q	80, 239
HLKDNTMYLJJNIF-UHFFFAOYSA-N	5.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C622OOH	1.3×10^{4}	12000	Wieser et al. (2023)	Q	437
$C_6H_{12}O_3$	2.9×10^{4}		Wang et al. (2017)	Q	80, 238
GWTGWFHICNOSTQ-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	80, 239
	1.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C624OOH	2.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.3×10^{3}		Wang et al. (2017)	Q	80, 239
DDEGWHJCSBWJSM-UHFFFAOYSA-N	8.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C64OH5OOH	1.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	7.8×10^{2}		Wang et al. (2017)	Q	80, 239
ZEOCDIHFKNFYIT-UHFFFAOYSA-N	6.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C65OH4OOH	1.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
PVVIDEIOKNUTFV-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C6OH5OOH	1.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	1.3×10^{3}		Wang et al. (2017)	Q	80, 239
HRDCBAWVKIWIOZ-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:CYHXOLAOOH	5.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	8.5×10^{4}		Wang et al. (2017)	Q	80, 239
UBIBQRDHLFTCKX-UHFFFAOYSA-N	6.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:H13M3C5OOH	3.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_4$	7.3×10^{6}		Wang et al. (2017)	Q	80, 239
KEIPMCKLLYLETP-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:H1MC5OOH	1.4×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	5.5×10^4		Wang et al. (2017)	Q	80, 239
NRUVZELSEXXOEO-UHFFFAOYSA-N	2.8×10^3		Wang et al. (2017)	Q	80, 240
MCM:H2M2C4CO3H	1.3×10^5		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	4.6×10^4		Wang et al. (2017)	Q	80, 239
NRXKHRBCIJLLIW-UHFFFAOYSA-N	1.2×10^2		Wang et al. (2017)	Q	80, 240
MCM:H2M3C4CO3H	2.0×10^5		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	5.0×10^4		Wang et al. (2017)	Q	80, 239
BSSSRXSGDLZQTD-UHFFFAOYSA-N	6.2×10^1		Wang et al. (2017)	Q	80, 240
MCM:H2MC5OOH	1.4×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	4.9×10^4		Wang et al. (2017)	Q	80, 239
VFABJBQUVDJTMS-UHFFFAOYSA-N	1.3×10^3		Wang et al. (2017)	Q	80, 240
MCM:H3M2C4CO3H	2.0×10^5		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	4.6×10^4		Wang et al. (2017)	Q	80, 239
BXUACBWFNFVFRM-UHFFFAOYSA-N	8.0		Wang et al. (2017)	Q	80, 240
MCM:H3M3C4CO3H	1.3×10^5		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	4.1×10^4		Wang et al. (2017)	Q	80, 239
QREFYDOYYWEEBY-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	80, 240
MCM:H3M3C5OOH	8.1×10^3		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	4.6×10^2		Wang et al. (2017)	Q	80, 239
SFWIETIRFCEPBV-UHFFFAOYSA-N	2.2×10^3		Wang et al. (2017)	Q	80, 240
MCM:HM22C3CO3H	1.3×10^5		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	3.5×10^4		Wang et al. (2017)	Q	80, 239
CFTUKLJUHGJIMT-UHFFFAOYSA-N	2.0×10^1		Wang et al. (2017)	Q	80, 240
MCM:HM22C4OOH	8.1×10^3		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	3.2×10^4		Wang et al. (2017)	Q	80, 239
RBKQZGUZSABUAQ-UHFFFAOYSA-N	1.3×10^3		Wang et al. (2017)	Q	80, 240
MCM:HM23C4OOH	1.4×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	6.9×10^4		Wang et al. (2017)	Q	80, 239
OEDZXCCMDSIVQE-UHFFFAOYSA-N	1.9×10^3		Wang et al. (2017)	Q	80, 240
MCM:HM2C43CO3H	2.0×10^5		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	5.5×10^4		Wang et al. (2017)	Q	80, 239
AAGQWOGOWVBCOC-UHFFFAOYSA-N	1.1×10^2		Wang et al. (2017)	Q	80, 240
MCM:HM33C3CO3H	1.3×10^5		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	3.8×10^4		Wang et al. (2017)	Q	80, 239
CJLFHOYFCBYSAF-UHFFFAOYSA-N	1.0×10^2		Wang et al. (2017)	Q	80, 240
MCM:HM33C4OOH	8.1×10^3		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	4.5×10^4		Wang et al. (2017)	Q	80, 239
IRDKGYBPQHNNSI-UHFFFAOYSA-N	6.0×10^3		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HO1C6OOH	1.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	3.7×10^{4}		Wang et al. (2017)	Q	80, 239
AODLLEVTDATZKZ-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO1MC5OOH	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	2.5×10^{4}		Wang et al. (2017)	Q	80, 239
XFJAYUAZOYAZNW-UHFFFAOYSA-N	2.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO2C54CO3H	2.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	4.3×10^{4}		Wang et al. (2017)	Q	80, 239
HFXNQHIGYFOTHL-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO2C6OOH	5.4×10^{3}	11000	Wieser et al. (2023)	Q	437
$C_6H_{14}O_3$	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
BVOYWPYSMMRYPX-UHFFFAOYSA-N	2.4×10^{4}		Wang et al. (2017)	Q	80, 239
	1.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO2M2C5OOH	8.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	4.1×10^{4}		Wang et al. (2017)	Q	80, 239
XDJWSJNLVSIJHD-UHFFFAOYSA-N	5.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO2MC5OOH	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	4.8×10^{4}		Wang et al. (2017)	Q	80, 239
AGNBGPUCVJMPGZ-UHFFFAOYSA-N	4.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO3C5CO3H	1.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	4.5×10^{4}		Wang et al. (2017)	Q	80, 239
NIDIDJCFEJYKBD-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HO3C6OOH	1.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	4.0×10^{4}		Wang et al. (2017)	Q	80, 239
WSWZWPBQPMRENX-UHFFFAOYSA-N	8.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO4C5CO3H	1.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	4.2×10^{4}		Wang et al. (2017)	Q	80, 239
YRMQNGAQYQCFSB-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HO5C5CO3H	8.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	4.0×10^{1}		Wang et al. (2017)	Q	80, 239
ZOLITBGWKBFVQG-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	80, 240
MCM:HO5C6OOH	1.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	7.6×10^{2}		Wang et al. (2017)	Q	80, 239
VKWHJFIJUJODAG-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:PHENOH	5.5×10^{10}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	4.5×10^{8}		Wang et al. (2017)	Q	80, 239
JRROYJLQPIXCRD-UHFFFAOYSA-N	1.2×10^{8}		Wang et al. (2017)	Q	80, 240
MCM:PHENOOH	1.4×10^{12}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_6$	2.0×10^{8}		Wang et al. (2017)	Q	80, 239
WQYYYMQUZFKHHO-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C622CO3H	3.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	3.5×10^{4}		Wang et al. (2017)	Q	80, 239
JSEAPEOJJJOJEL-UHFFFAOYSA-N	9.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C624CO3H	3.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	3.9×10^{4}		Wang et al. (2017)	Q	80, 239
VELNAHZLHYPPOS-UHFFFAOYSA-N	2.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C720OOH	1.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_3$	2.9×10^{5}		Wang et al. (2017)	Q	80, 239
LPMHECUYQWFTDP-UHFFFAOYSA-N	2.4×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:CRESOH	3.0×10^{10}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	1.7×10^{8}		Wang et al. (2017)	Q	80, 239
UMHUAUCNJCQCRC-UHFFFAOYSA-N	1.6×10^{9}		Wang et al. (2017)	Q	80, 240
MCM:CRESOOH	7.8×10^{11}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_6$	7.6×10^{7}		Wang et al. (2017)	Q	80, 239
POYQJFWARUGMBT-UHFFFAOYSA-N	2.5×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:H2M2C65OOH	7.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{16}O_3$	2.9×10^{4}		Wang et al. (2017)	Q	80, 239
MDRLNEUVCFZYIZ-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:H2M4C65OOH	1.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{16}O_3$	3.9×10^{4}		Wang et al. (2017)	Q	80, 239
HGFYTCXFDJYCQF-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:H2M5C65OOH	7.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{16}O_3$	1.0×10^{4}		Wang et al. (2017)	Q	80, 239
NIKXNAUPHRWTEG-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:H3M3C5CO3H	9.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_4$	3.8×10^{4}		Wang et al. (2017)	Q	80, 239
DTTYYTHTMWEWDN-UHFFFAOYSA-N	4.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:H3M3C6OOH	6.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{16}O_3$	3.3×10^{4}		Wang et al. (2017)	Q	80, 239
IWLJNMJTDMGLQI-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO3C76OOH	1.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{16}O_3$	2.0×10^{4}		Wang et al. (2017)	Q	80, 239
YDKPOQVDDHNRNK-UHFFFAOYSA-N	9.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO5C6CO3H	1.4×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_4$	3.3×10^{4}		Wang et al. (2017)	Q	80, 239
KSOZMYOJLUVTBJ-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HO6C7OOH	1.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{16}O_3$	5.9×10^{2}		Wang et al. (2017)	Q	80, 239
YGTQIECBHSKCOV-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:TLBIPER2OH	1.7×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	9.6×10^{5}		Wang et al. (2017)	Q	80, 239
CXEVRKZODGVABW-UHFFFAOYSA-N	2.6×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:TLBIPEROOH	3.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	3.8×10^{6}		Wang et al. (2017)	Q	80, 239
JAKOWCUSWIMTAF-UHFFFAOYSA-N	9.8×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:EBENZOLOH	2.5×10^{10}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	1.0×10^{8}		Wang et al. (2017)	Q	80, 239
BUWSXDLGJSAPEF-UHFFFAOYSA-N	6.0×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:EBENZOLOOH	6.3×10^{11}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_6$	4.8×10^{7}		Wang et al. (2017)	Q	80, 239
RHHRSXIXEXUGSZ-UHFFFAOYSA-N	3.9×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:EBZBPER2OH	1.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	6.3×10^{5}		Wang et al. (2017)	Q	80, 239
AUMASFBINMOOAH-UHFFFAOYSA-N	3.8×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:EBZBPEROOH	3.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	2.5×10^{6}		Wang et al. (2017)	Q	80, 239
SCDRKAWXSVOIOT-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:HO3C86OOH	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{18}O_3$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
SPJZDLLIJATZHB-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO6C7CO3H	1.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_{16}O_4$	2.9×10^{4}		Wang et al. (2017)	Q	80, 239
UKHVIUJOBBSNIJ-UHFFFAOYSA-N	9.1		Wang et al. (2017)	Q	80, 240
MCM:HO7C8OOH	1.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{18}O_3$	4.7×10^{2}		Wang et al. (2017)	Q	80, 239
NDXYTTLTSMWWGD-UHFFFAOYSA-N	7.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MXYBPER2OH	9.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	4.0×10^{5}		Wang et al. (2017)	Q	80, 239
HJWPGRMMUKJUOW-UHFFFAOYSA-N	1.5×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:MXYBPEROOH	2.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	1.5×10^{6}		Wang et al. (2017)	Q	80, 239
JLBHNTWNBASURB-UHFFFAOYSA-N	1.2×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:MXYOLOH	1.7×10^{10}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	7.4×10^{7}		Wang et al. (2017)	Q	80, 239
HYWULKMMJLAVGS-UHFFFAOYSA-N	1.5×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:MXYOLOOH	4.4×10^{11}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_6$	3.2×10^{7}		Wang et al. (2017)	Q	80, 239
GRFXDNYNQVBVKX-UHFFFAOYSA-N	3.2×10^{7}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:OXYBPER2OH	9.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	5.0×10^{5}		Wang et al. (2017)	Q	80, 239
VCLGCGXZSIRZEA-UHFFFAOYSA-N	4.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:OXYBPEROOH	2.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	1.5×10^{6}		Wang et al. (2017)	Q	80, 239
AMPOFIFBYJNSOH-UHFFFAOYSA-N	2.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:OXYOLOH	2.0×10^{10}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	1.2×10^{8}		Wang et al. (2017)	Q	80, 239
CAIZPBLFMULAII-UHFFFAOYSA-N	4.0×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:OXYOLOOH	5.3×10^{11}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_6$	5.5×10^{7}		Wang et al. (2017)	Q	80, 239
QYYRJAPHRBSJOE-UHFFFAOYSA-N	8.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PXYBPER2OH	9.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	5.0×10^{5}		Wang et al. (2017)	Q	80, 239
IOEDFCIBQPWSMP-UHFFFAOYSA-N	4.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:PXYBPEROOH	2.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	1.6×10^{6}		Wang et al. (2017)	Q	80, 239
LZVOCZWDZPUJRQ-UHFFFAOYSA-N	5.1×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PXYOLOH	2.0×10^{10}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	1.6×10^{8}		Wang et al. (2017)	Q	80, 239
YSBIHFSZRPVTOU-UHFFFAOYSA-N	9.6×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:PXYOLOOH	5.3×10^{11}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_6$	6.8×10^{7}		Wang et al. (2017)	Q	80, 239
ROOFTVJQSDLVOJ-UHFFFAOYSA-N	4.4×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:HO3C96OOH	8.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{20}O_3$	1.9×10^{4}		Wang et al. (2017)	Q	80, 239
GGTTUTGCXALAOI-UHFFFAOYSA-N	8.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO7C8CO3H	1.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{18}O_4$	2.6×10^{4}		Wang et al. (2017)	Q	80, 239
LZPDGAGYXQEGIA-UHFFFAOYSA-N	9.6		Wang et al. (2017)	Q	80, 240
MCM:HO8C9OOH	8.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{20}O_3$	3.8×10^{2}		Wang et al. (2017)	Q	80, 239
DDKPTZKAQLYQQK-UHFFFAOYSA-N	6.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:IPBENZOLOH	2.6×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	1.0×10^{8}		Wang et al. (2017)	Q	80, 239
MXOPSFWTSRHQGT-UHFFFAOYSA-N	1.5×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:IPBZBPR2OH	1.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	6.8×10^{5}		Wang et al. (2017)	Q	80, 239
ZYFWWFFTFWUTQU-UHFFFAOYSA-N	8.9×10^{5}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:IPBZBPROOH	2.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	2.6×10^{6}		Wang et al. (2017)	Q	80, 239
PFZQQVVUSVRBJH-UHFFFAOYSA-N	2.5×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:IPBZOLOOH	5.9×10^{11}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_6$	4.9×10^{7}		Wang et al. (2017)	Q	80, 239
CHCZSTHNGRHXBM-UHFFFAOYSA-N	3.6×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:METLBPR2OH	7.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	2.8×10^{5}		Wang et al. (2017)	Q	80, 239
WBMKIPDFTCRXQQ-UHFFFAOYSA-N	5.3×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:METLBPROOH	1.7×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	1.0×10^{6}		Wang et al. (2017)	Q	80, 239
JDOROKVPYHJTEM-UHFFFAOYSA-N	4.9×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:METOLOH	1.3×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	5.0×10^{7}		Wang et al. (2017)	Q	80, 239
JGSZPUTWQXTPGZ-UHFFFAOYSA-N	5.1×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:METOLOOH	3.5×10^{11}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_6$	2.3×10^{7}		Wang et al. (2017)	Q	80, 239
WHWNZVSDBMWGPT-UHFFFAOYSA-N	2.0×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:OETLBPR2OH	7.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	3.6×10^{5}		Wang et al. (2017)	Q	80, 239
HUTNYAIOWRBWAA-UHFFFAOYSA-N	7.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:OETLBPROOH	1.7×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
JWHYGBDQJAPXFD-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:OETOLOH	1.7×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	7.6×10^{7}		Wang et al. (2017)	Q	80, 239
RKSMHAQFVDQZCV-UHFFFAOYSA-N	5.1×10^{8}		Wang et al. (2017)	Q	80, 240
MCM:OETOLOOH	4.4×10^{11}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_6$	3.1×10^{7}		Wang et al. (2017)	Q	80, 239
HMIPOFAAVJMIHR-UHFFFAOYSA-N	4.5×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:PBENZOLOH	2.1×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	7.8×10^{7}		Wang et al. (2017)	Q	80, 239
PPOCUJCGHLIXAB-UHFFFAOYSA-N	2.8×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:PBENZOLOOH	5.6×10^{11}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_6$	3.7×10^{7}		Wang et al. (2017)	Q	80, 239
YYEAFIOCCPRRFC-UHFFFAOYSA-N	9.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PBZBPER2OH	1.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	5.0×10^{5}		Wang et al. (2017)	Q	80, 239
NXHGWQBANLWNAY-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PBZBPEROOH	2.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	2.0×10^{6}		Wang et al. (2017)	Q	80, 239
BDTBCPZZIFVKES-UHFFFAOYSA-N	2.0×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:PETLBPR2OH	7.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	3.6×10^{5}		Wang et al. (2017)	Q	80, 239
ZJSMOJBPUXMKGO-UHFFFAOYSA-N	2.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PETLBPROOH	1.7×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
HYHORQQVDRWXSH-UHFFFAOYSA-N	8.1×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PETOLOH	1.7×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	8.5×10^{7}		Wang et al. (2017)	Q	80, 239
WWMQWQMHOYSCPT-UHFFFAOYSA-N	1.6×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:PETOLOOH	4.4×10^{11}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_6$	3.6×10^{7}		Wang et al. (2017)	Q	80, 239
NWKQTACFFZGFMV-UHFFFAOYSA-N	6.6×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:TM123BP2OH	4.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	2.3×10^{5}		Wang et al. (2017)	Q	80, 239
XELNTWYHIBVYRB-UHFFFAOYSA-N	1.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:TM123BPOOH	1.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	8.7×10^{5}		Wang et al. (2017)	Q	80, 239
VYRKWTIFXGFOKI-UHFFFAOYSA-N	1.6×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:TM123OLOH	1.4×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	8.5×10^{7}		Wang et al. (2017)	Q	80, 239
CUPCKHHMKYENPF-UHFFFAOYSA-N	7.8×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:TM123OLOOH	3.6×10^{11}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_6$	3.8×10^{7}		Wang et al. (2017)	Q	80, 239
QKUAZMPWBBDUFL-UHFFFAOYSA-N	3.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:TM124BP2OH	4.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	2.3×10^{5}		Wang et al. (2017)	Q	80, 239
ALTMQDHYGSUKTA-UHFFFAOYSA-N	1.5×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:TM124BPOOH	1.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	7.1×10^{5}		Wang et al. (2017)	Q	80, 239
WAGRVRZIKOHUQN-UHFFFAOYSA-N	2.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:TM124OLOH	1.4×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	1.2×10^{8}		Wang et al. (2017)	Q	80, 239
BDZMWXRIFUJLAS-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:TM124OLOOH	3.6×10^{11}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_6$	5.4×10^{7}		Wang et al. (2017)	Q	80, 239
BWEFFYCDYKVJMY-UHFFFAOYSA-N	2.0×10^{5}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:TM135BP2OH	5.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	2.8×10^{5}		Wang et al. (2017)	Q	80, 239
UOFFRVMQLZOQAS-UHFFFAOYSA-N	1.2×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:TM135BPOOH	1.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	7.3×10^{5}		Wang et al. (2017)	Q	80, 239
JMJJTOHEWPZJQK-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:TM135OLOH	1.1×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	5.4×10^{7}		Wang et al. (2017)	Q	80, 239
QLKJHZCZIQIKHZ-UHFFFAOYSA-N	2.1×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:TM135OLOOH	2.9×10^{11}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_6$	2.1×10^{7}		Wang et al. (2017)	Q	80, 239
BLJZZZVPECPSDH-UHFFFAOYSA-N	6.5×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:APINAOOH	4.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_3$	1.5×10^{4}		Wang et al. (2017)	Q	80, 239
RYIWEMFTAFVTLU-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:APINBOOH	4.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_3$	1.8×10^{4}		Wang et al. (2017)	Q	80, 239
USRGRUOHOYDFID-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:APINCOOH	4.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_3$	1.6×10^{5}		Wang et al. (2017)	Q	80, 239
PONCTWLYBMTTOF-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:BPINAOOH	4.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_3$	1.6×10^{3}		Wang et al. (2017)	Q	80, 239
YIWAKBLZYMRLPO-UHFFFAOYSA-N	4.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:BPINBOOH	4.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_3$	1.2×10^{3}		Wang et al. (2017)	Q	80, 239
LNOABRBKZGHYLB-UHFFFAOYSA-N	5.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:BPINCOOH	4.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_3$	2.7×10^{5}		Wang et al. (2017)	Q	80, 239
ONJNLKNHLLSXIR-UHFFFAOYSA-N	3.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C918CO3H	2.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_4$	5.9×10^{1}		Wang et al. (2017)	Q	80, 239
NCSYYALRPIRWRM-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DMEBPR2OH	5.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_4$	2.0×10^{5}		Wang et al. (2017)	Q	80, 239
JNPNKLHEXQFLDW-UHFFFAOYSA-N	4.4×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:DMEBPROOH	1.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_5$	7.4×10^{5}		Wang et al. (2017)	Q	80, 239
FGEXZPMCUOXGAY-UHFFFAOYSA-N	3.0×10^{5}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DMEPHOLOH	8.9×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_5$	3.7×10^{7}		Wang et al. (2017)	Q	80, 239
KIALIUKUKYONFN-UHFFFAOYSA-N	4.9×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:DMEPHOLOOH	2.3×10^{11}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_6$	1.4×10^{7}		Wang et al. (2017)	Q	80, 239
NQWKUASPEMANIL-UHFFFAOYSA-N	3.2×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:HO3C106OOH	6.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{22}O_3$	1.6×10^{4}		Wang et al. (2017)	Q	80, 239
FUGKCLXVXWNPCD-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO8C9CO3H	8.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{20}O_4$	2.5×10^{4}		Wang et al. (2017)	Q	80, 239
UIPJRQQFQSAZPI-UHFFFAOYSA-N	7.3		Wang et al. (2017)	Q	80, 240
MCM:LIMAOOH	3.6×10^{4}	13000	Wieser et al. (2023)	Q	437
$C_{10}H_{18}O_3$	4.4×10^{4}		Wang et al. (2017)	Q	80, 238
FPMDSGWWEURSNO-UHFFFAOYSA-N	2.7×10^{4}		Wang et al. (2017)	Q	80, 239
	7.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:LIMBOOH	4.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_3$	2.9×10^{4}		Wang et al. (2017)	Q	80, 239
KUZZIHAARVNWSI-UHFFFAOYSA-N	2.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:LIMCOOH	3.6×10^{4}	13000	Wieser et al. (2023)	Q	437
$C_{10}H_{18}O_3$	5.3×10^{4}		Wang et al. (2017)	Q	80, 238
VVHMRXSQYYKNLC-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	80, 239
	4.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:DEMPHOLOH	8.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_5$	2.3×10^{7}		Wang et al. (2017)	Q	80, 239
ZTCJTCVANLKQAR-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:DEMPHOLOOH	2.1×10^{11}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_6$	1.1×10^{7}		Wang et al. (2017)	Q	80, 239
MGZZNFCOXGVYJN-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:DETLBPR2OH	4.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_4$	1.7×10^{5}		Wang et al. (2017)	Q	80, 239
DLRWBBGTDDBDMY-UHFFFAOYSA-N	8.5×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:DETLBPROOH	1.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_5$	4.2×10^{5}		Wang et al. (2017)	Q	80, 239
XWTOJCWARUYVPA-UHFFFAOYSA-N	1.1×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:HO3C116OOH	5.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{24}O_3$	1.3×10^{4}		Wang et al. (2017)	Q	80, 239
XCBVDNPGCYSIMS-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO3C126OOH	4.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{26}O_3$	1.0×10^{4}		Wang et al. (2017)	Q	80, 239
FENUAUYSPLOZDX-UHFFFAOYSA-N	4.7×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:BCAOOH	4.0×10^4		Wang et al. (2017)	Q	80, 238
$C_{15}H_{26}O_3$	3.6×10^3		Wang et al. (2017)	Q	80, 239
UHQMVBPMTRQRFN-UHFFFAOYSA-N	1.0×10^5		Wang et al. (2017)	Q	80, 240
MCM:BCBOOH	4.0×10^4		Wang et al. (2017)	Q	80, 238
$C_{15}H_{26}O_3$	1.0×10^4		Wang et al. (2017)	Q	80, 239
LZWWDZWHHIWFFS-UHFFFAOYSA-N	6.3×10^4		Wang et al. (2017)	Q	80, 240
MCM:BCCOOH	5.8×10^4		Wang et al. (2017)	Q	80, 238
$C_{15}H_{26}O_3$	3.7×10^4		Wang et al. (2017)	Q	80, 239
LYZHLRDUTRINQK-UHFFFAOYSA-N	2.5×10^4		Wang et al. (2017)	Q	80, 240
MCM:CATEC1OOH	7.4×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_6O_3$	1.4×10^3		Wang et al. (2017)	Q	80, 239
GQLFYNLDVCYDKN-UHFFFAOYSA-N	2.5×10^2		Wang et al. (2017)	Q	80, 240
MCM:MCATEC1OOH	4.6×10^4		Wang et al. (2017)	Q	80, 238
$C_7H_8O_3$	1.6×10^3		Wang et al. (2017)	Q	80, 239
XVDDPRZRYAGIKB-UHFFFAOYSA-N	2.2×10^2		Wang et al. (2017)	Q	80, 240
MCM:ECATEC1OOH	4.0×10^4		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_3$	8.3×10^2		Wang et al. (2017)	Q	80, 239
WXEIAPGLSOOSMJ-UHFFFAOYSA-N	5.3×10^2		Wang et al. (2017)	Q	80, 240
MCM:MXCTEC1OOH	3.0×10^4		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_3$	1.6×10^3		Wang et al. (2017)	Q	80, 239
OTSRNDWSIFNBPX-UHFFFAOYSA-N	8.3×10^6		Wang et al. (2017)	Q	80, 240
MCM:OCATEC1OOH	3.0×10^4		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_3$	1.7×10^3		Wang et al. (2017)	Q	80, 239
FFFASTPMSYAWLR-UHFFFAOYSA-N	1.4×10^3		Wang et al. (2017)	Q	80, 240
MCM:PCATEC1OOH	3.0×10^4		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_3$	3.1×10^3		Wang et al. (2017)	Q	80, 239
XEPXMQBYFZNYBF-UHFFFAOYSA-N	5.6×10^1		Wang et al. (2017)	Q	80, 240
MCM:STYRENOOH	3.2×10^6		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_3$	2.1×10^4		Wang et al. (2017)	Q	80, 239
PRSNAZGJNCSLPW-UHFFFAOYSA-N	4.4×10^4		Wang et al. (2017)	Q	80, 240
MCM:IPCATC1OOH	3.8×10^4		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	6.0×10^2		Wang et al. (2017)	Q	80, 239
LUGXJULPVOELPW-UHFFFAOYSA-N	5.8×10^2		Wang et al. (2017)	Q	80, 240
MCM:MTCTEC1OOH	2.3×10^4		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	7.6×10^2		Wang et al. (2017)	Q	80, 239
RXVYKZMASOKYNM-UHFFFAOYSA-N	6.5×10^6		Wang et al. (2017)	Q	80, 240
MCM:OTCTEC1OOH	2.3×10^4		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	8.9×10^2		Wang et al. (2017)	Q	80, 239
BNYRTZAXTAHDLR-UHFFFAOYSA-N	8.9×10^2		Wang et al. (2017)	Q	80, 240

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Table A3.4: Peroxides (ROOH) and peroxy radicals (ROO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PRCATC1OOH	3.2×10^4		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	5.9×10^2		Wang et al. (2017)	Q	80, 239
WDHGVTVSFNORIO-UHFFFAOYSA-N	6.0×10^2		Wang et al. (2017)	Q	80, 240
MCM:PTCTEC1OOH	2.3×10^4		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	1.6×10^3		Wang et al. (2017)	Q	80, 239
SXYSFXQBYZNKPP-UHFFFAOYSA-N	4.5×10^1		Wang et al. (2017)	Q	80, 240
MCM:T123CT1OOH	1.7×10^4		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	2.0×10^3		Wang et al. (2017)	Q	80, 239
XFULZEJTRUOVEV-UHFFFAOYSA-N	7.3×10^6		Wang et al. (2017)	Q	80, 240
MCM:T124CT1OOH	1.7×10^4		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	3.2×10^3		Wang et al. (2017)	Q	80, 239
XVSFIBYJDMNABQ-UHFFFAOYSA-N	2.7×10^6		Wang et al. (2017)	Q	80, 240
MCM:HCOCH2OOH	7.4×10^3		Wang et al. (2017)	Q	80, 238
$C_2H_4O_3$	1.4×10^2		Wang et al. (2017)	Q	80, 239
TUJPSEFVDYHSJJ-UHFFFAOYSA-N	4.2×10^1		Wang et al. (2017)	Q	80, 240
MCM:HCOCO3H	9.8×10^4		Wang et al. (2017)	Q	80, 238
$C_2H_2O_4$	3.9×10^2		Wang et al. (2017)	Q	80, 239
JOALXJIWVKUVBR-UHFFFAOYSA-N	1.6×10^1		Wang et al. (2017)	Q	80, 240
MCM:C3DIALOOH	5.6×10^6		Wang et al. (2017)	Q	80, 238
$C_3H_4O_4$	1.7×10^4		Wang et al. (2017)	Q	80, 239
VUPDPJIDXKCVGY-UHFFFAOYSA-N	4.7×10^1		Wang et al. (2017)	Q	80, 240
MCM:CHOC2H4OOH	5.8×10^3		Wang et al. (2017)	Q	80, 238
$C_3H_6O_3$	5.3×10^3		Wang et al. (2017)	Q	80, 239
XSASRUDTFFBDDK-UHFFFAOYSA-N	1.6×10^3		Wang et al. (2017)	Q	80, 240

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A3.5 Aldehydes (RCHO)

Table A3.5: Aldehydes (RCHO)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methanal	3.2×10^{1}	7100	Burkholder et al. (2019)	L	455
HCHO	3.2×10^{1}	7100	Burkholder et al. (2015)	L	455
(formaldehyde)	3.2×10^{1}	6800	Warneck and Williams (2012)	L	455
[50-00-0]	3.2×10^{1}	7100	Sander et al. (2011)	L	455
WSFSSNUMVMOOMR-UHFFFAOYSA-N	3.2×10^{1}	7100	Sander et al. (2006)	L	455
	3.2×10^{1}	6800	Staudinger and Roberts (2001)	L	455
	3.2×10^{1}	6800	Staudinger and Roberts (1996)	L	455
	3.5×10^{1}	5700	Liu et al. (2015)	M	455
	3.4×10^{1}	6400	Allou et al. (2011)	M	455
	5.3×10^{1}	1600	Seyfioglu and Odabasi (2007)	M	455
	9.9×10^{1}		Kim et al. (2000)	M	87, 455
	3.1×10^{1}	6500	Zhou and Mopper (1990)	M	456, 455
	3.1×10^{1}	7200	Betterton and Hoffmann (1988)	M	455
			Dong and Dasgupta (1986)	M	457
			Ledbury and Blair (1925)	M	458
			Blair and Ledbury (1925)	M	458
	3.0×10^{1}		Lide and Frederikse (1995)	V	455
	2.3		Hwang et al. (1992)	V	455
	6.9×10^{1}	6400	Chameides (1984)	T	455
	2.9×10^{1}	7200	Bell (1966)	X	459, 455
	5.9×10^{1}		Gaffney and Senum (1984)	X	455, 389
	4.5×10^{1}		Lee and Zhou (1993)	C	87, 455
			Hough (1991)	C	458
	1.4×10^{2}		Warneck (1988)	C	455
	7.8×10^{-2}		Wang et al. (2017)	Q	80, 238
	4.9×10^{-2}		Wang et al. (2017)	Q	80, 239
	1.0×10^{-2}		Wang et al. (2017)	Q	80, 240
	2.8×10^{-2}		Hilal et al. (2008)	Q	
	7.5×10^{-2}		Modarresi et al. (2007)	Q	67
	4.3×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	9.0×10^{-2}		English and Carroll (2001)	Q	230, 231
	6.2×10^{-2}		Katritzky et al. (1998)	Q	
	1.8×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.0×10^{2}		Meylan and Howard (1991)	Q	455
	4.2×10^{-2}		Abraham et al. (1990)	?	
	6.2×10^{1}		Seinfeld (1986)	?	21, 455
			Lelieveld and Crutzen (1991)	W	458
			Pandis and Seinfeld (1989)	W	458

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethanal	1.3×10^{-1}	5900	Burkholder et al. (2019)	L	460
CH_3CHO	1.3×10^{-1}	5900	Burkholder et al. (2015)	L	460
(acetaldehyde)	1.5×10^{-1}	5600	Brockbank (2013)	L	1
[75-07-0]	1.3×10^{-1}	5900	Sander et al. (2011)	L	
IKHGUXGNUITLKF-UHFFFAOYSA-N	1.3×10^{-1}	5900	Sander et al. (2006)	L	
	1.3×10^{-1}	5700	Staudinger and Roberts (2001)	L	
	1.4×10^{-1}	5600	Staudinger and Roberts (1996)	L	
	1.7×10^{-1}	5600	Wieland et al. (2015)	M	461
	1.5×10^{-1}	6400	Ji and Evans (2007)	M	
	1.1×10^{-1}		Straver and de Loos (2005)	M	
	1.5×10^{-1}		Marin et al. (1999)	M	
	1.3×10^{-1}	5700	Benkelberg et al. (1995)	M	
	1.7×10^{-1}	5000	Zhou and Mopper (1990)	M	456
	7.1×10^{-2}		Guitart et al. (1989)	M	14
	1.2×10^{-1}	6300	Betterton and Hoffmann (1988)	M	460
	1.2×10^{-1}	5800	Snider and Dawson (1985)	M	
	8.3×10^{-2}		Richon et al. (1985)	M	38
	1.6×10^{-1}		Mazza (1980)	M	
	2.5×10^{-1}		Vitenberg et al. (1974)	M	373
	1.5×10^{-1}		Buttery et al. (1969)	M	
	1.2×10^{-1}		Marin et al. (1999)	V	
	1.2×10^{-1}		Hwang et al. (1992)	V	
	7.8×10^{-2}		Yaws (2003)	X	258
	1.7×10^{-2}	4500	Janini and Quaddora (1986)	X	298
	1.7×10^{-1}	4700	Goldstein (1982)	X	298
	1.5×10^{-1}		Gaffney and Senum (1984)	X	389
	1.5×10^{-1}		Pierotti et al. (1959)	X	462
	1.8×10^{-1}		Dupeux et al. (2022)	Q	259
	9.0×10^{-2}		Keshavarz et al. (2022)	Q	
	9.8×10^{-2}		Duchowicz et al. (2020)	Q	
	9.8×10^{-2}		Wang et al. (2017)	Q	80, 238
	3.4×10^{-1}		Wang et al. (2017)	Q	80, 239
	1.3×10^{-1}		Wang et al. (2017)	Q	80, 240
	1.5×10^{-1}		Li et al. (2014)	Q	241
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.1×10^{-1}		Hilal et al. (2008)	Q	
	1.0×10^{-1}		Modarresi et al. (2007)	Q	67
		5200	Kühne et al. (2005)	Q	
	1.5×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	6.6×10^{-2}		Yao et al. (2002)	Q	229
	1.4×10^{-1}		English and Carroll (2001)	Q	230, 231
	1.4×10^{-1}		Marin et al. (1999)	Q	
	7.7×10^{-2}		Katritzky et al. (1998)	Q	
	1.5×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.3×10^{-1}		Suzuki et al. (1992)	Q	232

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.5×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	1.5×10^{-1}		Mackay et al. (2006c)	?	21
		5800	Kühne et al. (2005)	?	
	1.0×10^{-1}		Yaws (1999)	?	21
	9.8×10^{-2}		Yaws and Yang (1992)	?	21
	1.5×10^{-1}		Abraham et al. (1990)	?	
ethanedial	4.1×10^{3}	7500	Burkholder et al. (2019)	L	460
OHCCHO	4.1×10^{3}	7500	Burkholder et al. (2015)	L	460
(glyoxal)	4.1×10^{3}	7500	Sander et al. (2011)	L	460
[107-22-2]	4.9×10^{5}		Kampf et al. (2013)	M	460, 463
LEQAOMBKQFMDFZ-UHFFFAOYSA-N	4.1×10^{3}	7500	Ip et al. (2009)	M	460
			Volkamer et al. (2009)	M	464
	2.6×10^{5}		Kroll et al. (2005)	M	460, 465
	3.6×10^{3}		Zhou and Mopper (1990)	M	460, 70
	$>3.0\times10^{3}$		Betterton and Hoffmann (1988)	M	460
	1.4×10^{4}		Lee and Zhou (1993)	C	87, 460
	2.0×10^{2}		Keshavarz et al. (2022)	Q	
	1.6×10^{1}		Duchowicz et al. (2020)	Q	299
	8.9×10^{1}		Wang et al. (2017)	Q	80, 238
	9.6		Wang et al. (2017)	Q	80, 239
	1.2×10^{-2}		Wang et al. (2017)	Q	80, 240
	3.1×10^{4}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{3}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	245
	3.0×10^{3}		Duchowicz et al. (2020)	?	185, 21
	2.7×10^{5}		Woo and McNeill (2015)	?	466
propanal	9.9×10^{-2}	4300	Burkholder et al. (2019)	L	
C_2H_5CHO	9.9×10^{-2}	4300	Burkholder et al. (2015)	L	
(propionaldehyde)	1.3×10^{-1}	5500	Brockbank (2013)	L	1
[123-38-6]	9.9×10^{-2}	4300	Sander et al. (2011)	L	
NBBJYMSMWIIQGU-UHFFFAOYSA-N	9.9×10^{-2}	4300	Sander et al. (2006)	L	
	1.3×10^{-1}		Liu et al. (2015)	M	72
	9.1×10^{-2}		Kim and Kim (2014)	M	
	1.3×10^{-1}	5800	Ji and Evans (2007)	M	
	1.3×10^{-1}	5700	Zhou and Mopper (1990)	M	456
	6.1×10^{-2}		Richon et al. (1985)	M	38
	1.2×10^{-1}		Mazza (1980)	M	
	1.3×10^{-1}		Buttery et al. (1969)	M	
	7.5×10^{-2}		Buttery et al. (1965)	M	
	1.3×10^{-1}		Mackay et al. (2006c)	V	
	1.3×10^{-2}		Mackay et al. (1995)	V	
	3.2×10^{-2}	3200	Djerki and Laub (1988)	V	
	1.6×10^{-1}		Amoore and Buttery (1978)	V	
	4.3×10^{-2}		Yaws (2003)	X	258
	5.2×10^{-2}	5600	Schaffer and Daubert (1969)	X	298
	2.7×10^{-2}	2400	Janini and Quaddora (1986)	X	298

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	9.8×10^{-2}		Dupeux et al. (2022)	Q	259
	1.2×10^{-1}		Keshavarz et al. (2022)	Q	
	9.9×10^{-2}		Duchowicz et al. (2020)	Q	184
	8.0×10^{-2}		Wang et al. (2017)	Q	80, 238
	2.4×10^{-1}		Wang et al. (2017)	Q	80, 239
	8.0×10^{-2}		Wang et al. (2017)	Q	80, 240
	1.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Modarresi et al. (2007)	Q	67
		5500	Kühne et al. (2005)	Q	
	1.4×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	1.1×10^{-1}		English and Carroll (2001)	Q	230, 231
	5.8×10^{-2}		Katritzky et al. (1998)	Q	
	1.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	7.3×10^{-2}		Russell et al. (1992)	Q	279
	1.0×10^{-1}		Suzuki et al. (1992)	Q	232
	1.3×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	1.3×10^{-1}		Mackay et al. (2006c)	?	21
		5000	Kühne et al. (2005)	?	
	2.3×10^{-1}		Yaws (1999)	?	21
	1.3×10^{-1}		Abraham et al. (1990)	?	
propanedial $C_3H_4O_2$ (malonaldehyde) [542-78-9] WSMYVTOQOOLQHP-UHFFFAOYSA-N	7.3×10^{1}		Wang et al. (2017)	Q	80, 238
	6.0×10^{1}		Wang et al. (2017)	Q	80, 239
	4.1		Wang et al. (2017)	Q	80, 240
MCM:C32OH13CO $C_3H_4O_3$ NVXLIZQNSVLKPO-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	80, 238
	5.5×10^{3}		Wang et al. (2017)	Q	80, 239
	8.7		Wang et al. (2017)	Q	80, 240
MCM:CH3CHOHCHO $C_3H_6O_2$ BSABBBMNWQWLLU-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	80, 238
	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
	3.1		Wang et al. (2017)	Q	80, 240
MCM:HOC2H4CHO $C_3H_6O_2$ AKXKFZDCRYJKTF-UHFFFAOYSA-N	3.6×10^{1}	9900	Wieser et al. (2023)	Q	437
	2.2×10^{2}		Wang et al. (2017)	Q	80, 238
	8.3×10^{2}		Wang et al. (2017)	Q	80, 239
	6.6×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
butanal	9.5×10^{-2}	6200	Burkholder et al. (2019)	L	
C_3H_7CHO	9.5×10^{-2}	6200	Burkholder et al. (2015)	L	
(butyraldehyde)	9.1×10^{-2}	6000	Brockbank (2013)	L	1
[123-72-8]	9.5×10^{-2}	6200	Sander et al. (2011)	L	
ZTQSAGDEMFDKMZ-UHFFFAOYSA-N	9.5×10^{-2}	6200	Sander et al. (2006)	L	
	6.1×10^{-2}		Kim and Kim (2014)	M	
	8.9×10^{-2}	6200	Ji and Evans (2007)	M	
	9.5×10^{-2}	6200	Zhou and Mopper (1990)	M	456
	8.6×10^{-2}		Buttery et al. (1969)	M	
	6.4×10^{-2}		Buttery et al. (1965)	M	
	6.5×10^{-2}		Mackay et al. (2006c)	V	
	6.5×10^{-2}		Mackay et al. (1995)	V	
	1.0×10^{-1}		Hwang et al. (1992)	V	
	8.7×10^{-2}	3500	Djerki and Laub (1988)	V	
	6.7×10^{-2}		Amoore and Buttery (1978)	V	
	8.4×10^{-2}		Yaws (2003)	X	258
	8.3×10^{-2}		Yaws (2003)	X	237
	5.4×10^{-2}	4000	Janini and Quaddora (1986)	X	298
	6.8×10^{-2}		Dupeux et al. (2022)	Q	259
	1.6×10^{-1}		Keshavarz et al. (2022)	Q	
	9.9×10^{-2}		Duchowicz et al. (2020)	Q	
	6.3×10^{-2}		Wang et al. (2017)	Q	80, 238
	1.4×10^{-1}		Wang et al. (2017)	Q	80, 239
	6.3×10^{-2}		Wang et al. (2017)	Q	80, 240
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	5.8×10^{-2}		Ghargheizi et al. (2010)	Q	246
	9.0×10^{-2}		Hilal et al. (2008)	Q	
	1.1×10^{-1}		Modarresi et al. (2007)	Q	67
		5900	Kühne et al. (2005)	Q	
	6.7×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	5.3×10^{-2}		Yao et al. (2002)	Q	229
	8.6×10^{-2}		English and Carroll (2001)	Q	230, 231
	5.4×10^{-2}		Katritzky et al. (1998)	Q	
	9.5×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	8.6×10^{-2}		Russell et al. (1992)	Q	279
	7.9×10^{-2}		Suzuki et al. (1992)	Q	232
	8.6×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	8.6×10^{-2}		Mackay et al. (2006c)	?	21
		6400	Kühne et al. (2005)	?	
	8.4×10^{-2}		Yaws (1999)	?	21
	8.6×10^{-2}		Abraham et al. (1990)	?	

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methylpropanal	5.1×10^{-2}		Burkholder et al. (2019)	L	
C_4H_8O	5.1×10^{-2}		Brockbank (2013)	L	
(isobutyraldehyde)	3.2×10^{-2}	7600	Bruneel et al. (2016)	M	
[78-84-2]	5.9×10^{-3}	4500	Strekowski and George (2005)	M	
AMIMRNSIRUDHCM-UHFFFAOYSA-N	3.3×10^{-2}		Karl et al. (2003)	M	
	3.4×10^{-2}		Pollien et al. (2003)	M	
	5.0×10^{-2}		Amoore and Buttery (1978)	M	
	5.5×10^{-2}		Duchowicz et al. (2020)	V	186
	5.5×10^{-2}		HSDB (2015)	V	
	6.7×10^{-2}		Amoore and Buttery (1978)	V	
	5.8×10^{-2}		Yaws (2003)	X	258
	4.5×10^{-2}		Dupeux et al. (2022)	Q	259
	3.8×10^{-2}		Duchowicz et al. (2020)	Q	
	7.4×10^{-2}		Wang et al. (2017)	Q	80, 238
	1.1×10^{-1}		Wang et al. (2017)	Q	80, 239
	4.3×10^{-2}		Wang et al. (2017)	Q	80, 240
	7.0×10^{-2}		Hilal et al. (2008)	Q	
		5000	Kühne et al. (2005)	Q	
	5.2×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	3.7×10^{-2}		Yao et al. (2002)	Q	229, 267
	5.2×10^{-2}		English and Carroll (2001)	Q	230, 274
	5.4×10^{-2}		Katritzky et al. (1998)	Q	
	8.2×10^{-2}		Nirmalakhandan et al. (1997)	Q	
		5100	Kühne et al. (2005)	?	
	5.7×10^{-2}		Yaws (1999)	?	21
	5.1×10^{-2}		Abraham et al. (1990)	?	
2-methylpropanedial	6.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_2$	1.2×10^{1}		Wang et al. (2017)	Q	80, 239
[16002-19-0]	1.9		Wang et al. (2017)	Q	80, 240
VXYSFSCCSQAYJV-UHFFFAOYSA-N					
MCM:MALDIAL	2.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_2$	4.6×10^{2}		Wang et al. (2017)	Q	80, 239
JGEMYUOFGVHXKV-UHFFFAOYSA-N	6.5		Wang et al. (2017)	Q	80, 240
MCM:C3MDIALOH	1.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_3$	2.0×10^{3}		Wang et al. (2017)	Q	80, 239
SQHUBVCIVAIUAB-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	80, 240
MCM:C41OH	2.5×10^{7}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	3.7×10^{7}		Wang et al. (2017)	Q	80, 239
YTBSYETUWUMLBZ-UHFFFAOYSA-N	1.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C41OOH	3.3×10^{9}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_5$	3.6×10^{8}		Wang et al. (2017)	Q	80, 239
ROHPNOOUQDXFHZ-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	80, 240

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C4OCCOHCOH	1.4×10^4		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	5.0×10^4		Wang et al. (2017)	Q	80, 239
DFFAMJFPVBTTBX-UHFFFAOYSA-N	3.5×10^2		Wang et al. (2017)	Q	80, 240
MCM:CHOC3DIOL	2.6×10^5		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	2.2×10^5		Wang et al. (2017)	Q	80, 239
CQSYGAZTCJHVFE-UHFFFAOYSA-N	3.6×10^3		Wang et al. (2017)	Q	80, 240
MCM:HC3CCHO	3.0×10^1		Wang et al. (2017)	Q	80, 238
$C_4H_6O_2$	8.7×10^1		Wang et al. (2017)	Q	80, 239
PPNVQCFSKPIRKK-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	80, 240
MCM:HC3CHO	7.1×10^2		Wang et al. (2017)	Q	80, 238
$C_4H_6O_2$	3.7×10^3		Wang et al. (2017)	Q	80, 239
FXCMZPXXCRHRNK-UHFFFAOYSA-N	2.5×10^4		Wang et al. (2017)	Q	80, 240
MCM:HMACROH	1.5×10^7		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	8.5×10^7		Wang et al. (2017)	Q	80, 239
OUEKYUKJSLEOIU-UHFFFAOYSA-N	1.3×10^4		Wang et al. (2017)	Q	80, 240
MCM:HMACR	4.1×10^2		Wang et al. (2017)	Q	80, 238
$C_4H_6O_2$	2.0×10^2		Wang et al. (2017)	Q	80, 239
QVBICLGJAQXLSA-UHFFFAOYSA-N	1.1×10^2		Wang et al. (2017)	Q	80, 240
MCM:HO13C3CHO	2.6×10^4		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	2.3×10^5		Wang et al. (2017)	Q	80, 239
NKVLMFFGFYHDNE-UHFFFAOYSA-N	3.2×10^3		Wang et al. (2017)	Q	80, 240
MCM:HO2C3CHO	2.1×10^2		Wang et al. (2017)	Q	80, 238
$C_4H_8O_2$	1.4×10^3		Wang et al. (2017)	Q	80, 239
HSJKGGMUJITCBW-UHFFFAOYSA-N	3.6×10^1		Wang et al. (2017)	Q	80, 240
MCM:HO3C3CHO	1.1×10^1		Wang et al. (2017)	Q	80, 238
$C_4H_8O_2$	8.9×10^1		Wang et al. (2017)	Q	80, 239
UIKQNMXWCYQNCS-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	80, 240
MCM:HOC3H6CHO	1.7×10^2		Wang et al. (2017)	Q	80, 238
$C_4H_8O_2$	2.8×10^3		Wang et al. (2017)	Q	80, 239
PIAOXUVIBAKVSP-UHFFFAOYSA-N	6.5×10^2		Wang et al. (2017)	Q	80, 240
MCM:HOHOC4DIAL	6.3×10^5		Wang et al. (2017)	Q	80, 238
$C_4H_6O_4$	3.0×10^6		Wang et al. (2017)	Q	80, 239
UUWVJXZLAWXQBU-UHFFFAOYSA-N	2.8×10^2		Wang et al. (2017)	Q	80, 240
MCM:HOIPRCHO	2.1×10^2		Wang et al. (2017)	Q	80, 238
$C_4H_8O_2$	6.8×10^2		Wang et al. (2017)	Q	80, 239
JTMCAHGCWBGWRV-UHFFFAOYSA-N	2.5×10^1		Wang et al. (2017)	Q	80, 240
MCM:IBUTALOH	6.6		Wang et al. (2017)	Q	80, 238
$C_4H_8O_2$	4.4×10^1		Wang et al. (2017)	Q	80, 239
HNVAGBIANFAIIL-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	80, 240

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MACROH	8.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	3.6×10^{4}		Wang et al. (2017)	Q	80, 239
JBCPUXACCOWZEB-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
pentanal	6.6×10^{-2}	6500	Brockbank (2013)	L	1
C_4H_9CHO	6.8×10^{-2}		Liu et al. (2015)	M	72
(valeraldehyde)	3.9×10^{-2}		Kim and Kim (2014)	M	
[110-62-3]	7.1×10^{-2}	6100	Ji and Evans (2007)	M	
HGBOYTHUEUWSSQ-UHFFFAOYSA-N	6.3×10^{-2}	6300	Zhou and Mopper (1990)	M	456
	6.7×10^{-2}		Buttery et al. (1969)	M	
	5.8×10^{-2}		Buttery et al. (1965)	M	
	2.4×10^{-1}	3800	Djerki and Laub (1988)	V	
	6.4×10^{-2}		Amoore and Buttery (1978)	V	
	3.0×10^{-2}		Yaws (2003)	X	258
	3.0×10^{-2}		Yaws (2003)	X	237
	6.1×10^{-2}		Dupeux et al. (2022)	Q	259
	2.2×10^{-1}		Keshavarz et al. (2022)	Q	
	9.8×10^{-2}		Duchowicz et al. (2020)	Q	299
	5.8×10^{-2}		Wang et al. (2017)	Q	80, 238
	8.9×10^{-2}		Wang et al. (2017)	Q	80, 239
	3.2×10^{-2}		Wang et al. (2017)	Q	80, 240
	5.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
	7.2×10^{-2}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	67
		6200	Kühne et al. (2005)	Q	
	6.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.9×10^{-2}		Yao et al. (2002)	Q	229, 267
	6.7×10^{-2}		English and Carroll (2001)	Q	230, 231
	7.3×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	6.1×10^{-2}		Suzuki et al. (1992)	Q	232
	6.2×10^{-2}		Meylan and Howard (1991)	Q	
	6.7×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	6.7×10^{-2}		Mackay et al. (2006c)	?	21
		5500	Kühne et al. (2005)	?	
	3.0×10^{-2}		Yaws (1999)	?	21
	4.4×10^{-2}		Yaws and Yang (1992)	?	21, 38
	6.7×10^{-2}		Abraham et al. (1990)	?	
2-methylbutanal	2.5×10^{-2}	5600	Brockbank (2013)	L	1
$C_5H_{10}O$	2.3×10^{-2}		Pollien et al. (2003)	M	
[96-17-3]	5.9×10^{-2}		Wang et al. (2017)	Q	80, 238
BYGQBDHUGHBGMD-UHFFFAOYSA-N	8.7×10^{-2}		Wang et al. (2017)	Q	80, 239
	3.9×10^{-2}		Wang et al. (2017)	Q	80, 240
	9.5×10^{-3}		Hertel et al. (2007)	Q	467

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methylbutanal	1.1×10^{-2}	10000	Bruneel et al. (2016)	M	33
$C_5H_{10}O$	2.4×10^{-2}	6100	Wieland et al. (2015)	M	468
(isovaleraldehyde)	2.1×10^{-2}		Kim and Kim (2014)	M	
[590-86-3]	2.6×10^{-2}		Pollien et al. (2003)	M	
YGHRJJRRZDOVPD-UHFFFAOYSA-N	2.0×10^{-2}		Nelson and Hoff (1968)	M	297
	2.4×10^{-2}		Duchowicz et al. (2020)	V	186
	2.5×10^{-2}		HSDB (2015)	V	
	5.2×10^{-2}		Yaws (2003)	X	237
	3.8×10^{-2}		Duchowicz et al. (2020)	Q	
	5.9×10^{-2}		Wang et al. (2017)	Q	80, 238
	1.1×10^{-1}		Wang et al. (2017)	Q	80, 239
	4.5×10^{-2}		Wang et al. (2017)	Q	80, 240
	5.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
	7.3×10^{-2}		Hilal et al. (2008)	Q	
	9.1×10^{-2}		Modarresi et al. (2007)	Q	67
	9.8×10^{-3}		Hertel et al. (2007)	Q	467
MCM:C4MDIAL	1.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_2$	6.5×10^{2}		Wang et al. (2017)	Q	80, 239
USBJWIKCHJDWPF-UHFFFAOYSA-N	2.8		Wang et al. (2017)	Q	80, 240
MCM:CO1M22CHO	3.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_2$	8.9		Wang et al. (2017)	Q	80, 239
WNBFTLCNQKKVHC-UHFFFAOYSA-N	3.4×10^{-1}		Wang et al. (2017)	Q	80, 240
2,2-dimethylpropanal	4.1×10^{-2}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O$	5.6×10^{-2}		Wang et al. (2017)	Q	80, 239
(pivaldehyde)	2.8×10^{-2}		Wang et al. (2017)	Q	80, 240
[630-19-3]					
FJJYHTVHBVXEEQ-UHFFFAOYSA-N					
MCM:C3EDIALOH	1.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	2.6×10^{3}		Wang et al. (2017)	Q	80, 239
QTDYRJFEJDMBDI-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:C3M3OH2CHO	1.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	6.5×10^{1}		Wang et al. (2017)	Q	80, 239
VKYKDJZVZBURQF-UHFFFAOYSA-N	6.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C42CHO	2.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	3.2×10^{5}		Wang et al. (2017)	Q	80, 239
NGVSSTUGOBBIBC-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C4M2AL2OH	3.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	5.0×10^{6}		Wang et al. (2017)	Q	80, 239
NUHRTSFMSDZSTE-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C4OHCHO	8.3		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	5.6×10^{1}		Wang et al. (2017)	Q	80, 239
SUTLBTHMXYSMSZ-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	80, 240

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C514OH	1.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	8.7×10^{5}		Wang et al. (2017)	Q	80, 239
UIVALZXFWDRKKE-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C57OH	1.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	6.8×10^{7}		Wang et al. (2017)	Q	80, 239
ZKDSJDSEVDWBAC-UHFFFAOYSA-N	1.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C58OH	1.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	1.4×10^{8}		Wang et al. (2017)	Q	80, 239
HTPZSALIZDTBIL-UHFFFAOYSA-N	2.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C5DIALOH	3.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_3$	5.8×10^{4}		Wang et al. (2017)	Q	80, 239
KBKQEUDBRUGUIQ-UHFFFAOYSA-N	3.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:H13C43CHO	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	1.7×10^{5}		Wang et al. (2017)	Q	80, 239
KJLUILOCNALPNM-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:H2M2C3CHO	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	6.2×10^{2}		Wang et al. (2017)	Q	80, 239
FXFBPKDQLDOIRG-UHFFFAOYSA-N	2.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HC4ACHO	4.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_2$	4.6×10^{3}		Wang et al. (2017)	Q	80, 239
BSHDRMLUCYMQOP-UHFFFAOYSA-N	1.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HC4CCHO	1.2×10^{3}	11000	Wieser et al. (2023)	Q	437
$C_5H_8O_2$	4.8×10^{2}		Wang et al. (2017)	Q	80, 238
GCHJBJOOADXJFT-UHFFFAOYSA-N	4.1×10^{3}		Wang et al. (2017)	Q	80, 239
	5.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HM22CHO	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	3.7×10^{2}		Wang et al. (2017)	Q	80, 239
JJMOMMLADQPZNY-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HO24C4CHO	2.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	3.6×10^{5}		Wang et al. (2017)	Q	80, 239
WDKLWOBHKQJYSU-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO2C43CHO	2.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	6.9×10^{2}		Wang et al. (2017)	Q	80, 239
ZURZPPULRFXVLF-UHFFFAOYSA-N	3.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HO2C4CHO	1.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	2.1×10^{3}		Wang et al. (2017)	Q	80, 239
HFZMJAMTNAAZQE-UHFFFAOYSA-N	4.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO3C4CHO	1.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	7.8×10^{2}		Wang et al. (2017)	Q	80, 239
WRWLNLBWBJEUPI-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HOBUT2CHO	1.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	1.6×10^{3}		Wang et al. (2017)	Q	80, 239
PLBZJQQQFIOXRU-UHFFFAOYSA-N	2.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HOIBUTCHO	1.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	2.0×10^{3}		Wang et al. (2017)	Q	80, 239
RWXBAXNFTXQJAY-UHFFFAOYSA-N	4.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MBOBCO	7.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	4.4×10^{4}		Wang et al. (2017)	Q	80, 239
YDXYYBJRCIQQSF-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PROL1MCHO	5.8		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	4.2×10^{1}		Wang et al. (2017)	Q	80, 239
MEHIGMLPKIJWEA-UHFFFAOYSA-N	7.4×10^{-1}		Wang et al. (2017)	Q	80, 240
hexanal	4.5×10^{-2}	6400	Brockbank (2013)	L	1
$C_5H_{11}CHO$	2.3×10^{-2}	5200	Kutsuna and Kaneyasu (2021)	M	
[66-25-1]	2.9×10^{-2}	8900	Bruneel et al. (2016)	M	
JARKCYVAAOWBJS-UHFFFAOYSA-N	4.7×10^{-2}		Souchon et al. (2004)	M	
	3.2×10^{-2}		Karl et al. (2003)	M	
	1.6×10^{-1}	4900	Meynier et al. (2003)	M	38
	2.7×10^{-2}		van Ruth et al. (2002)	M	14
	2.2×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 361
	1.6×10^{-2}		van Ruth et al. (2001)	M	14
	4.9×10^{-2}	6500	Zhou and Mopper (1990)	M	456
	4.6×10^{-2}		Buttery et al. (1969)	M	
	5.8×10^{-2}		Buttery et al. (1965)	M	
	3.5×10^{-2}		Amoore and Buttery (1978)	V	
	2.8×10^{-2}		Yaws (2003)	X	258
	2.8×10^{-2}		Yaws (2003)	X	237, 38
	4.8×10^{-2}		Sieg et al. (2008)	C	
	4.6×10^{-2}		Meynier et al. (2003)	C	
	3.1×10^{-2}		Nahon et al. (2000)	C	14
	4.2×10^{-2}		Dupeux et al. (2022)	Q	259
	3.0×10^{-1}		Keshavarz et al. (2022)	Q	
	9.8×10^{-2}		Duchowicz et al. (2020)	Q	299
	4.6×10^{-2}		Wang et al. (2017)	Q	80, 238
	5.8×10^{-2}		Wang et al. (2017)	Q	80, 239
	5.5×10^{-2}		Wang et al. (2017)	Q	80, 240
	4.6×10^{-2}		Li et al. (2014)	Q	241
	4.3×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
	5.8×10^{-2}		Hilal et al. (2008)	Q	
	9.8×10^{-2}		Modarresi et al. (2007)	Q	67
	1.1×10^{-2}		Hertel et al. (2007)	Q	467

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		6600	Kühne et al. (2005)	Q	
	4.6×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.6×10^{-2}		Yao et al. (2002)	Q	229
	5.2×10^{-2}		English and Carroll (2001)	Q	230, 260
	4.8×10^{-2}		Katritzky et al. (1998)	Q	
	5.8×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	4.6×10^{-2}		Suzuki et al. (1992)	Q	232
	4.6×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	4.6×10^{-2}		Mackay et al. (2006c)	?	21
		6900	Kühne et al. (2005)	?	
	3.8×10^{-2}		Yaws (1999)	?	21, 38
	1.9×10^{-2}		Yaws and Yang (1992)	?	21, 38
	4.6×10^{-2}		Abraham et al. (1990)	?	
pentanedial	3.0×10^{2}	9200	Olson (1998)	M	
$OHC(CH_2)_3CHO$	4.1×10^{2}		HSDB (2015)	Q	99
(glutaraldehyde)		8800	Kühne et al. (2005)	Q	
[111-30-8]		9100	Kühne et al. (2005)	?	
SXRSQZLOMIGNAQ-UHFFFAOYSA-N					
2-methylpentanal	5.3×10^{-2}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O$	5.6×10^{-2}		Wang et al. (2017)	Q	80, 239
(2-methylvaleraldehyde)	3.5×10^{-2}		Wang et al. (2017)	Q	80, 240
[123-15-9]	2.7×10^{-2}		HSDB (2015)	Q	99
FTZILAQGHINQQR-UHFFFAOYSA-N		5700	Kühne et al. (2005)	Q	
		5300	Kühne et al. (2005)	?	
hexanedial	4.2×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_2$	1.7×10^{2}		Wang et al. (2017)	Q	80, 239
(adipaldehyde)	3.2×10^{1}		Wang et al. (2017)	Q	80, 240
[1072-21-5]					
UMHJEEQLYBKSAN-UHFFFAOYSA-N					
MCM:M22C3CHO	3.2×10^{-2}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O$	6.5×10^{-2}		Wang et al. (2017)	Q	80, 239
LTNUSYNQZJZUSY-UHFFFAOYSA-N	3.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:M2C43CHO	6.2×10^{-2}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O$	6.0×10^{-2}		Wang et al. (2017)	Q	80, 239
AKUUEDVRXOZTBF-UHFFFAOYSA-N	3.7×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:M33C3CHO	3.2×10^{-2}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O$	5.0×10^{-2}		Wang et al. (2017)	Q	80, 239
QYPLKDUOPJZROX-UHFFFAOYSA-N	2.6×10^{-2}		Wang et al. (2017)	Q	80, 240
3-methylpentanal	3.8×10^{-2}		Yaws (2003)	X	237
$C_6H_{12}O$	5.3×10^{-2}		Wang et al. (2017)	Q	80, 238
[15877-57-3]	7.8×10^{-2}		Wang et al. (2017)	Q	80, 239
YJWJGLQYQJGEEP-UHFFFAOYSA-N	4.5×10^{-2}		Wang et al. (2017)	Q	80, 240
	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	246

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methylpentanal $C_6H_{12}O$ [1119-16-0] JGEGJYXHCFUMJF-UHFFFAOYSA-N	3.8×10^{-2} 3.8×10^{-2}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
2-ethylbutanal $C_6H_{12}O$ [97-96-1] UNNGUFMVYQJGTD-UHFFFAOYSA-N	4.0×10^{-2} 3.7×10^{-2}		Yaws (2003) Dupeux et al. (2022)	X Q	258 259
MCM:C518CHO $C_6H_{10}O_2$ XEAYIEUKFACAKS-UHFFFAOYSA-N	3.2×10^{2} 5.3×10^{2} 2.8×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:C615OH $C_6H_{10}O_3$ LOUHJSYYTNSRBN-UHFFFAOYSA-N	4.9×10^{3} 4.4×10^{4} 3.7×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:C623OH $C_6H_{12}O_4$ ASGSKBSLHTVURJ-UHFFFAOYSA-N	3.2×10^{8} 6.2×10^{8} 1.9×10^{4}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:C67OH $C_6H_{12}O_3$ SIBVVDHXFPINCX-UHFFFAOYSA-N	1.3×10^{5} 3.5×10^{5} 4.6×10^{2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:C68OH $C_6H_{12}O_3$ RJKLRJTWLKKQSE-UHFFFAOYSA-N	1.3×10^{5} 3.6×10^{5} 3.6×10^{2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:C6DIALOH $C_6H_{10}O_3$ GATFIJYWERJMGU-UHFFFAOYSA-N	1.2×10^{5} 4.7×10^{5} 2.6×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:CO1C6OH $C_6H_{12}O_2$ FPFTWHJPEMPAGE-UHFFFAOYSA-N	1.3×10^{2} 1.9×10^{3} 1.4×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:CO1H63OH $C_6H_{12}O_3$ TWSXDPXQZVBPJU-UHFFFAOYSA-N	4.1×10^{5} 2.5×10^{6} 2.8×10^{4}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:H2M2C4CHO $C_6H_{12}O_2$ NEJZWIVQOAKZHY-UHFFFAOYSA-N	9.3×10^{1} 1.3×10^{3} 2.0×10^{2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:H2M3C4CHO $C_6H_{12}O_2$ GUXDGBBNSMURMG-UHFFFAOYSA-N	1.5×10^{2} 1.8×10^{3} 1.5×10^{2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:H3M3C4CHO $C_6H_{12}O_2$ HKXRCBUXVFAKDA-UHFFFAOYSA-N	9.3×10^{1} 5.5×10^{2} 1.2×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HM22C3CHO	9.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	1.1×10^{3}		Wang et al. (2017)	Q	80, 239
VOISQCUJWIZDHK-UHFFFAOYSA-N	5.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HM2C43CHO	1.5×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	1.7×10^{3}		Wang et al. (2017)	Q	80, 239
QQZFDCJFBSAIBQ-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HM33C3CHO	9.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	1.0×10^{3}		Wang et al. (2017)	Q	80, 239
YHMMFPKTSXQULG-UHFFFAOYSA-N	2.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO2C54CHO	1.5×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	1.3×10^{3}		Wang et al. (2017)	Q	80, 239
ZHZOUKIXPREHLS-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO3C5CHO	1.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	1.5×10^{3}		Wang et al. (2017)	Q	80, 239
HAPLZPWSLJPZBM-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO5C5CHO	6.9		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	4.0×10^{1}		Wang et al. (2017)	Q	80, 239
BRZMRZVKWQWYPJ-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	80, 240
heptanal	3.4×10^{-2}	7500	Brockbank (2013)	L	1
$C_6H_{13}CHO$	3.5×10^{-2}		Souchon et al. (2004)	M	
[111-71-7]	2.0×10^{-2}		van Ruth et al. (2002)	M	14
FXHGMKSSBGDXIY-UHFFFAOYSA-N	1.9×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 361
	1.1×10^{-2}		van Ruth et al. (2001)	M	14
	3.3×10^{-2}	7500	Zhou and Mopper (1990)	M	456
	3.7×10^{-2}		Buttery et al. (1969)	M	
	6.0×10^{-2}		Buttery et al. (1965)	M	
	5.4×10^{-2}		Amoore and Buttery (1978)	V	
	2.1×10^{-2}		Yaws (2003)	X	258
	2.0×10^{-2}		Yaws (2003)	X	237, 38
	3.7×10^{-2}		Sieg et al. (2008)	C	
	3.0×10^{-2}		Dupeux et al. (2022)	Q	259
	5.3×10^{-2}		Keshavarz et al. (2022)	Q	
	9.8×10^{-2}		Duchowicz et al. (2020)	Q	184
	3.6×10^{-2}		Wang et al. (2017)	Q	80, 238
	4.3×10^{-2}		Wang et al. (2017)	Q	80, 239
	2.5×10^{-2}		Wang et al. (2017)	Q	80, 240
	3.7×10^{-2}		Li et al. (2014)	Q	241
	3.3×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
	3.7×10^{-2}		Hilal et al. (2008)	Q	
	8.1×10^{-2}		Modarresi et al. (2007)	Q	67

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		6900	Kühne et al. (2005)	Q	
	3.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.2×10^{-2}		Yao et al. (2002)	Q	229
	3.9×10^{-2}		English and Carroll (2001)	Q	230, 274
	4.7×10^{-2}		Katritzky et al. (1998)	Q	
	4.5×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	3.6×10^{-2}		Suzuki et al. (1992)	Q	232
	3.7×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		7100	Kühne et al. (2005)	?	
	2.8×10^{-2}		Yaws (1999)	?	21, 38
	2.3×10^{-2}		Yaws and Yang (1992)	?	21, 38
	3.7×10^{-2}		Abraham et al. (1990)	?	
MCM:C622CHO	5.8×10^{3}	11000	Wieser et al. (2023)	Q	437
$C_7H_{12}O_2$	2.5×10^{2}		Wang et al. (2017)	Q	80, 238
JWVBPJJNIHELFZ-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	80, 239
	7.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C624CHO	5.8×10^{3}	11000	Wieser et al. (2023)	Q	437
$C_7H_{12}O_2$	2.5×10^{2}		Wang et al. (2017)	Q	80, 238
AIMYSSDKEKDSEU-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 239
	2.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C728OH	2.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_4$	1.2×10^{9}		Wang et al. (2017)	Q	80, 239
RQDWEXZQVQBWBC-UHFFFAOYSA-N	2.2×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C730OH	2.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_4$	3.4×10^{9}		Wang et al. (2017)	Q	80, 239
ROYLBPWMPALPRM-UHFFFAOYSA-N	1.3×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:H3M3C5CHO	7.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_2$	1.1×10^{3}		Wang et al. (2017)	Q	80, 239
PUMVOOYIPAYIQQ-UHFFFAOYSA-N	5.6×10^{1}		Wang et al. (2017)	Q	80, 240
octanal	2.0×10^{-2}	7300	Brockbank (2013)	L	1
$C_7H_{15}CHO$	2.1×10^{-2}		van Ruth et al. (2002)	M	14
[124-13-0]	1.9×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 361
NUJGJRNETVAIRJ-UHFFFAOYSA-N	8.8×10^{-3}		van Ruth et al. (2001)	M	14
	2.1×10^{-2}		Li and Carr (1993)	M	
	2.1×10^{-2}	7400	Zhou and Mopper (1990)	M	456
	1.9×10^{-2}		Buttery et al. (1969)	M	
	7.5×10^{-2}		Buttery et al. (1965)	M	
	2.9×10^{-2}		Amoore and Buttery (1978)	V	
	1.3×10^{-2}		Yaws (2003)	X	258
	1.3×10^{-2}		Yaws (2003)	X	237, 38
	1.9×10^{-2}		Sieg et al. (2008)	C	
	1.9×10^{-2}		Nahon et al. (2000)	C	14
	2.8×10^{-2}		Dupeux et al. (2022)	Q	259
	7.1×10^{-2}		Keshavarz et al. (2022)	Q	

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.7×10^{-2}		Duchowicz et al. (2020)	Q	
	2.4×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	7.0×10^{-2}		Modarresi et al. (2007)	Q	67
		7300	Kühne et al. (2005)	Q	
	5.2×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	2.0×10^{-2}		Yao et al. (2002)	Q	229
	3.1×10^{-2}		English and Carroll (2001)	Q	230, 231
	4.5×10^{-2}		Katritzky et al. (1998)	Q	
	3.6×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	2.8×10^{-2}		Suzuki et al. (1992)	Q	232
	1.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		6200	Kühne et al. (2005)	?	
	1.8×10^{-2}		Yaws (1999)	?	21, 38
	2.0		Yaws and Yang (1992)	?	21, 38
	1.9×10^{-2}		Abraham et al. (1990)	?	
2-ethylhexanal	1.2×10^{-2}	5400	Brockbank (2013)	L	1
$C_8H_{16}O$	1.3×10^{-2}		Duchowicz et al. (2020)	V	186
[123-05-7]	1.2×10^{-2}		HSDB (2015)	V	
LGYNIFWIKSEESD-UHFFFAOYSA-N	2.4×10^{-2}		Yaws (2003)	X	258
	2.4×10^{-2}		Yaws (2003)	X	237
	2.1×10^{-2}		Dupeux et al. (2022)	Q	259
	3.8×10^{-2}		Duchowicz et al. (2020)	Q	
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.7×10^{-2}		Hilal et al. (2008)	Q	
	2.4×10^{-2}		Modarresi et al. (2007)	Q	67
MCM:C729CHO	8.0×10^{2}	10000	Wieser et al. (2023)	Q	437
$C_8H_{12}O_2$	7.1×10^{1}		Wang et al. (2017)	Q	80, 238
MEGRLTONSLAOOM-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	80, 239
	6.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C810OH	6.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_3$	1.7×10^{5}		Wang et al. (2017)	Q	80, 239
WBGXLUPQADVOIR-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C822OH	2.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_2$	1.8×10^{3}		Wang et al. (2017)	Q	80, 239
CCTLWIOCAVSPLW-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C824OH	3.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_3$	1.9×10^{5}		Wang et al. (2017)	Q	80, 239
RBBQERVBTKJTLF-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C826OH	7.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_4$	3.0×10^{8}		Wang et al. (2017)	Q	80, 239
LLAUXDLXTPQIPI-UHFFFAOYSA-N	2.6×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C830OH	2.5×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_2$	1.6×10^{3}		Wang et al. (2017)	Q	80, 239
KODLEZWYEGWLGP-UHFFFAOYSA-N	6.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C831OH	6.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_3$	2.1×10^{5}		Wang et al. (2017)	Q	80, 239
YTEDFRLZFCPFBH-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C89OH	2.5×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_2$	2.3×10^{3}		Wang et al. (2017)	Q	80, 239
KMZPPEYMMZMCIQ-UHFFFAOYSA-N	2.2×10^{3}		Wang et al. (2017)	Q	80, 240
nonanal	1.1×10^{-2}	6800	Brockbank (2013)	L	1
$C_8H_{17}CHO$	1.0×10^{-2}	6700	Zhou and Mopper (1990)	M	456
[124-19-6]	1.3×10^{-2}		Buttery et al. (1969)	M	
GYHFUZHODSMOHU-UHFFFAOYSA-N	7.1×10^{-2}		Buttery et al. (1965)	M	
	1.3×10^{-2}		Amoore and Buttery (1978)	V	
	1.0×10^{-2}		Yaws (2003)	X	258
	1.0×10^{-2}		Yaws (2003)	X	237, 38
	1.4×10^{-2}		Sieg et al. (2008)	C	
	1.8×10^{-2}		Dupeux et al. (2022)	Q	259
	9.6×10^{-2}		Keshavarz et al. (2022)	Q	
	9.7×10^{-2}		Duchowicz et al. (2020)	Q	184
	1.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.4×10^{-2}		Hilal et al. (2008)	Q	
	5.9×10^{-2}		Modarresi et al. (2007)	Q	67
	1.3×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.8×10^{-2}		Yao et al. (2002)	Q	229
	2.3×10^{-2}		English and Carroll (2001)	Q	230, 231
	2.8×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	2.1×10^{-2}		Suzuki et al. (1992)	Q	232
	2.0×10^{-2}		Meylan and Howard (1991)	Q	
	1.3×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	1.5×10^{-2}		Yaws (1999)	?	21, 38
	6.9×10^{-3}		Yaws and Yang (1992)	?	21, 38
	1.3×10^{-2}		Abraham et al. (1990)	?	

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
3,5,5-trimethylhexanal $C_9H_{18}O$ [5435-64-3] WTPYRCJDOZVZON-UHFFFAOYSA-N	2.0×10^{-2}		HSDB (2015)	Q	99
decanal	6.3×10^{-3}	8900	Brockbank (2013)	L	1
$C_9H_{19}CHO$	4.3×10^{-3}		Helburn et al. (2008)	M	
[112-31-2]	6.0×10^{-3}	8700	Zhou and Mopper (1990)	M	456
KSMVZQYAVGTKIV-UHFFFAOYSA-N	1.7×10^{-1}		Buttery et al. (1965)	M	
	1.3×10^{-2}		Yaws (2003)	X	258
	1.3×10^{-2}		Yaws (2003)	X	237
	5.5×10^{-3}		Sieg et al. (2008)	C	
	1.9×10^{-2}		Dupeux et al. (2022)	Q	259
	1.8×10^{-1}		Keshavarz et al. (2022)	Q	
	9.7×10^{-2}		Duchowicz et al. (2020)	Q	299
	2.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	8.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.6×10^{-2}		Hilal et al. (2008)	Q	
	5.1×10^{-2}		Modarresi et al. (2007)	Q	67
		7900	Kühne et al. (2005)	Q	
	5.6×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	3.8×10^{-2}		Katritzky et al. (1998)	Q	
	5.5×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		8500	Kühne et al. (2005)	?	
MCM:C918CHO	1.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_2$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
GWMMOZICECYZLL-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	80, 240
hydroxycitronellal $C_{10}H_{20}O_2$ [107-75-5] WPFVBOQKRVRMJB-UHFFFAOYSA-N	9.4×10^{2}		Dupeux et al. (2022)	Q	259
undecanal	7.0×10^{-3}		Yaws (2003)	X	258
$C_{11}H_{22}O$	6.9×10^{-3}		Yaws (2003)	X	237
[112-44-7]	1.5×10^{-2}		Dupeux et al. (2022)	Q	259
KMPQYAYAQWNLME-UHFFFAOYSA-N	2.2×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
		8300	Kühne et al. (2005)	Q	
		8300	Kühne et al. (2005)	?	

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dodecanal	5.2×10^{-3}		Yaws (2003)	X	258
$C_{12}H_{24}O$	5.2×10^{-3}		Yaws (2003)	X	237
[112-54-9]	1.2×10^{-2}		Dupeux et al. (2022)	Q	259
HFJRKMMYBMWEAD-UHFFFAOYSA-N	2.3×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
1-tridecanal	5.8×10^{-3}		Yaws (2003)	X	258
$C_{13}H_{26}O$	5.8×10^{-3}		Yaws (2003)	X	237
[10486-19-8]	9.6×10^{-3}		Dupeux et al. (2022)	Q	259
BGEHHAVMRVXCGR-UHFFFAOYSA-N	2.4×10^{-3}		Gharagheizi et al. (2012)	Q	
	5.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
1-tetradecanal	8.0×10^{-4}		Yaws (2003)	X	258
$C_{14}H_{28}O$	6.2×10^{-3}		Dupeux et al. (2022)	Q	259
[124-25-4]	2.6×10^{-3}		Gharagheizi et al. (2012)	Q	
UHUFTBALEZWWIH-UHFFFAOYSA-N					
aquaflora	5.2×10^{-1}		Dupeux et al. (2022)	Q	259
$C_{12}H_{18}O$					
[1339119-15-1]					
BFTAXJRKNXWMMX-UHFFFAOYSA-N					
starfleur	1.4×10^{-1}		Dupeux et al. (2022)	Q	259
$C_{13}H_{24}O$					
(3-(4-isobutylcyclohexyl)propanal)					
[1254940-85-6]					
XUTZHJNXAOHUTM-UHFFFAOYSA-N					
MCM:C126CO	8.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{18}O_2$	1.7×10^{2}		Wang et al. (2017)	Q	80, 239
IWMJDJFLMSAAES-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C126OH	2.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_2$	2.1×10^{3}		Wang et al. (2017)	Q	80, 239
PQYIIYBUHROKIY-UHFFFAOYSA-N	4.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C127OH	5.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_3$	7.1×10^{6}		Wang et al. (2017)	Q	80, 239
QHKXYVNBHFONML-UHFFFAOYSA-N	3.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C126CHO	6.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{20}O_2$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
ZDIXDRBTLRZYNM-UHFFFAOYSA-N	4.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C1311OH	4.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_3$	8.3×10^{6}		Wang et al. (2017)	Q	80, 239
CBUCUSJJCJUTML-UHFFFAOYSA-N	6.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C1313OH	7.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_4$	4.3×10^{8}		Wang et al. (2017)	Q	80, 239
XIWFBNXBOAYHAJ-UHFFFAOYSA-N	8.3×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C136OH	2.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_2$	2.0×10^{3}		Wang et al. (2017)	Q	80, 239
GEHGNVSPJQGFQG-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	80, 240
propenal	1.3×10^{-1}	5500	Burkholder et al. (2019)	L	469
CH_2CHCHO	7.2×10^{-2}	5100	Brockbank (2013)	L	1
(acrolein)	7.2×10^{-2}	5100	Snider and Dawson (1985)	M	
[107-02-8]	1.0×10^{-1}		Mackay et al. (2006c)	V	
HGINCPLSRVDWNT-UHFFFAOYSA-N	2.3		Lide and Frederikse (1995)	V	
	1.0×10^{-2}		Mackay et al. (1995)	V	
	7.0×10^{-2}		Hwang et al. (1992)	V	
	1.3×10^{-1}		Suntio et al. (1988)	V	12
	1.0×10^{-1}	3800	Goldstein (1982)	X	298
	2.2		Howard (1989)	X	412
	8.1×10^{-2}		Gaffney and Senum (1984)	X	389
	1.8×10^{-1}		Suntio et al. (1988)	C	12
	1.4×10^{-1}		Ryan et al. (1988)	C	
	1.2×10^{-1}		Keshavarz et al. (2022)	Q	
	3.5×10^{-1}		Duchowicz et al. (2020)	Q	
	2.2×10^{-1}		Wang et al. (2017)	Q	80, 238
	1.9×10^{-1}		Wang et al. (2017)	Q	80, 239
	2.1×10^{-1}		Wang et al. (2017)	Q	80, 240
	5.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	9.5×10^{-2}		Hilal et al. (2008)	Q	
	6.3×10^{-1}		Modarresi et al. (2007)	Q	67
		4600	Kühne et al. (2005)	Q	
	8.1×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	7.5×10^{-2}		Mackay et al. (2006c)	?	21
		3800	Kühne et al. (2005)	?	
	1.2×10^{-1}		Yaws (1999)	?	21, 12
2-methylpropenal	4.5×10^{-2}	4600	Burkholder et al. (2019)	L	
C_4H_6O	6.4×10^{-2}		Burkholder et al. (2015)	L	
(methacrolein)	4.5×10^{-2}	4600	Brockbank (2013)	L	1
[78-85-3]	4.8×10^{-2}	4300	Ji and Evans (2007)	M	
STNJBCKSHOAVAJ-UHFFFAOYSA-N	6.4×10^{-2}		Iraci et al. (1999)	M	
	4.2×10^{-2}	5300	Allen et al. (1998)	M	
	5.2×10^{-2}		HSDB (2015)	V	
	4.7×10^{-2}		Yaws (2003)	X	258
	4.7×10^{-2}		Yaws (2003)	X	237
	7.3×10^{-2}		Dupeux et al. (2022)	Q	259
	1.6×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.5×10^{-1}		Wang et al. (2017)	Q	80, 238
	1.4×10^{-1}		Wang et al. (2017)	Q	80, 239

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.3×10^{-2}		Wang et al. (2017)	Q	80, 240
	1.6×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	4.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
	9.5×10^{-2}		Hilal et al. (2008)	Q	
	1.1×10^{-1}		Modarresi et al. (2007)	Q	67
		4000	Kühne et al. (2005)	Q	
	4.3×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		4800	Kühne et al. (2005)	?	
	4.8×10^{-2}		Yaws (1999)	?	21
2-butenal C_4H_6O [4170-30-3] MLUCVPSAIODCQM-UHFFFAOYSA-N	2.9×10^{-1}		Wang et al. (2017)	Q	80, 238
	1.6×10^{-1}		Wang et al. (2017)	Q	80, 239
	1.6		Wang et al. (2017)	Q	80, 240
	9.7×10^{-2}		Hilal et al. (2008)	Q	
	3.9×10^{-1}		Modarresi et al. (2007)	Q	67
	2.7×10^{-1}		Nirmalakhandan et al. (1997)	Q	
			Burkholder et al. (2019)	W	470
(E)-2-butenal $CH_3CHCHCHO$ (crotonaldehyde) [123-73-9] MLUCVPSAIODCQM-NSCUHMNNSA-N	5.4×10^{-1}	5300	Brockbank (2013)	L	1
	5.0×10^{-1}		Buttery et al. (1971)	M	
	4.4×10^{-2}		Mackay et al. (2006c)	V	
	4.4×10^{-2}		Mackay et al. (1995)	V	
	7.6×10^{-1}		Yaws (2003)	X	258
	5.9×10^{-1}	3600	Goldstein (1982)	X	298
	5.0×10^{-1}		Gaffney and Senum (1984)	X	389
	1.5		Dupeux et al. (2022)	Q	259
	1.6×10^{-1}		Keshavarz et al. (2022)	Q	
	1.2×10^{-1}		Duchowicz et al. (2020)	Q	299
	3.9×10^{-1}		Modarresi et al. (2007)	Q	67
		5000	Kühne et al. (2005)	Q	
	5.2×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	3.1×10^{-1}		Suzuki et al. (1992)	Q	232
	5.1×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		4300	Kühne et al. (2005)	?	
	5.9×10^{-1}		Yaws (1999)	?	21, 12
	5.1×10^{-1}		Abraham et al. (1990)	?	
2-hexenal $C_6H_{10}O$ [505-57-7] MBDOYVRWFFCFHM-UHFFFAOYSA-N	3.0×10^{-1}		Keshavarz et al. (2022)	Q	
	1.2×10^{-1}		Duchowicz et al. (2020)	Q	
	6.2×10^{-2}		Hilal et al. (2008)	Q	
	2.5×10^{-1}		Modarresi et al. (2007)	Q	67
	8.6×10^{-2}		English and Carroll (2001)	Q	230, 260
	1.7×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	2.0×10^{-1}		Duchowicz et al. (2020)	?	185, 21

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(*E*)-2-hexenal	1.4×10^{-1}		Karl et al. (2003)	M	
$C_3H_7CHCHCHO$	9.0×10^{-1}	5700	Meynier et al. (2003)	M	38
(*trans*-2-hexenal)	2.0×10^{-1}		Buttery et al. (1971)	M	
[6728-26-3]	2.0×10^{-1}		Meynier et al. (2003)	C	
MBDOYVRWFFCFHM-SNAWJCMRSA-N	2.1×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	1.8×10^{-1}		Suzuki et al. (1992)	Q	232
(*E*,*E*)-2,4-hexadienal	1.0		Buttery et al. (1971)	M	
$CH_3CHCHCHCHCHO$	3.0×10^{-1}		Keshavarz et al. (2022)	Q	
(*trans-trans*-2,4-hexadienal)	1.4×10^{-1}		Duchowicz et al. (2020)	Q	184
[142-83-6]	3.9×10^{-1}		Hilal et al. (2008)	Q	
BATOPAZDIZEVQF-MQQKCMAXSA-N	4.7×10^{-1}		Modarresi et al. (2007)	Q	67
	1.5		Suzuki et al. (1992)	Q	232
	1.0		Duchowicz et al. (2020)	?	185, 21
2-heptenal	5.0×10^{-2}		Hilal et al. (2008)	Q	
$C_7H_{12}O$					
[2463-63-0]					
NDFKTBCGKNOHPJ-UHFFFAOYSA-N					
trans-2-heptenal	1.3		Abney (2021)	Q	399
$C_7H_{12}O$					
[18829-55-5]					
NDFKTBCGKNOHPJ-AATRIKPKSA-N					
(*Z*)-4-heptenal	8.8×10^{-2}		Straver and de Loos (2005)	M	
$C_7H_{12}O$					
(*cis*-4-heptenal)					
[6728-31-0]					
VVGOCOMZRGWHPI-ARJAWSKDSA-N					
2-octenal	7.1×10^{-2}		Keshavarz et al. (2022)	Q	
$C_8H_{14}O$	1.2×10^{-1}		Duchowicz et al. (2020)	Q	299
[2363-89-5]	4.1×10^{-2}		Hilal et al. (2008)	Q	
LVBXEMGDVWVTGY-UHFFFAOYSA-N	1.9×10^{-1}		Modarresi et al. (2007)	Q	67
	5.2×10^{-2}		English and Carroll (2001)	Q	230, 231
	1.0×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.3×10^{-1}		Duchowicz et al. (2020)	?	185, 21
(*E*)-2-octenal	1.3×10^{-1}		Buttery et al. (1971)	M	
$C_8H_{14}O$	1.4×10^{-1}		Yaffe et al. (2003)	Q	248, 249
(*trans*-2-octenal)	1.1×10^{-1}		Suzuki et al. (1992)	Q	232
[2548-87-0]			Betterton (1992)	W	471
LVBXEMGDVWVTGY-VOTSOKGWSA-N					
2-ethyl-2-hexenal	5.2×10^{-2}	5800	Brockbank (2013)	L	1
$C_8H_{14}O$					
[645-62-5]					
PYLMCYQHBRSDND-UHFFFAOYSA-N					

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(*E*)-2-nonenal $C_9H_{16}O$ (*trans*-2-nonenal) [18829-56-6] BSAIUMLZVGUGKX-BQYQJAHWSA-N	5.8×10^{-2}		Roberts and Pollien (1997)	M	
trans-2,*cis*-6-nonadienal $C_9H_{14}O$ [557-48-2] HZYHMHHBBBSGHB-ODYTWBPASA-N	8.2×10^{-2}	7100	Ömür-Özbek and Dietrich (2005)	M	
3,7-dimethyl-6-octenal $C_{10}H_{18}O$ (citronellal) [106-23-0] NEHNMFOYXAPHSD-UHFFFAOYSA-N	2.5×10^{-2} 3.8×10^{-2}	4500	van Roon et al. (2005) HSDB (2015)	V Q	 99
3,7-dimethyl-2,6-octadienal $C_{10}H_{16}O$ (citral) [5392-40-5] WTEVQBCEXWBHNA-UHFFFAOYSA-N	2.9×10^{-1} 5.2 2.3×10^{-1}	6700	Wu et al. (2022b) Dupeux et al. (2022) HSDB (2015)	M Q Q	 259 99
tillenal $C_{11}H_{18}O$ (3-(4,4-dimethyl-1-cyclohexen-1-yl)propanal) [850997-10-3] IHMKWBJKOWYASH-UHFFFAOYSA-N	3.4×10^{-1}		Dupeux et al. (2022)	Q	259
lilybelle $C_{12}H_{20}O$ [1378867-81-2] VZZSYXAVGYODQG-UHFFFAOYSA-N	4.5×10^{-1}		Dupeux et al. (2022)	Q	259
mugoxal $C_{13}H_{22}O$ (3-(4-*tert*-butylcyclohexen-1-yl)propanal) WGWWNPFQPHLSIM-UHFFFAOYSA-N	6.7×10^{-1}		Dupeux et al. (2022)	Q	259
orange oil $C_{15}H_{22}O$ [8028-48-6] NOPLRNXKHZRXHT-UHFFFAOYSA-N	6.3×10^{-4}		Maniere et al. (2011)	?	241, 165

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benzaldehyde	4.0×10^{-1}	5200	Brockbank (2013)	L	1, 472
C_6H_5CHO	3.8×10^{-1}	5500	Staudinger and Roberts (2001)	L	
[100-52-7]	3.9×10^{-1}	4800	Staudinger and Roberts (1996)	L	
HUMNYLRZRPPJDN-UHFFFAOYSA-N	3.2×10^{-1}	6300	Allou et al. (2011)	M	
	3.4×10^{-1}		Souchon et al. (2004)	M	
	3.5×10^{-1}	7000	Allen et al. (1998)	M	
	4.2×10^{-1}	4600	Zhou and Mopper (1990)	M	456
	3.7×10^{-1}	5100	Betterton and Hoffmann (1988)	M	460
	1.6×10^{-1}		Mackay et al. (2006c)	V	
	1.6×10^{-1}		Mackay et al. (1995)	V	
	3.6×10^{-1}		Hine and Mookerjee (1975)	V	
	3.5×10^{-1}	5400	Bagno et al. (1991)	T	473
	3.9×10^{-1}		Yaws (2003)	X	258
	3.6×10^{-1}		Gaffney and Senum (1984)	X	389
	3.7×10^{-1}		Schüürmann (2000)	C	21
	8.4×10^{-1}		Dupeux et al. (2022)	Q	259
	5.3×10^{-2}		Keshavarz et al. (2022)	Q	
	6.6×10^{-1}		Duchowicz et al. (2020)	Q	184
	3.0		Wang et al. (2017)	Q	80, 238
	1.3		Wang et al. (2017)	Q	80, 239
	1.6		Wang et al. (2017)	Q	80, 240
	3.6×10^{-1}		Li et al. (2014)	Q	241
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	7.7×10^{-1}		Hilal et al. (2008)	Q	
	1.2		Modarresi et al. (2007)	Q	67
	2.6×10^{-2}		Emel'yanenko et al. (2007)	Q	415
	2.6×10^{-2}		Hertel and Sommer (2006)	Q	415
		5800	Kühne et al. (2005)	Q	
	3.7×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	5.4×10^{-1}		English and Carroll (2001)	Q	230, 274
	2.4×10^{-1}		Katritzky et al. (1998)	Q	
	7.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	3.6×10^{-1}		Suzuki et al. (1992)	Q	232
	3.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	4.4×10^{-1}		Mackay et al. (2006c)	?	21
		5400	Kühne et al. (2005)	?	
	4.0×10^{-1}		Yaws (1999)	?	21
	3.6×10^{-1}		Abraham et al. (1990)	?	
phenylacetaldehyde	1.6		Dupeux et al. (2022)	Q	259
$C_6H_5CH_2CHO$	2.8		Wang et al. (2017)	Q	80, 238
[122-78-1]	3.6		Wang et al. (2017)	Q	80, 239
DTUQWGWMVIHBKE-UHFFFAOYSA-N	3.6		Wang et al. (2017)	Q	80, 240
	1.0×10^{-1}		Emel'yanenko et al. (2007)	Q	415
	1.0×10^{-1}		Hertel and Sommer (2005)	Q	415

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methylbenzaldehyde	3.1×10^{-1}	6900	Ji et al. (2008)	M	
C_8H_8O	1.9		Wang et al. (2017)	Q	80, 238
(o-tolualdehyde)	1.7		Wang et al. (2017)	Q	80, 239
[529-20-4]	8.7×10^{-1}		Wang et al. (2017)	Q	80, 240
BTFQKIATRPGRBS-UHFFFAOYSA-N	3.3×10^{-1}		HSDB (2015)	Q	99
3-methylbenzaldehyde	3.5×10^{-1}	7200	Brockbank (2013)	L	1
C_8H_8O	3.0×10^{-1}	5800	Wu et al. (2022b)	M	
(m-tolualdehyde)	3.5×10^{-1}	7200	Ji et al. (2008)	M	
[620-23-5]	1.9		Wang et al. (2017)	Q	80, 238
OVWYEQOVUDKZNU-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 239
	1.7		Wang et al. (2017)	Q	80, 240
	3.3×10^{-1}		HSDB (2015)	Q	99
4-methylbenzaldehyde	5.3×10^{-1}	7200	Brockbank (2013)	L	1
C_8H_8O	4.6×10^{-1}	6400	Wu et al. (2022b)	M	
(p-tolualdehyde)	5.3×10^{-1}	7200	Ji et al. (2008)	M	
[104-87-0]	5.7×10^{-1}		Duchowicz et al. (2020)	V	186
FXLOVSHXALFLKQ-UHFFFAOYSA-N	5.8×10^{-1}		HSDB (2015)	V	
	5.4×10^{-1}		Abraham et al. (1994a)	R	
	3.3×10^{-1}		Duchowicz et al. (2020)	Q	
	1.9		Wang et al. (2017)	Q	80, 238
	1.3		Wang et al. (2017)	Q	80, 239
	3.0		Wang et al. (2017)	Q	80, 240
	7.9×10^{-1}		Hilal et al. (2008)	Q	
	5.3×10^{-1}		Modarresi et al. (2007)	Q	67
	4.8×10^{-1}		English and Carroll (2001)	Q	230, 231
	6.5×10^{-1}		Katritzky et al. (1998)	Q	
	5.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	5.6×10^{-1}		Yaws (1999)	?	21
terephthaldialdehyde	1.6×10^{1}		Abraham et al. (2019)	Q	
$C_8H_6O_2$					
[623-27-8]					
KUCOHFSKRZZVRO-UHFFFAOYSA-N					
2-hydroxybenzaldehyde	1.1	6200	Ji et al. (2008)	M	
$C_6H_4(OH)CHO$	1.8		Duchowicz et al. (2020)	V	186
(2-formylphenol; salicylaldehyde)	4.6		Duchowicz et al. (2020)	Q	
[90-02-8]	4.0×10^{3}		McFall et al. (2020)	Q	474
SMQUZDBALVYZAC-UHFFFAOYSA-N	6.2		Raventos-Duran et al. (2010)	Q	271, 243
	9.9		Raventos-Duran et al. (2010)	Q	244
	6.2		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{1}		Hilal et al. (2008)	Q	
	1.8		Yaws (1999)	?	21, 475

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-hydroxybenzaldehyde	3.9×10^3		Gaffney and Senum (1984)	X	389
$C_6H_4(OH)CHO$	9.6×10^3		Keshavarz et al. (2022)	Q	
(3-formylphenol)	1.8×10^4		Duchowicz et al. (2020)	Q	299
[100-83-4]	1.2×10^3		Raventos-Duran et al. (2010)	Q	242, 243
IAVREABSGIHHMO-UHFFFAOYSA-N	1.6×10^4		Raventos-Duran et al. (2010)	Q	244
	6.2×10^3		Raventos-Duran et al. (2010)	Q	245
	5.3×10^3		Hilal et al. (2008)	Q	
	7.9×10^2		Modarresi et al. (2007)	Q	67
	1.2×10^3		Katritzky et al. (1998)	Q	
	3.0×10^4		Nirmalakhandan et al. (1997)	Q	
	3.9×10^3		Duchowicz et al. (2020)	?	185, 21
	3.8×10^3		Abraham et al. (1990)	?	
4-hydroxybenzaldehyde	1.9×10^4	8600	Parsons et al. (1971)	T	417
$C_6H_4(OH)CHO$	9.6×10^3		Keshavarz et al. (2022)	Q	
(4-formylphenol)	2.1×10^4		Duchowicz et al. (2020)	Q	
[123-08-0]	1.2×10^3		Gharagheizi et al. (2012)	Q	
RGHHSNMVTDWUBI-UHFFFAOYSA-N	1.2×10^3		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^3		Raventos-Duran et al. (2010)	Q	244
	6.2×10^3		Raventos-Duran et al. (2010)	Q	245
	8.8×10^2		Hilal et al. (2008)	Q	
	1.6×10^3		Modarresi et al. (2007)	Q	67
	3.0×10^4		Nirmalakhandan et al. (1997)	Q	
	1.9×10^4		Duchowicz et al. (2020)	?	185, 21
	1.9×10^4		Abraham et al. (1990)	?	
2-methoxybenzaldehyde $C_8H_8O_2$ [135-02-4] PKZJLOCLABXVMC-UHFFFAOYSA-N	1.0×10^1	8900	Ji et al. (2008)	M	
3-methoxybenzaldehyde $C_8H_8O_2$ [591-31-1] WMPDAIZRQDCGFH-UHFFFAOYSA-N	5.1	8800	Ji et al. (2008)	M	
4-methoxybenzaldehyde $C_8H_8O_2$ [123-11-5] ZRSNZINYAWTAHE-UHFFFAOYSA-N	2.4×10^1	8700	Ji et al. (2008)	M	
3-phenyl-2-propenal	2.8		HSDB (2015)	V	
C_9H_8O	1.4	6300	van Roon et al. (2005)	V	
(cinnamaldehyde) [104-55-2] KJPRLNWUNMBNBZ-QPJJXVBHSA-N					

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-dimethylbenzaldehyde $C_9H_{10}O$ [5779-93-1] UIFVCPMLQXKEEU-UHFFFAOYSA-N	1.2 2.1 7.6×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
3,4-dimethylbenzaldehyde $C_9H_{10}O$ [5973-71-7] POQJHLBMLVTHAU-UHFFFAOYSA-N	1.2 1.5 3.8		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
3,5-dimethylbenzaldehyde $C_9H_{10}O$ [5779-95-3] NBEFMISJJNGCIZ-UHFFFAOYSA-N	1.2 9.6×10^{-1} 2.0		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
2-naphthaldehyde $C_{11}H_8O$ [66-99-9] PJKVFARRVXDXAD-UHFFFAOYSA-N	6.0×10^{1}		Abraham et al. (2019)	Q	
cyclemax $C_{12}H_{16}O$ (4-(1-methylethyl)- benzenepropanal) [7775-00-0] RLEFOSDUWZYGOS-UHFFFAOYSA-N	7.8×10^{-1}		Dupeux et al. (2022)	Q	259
bourgeonal $C_{13}H_{18}O$ [18127-01-0] FZJUFJKVIYFBSY-UHFFFAOYSA-N	1.1		Dupeux et al. (2022)	Q	259
florhydral $C_{13}H_{18}O$ [125109-85-5] OHRBQTOZYGEWCJ-UHFFFAOYSA-N	4.9×10^{-1}		Dupeux et al. (2022)	Q	259
cyclamen aldehyde $C_{13}H_{18}O$ [103-95-7] ZFNVDHOSLNRHNN-UHFFFAOYSA-N	2.3×10^{-1}		Dupeux et al. (2022)	Q	259
mimosal $C_{13}H_{16}O$ (4-methyl-5-(4-methylphenyl)pent- 4-enal) [1226911-69-8] LBKHGAIELUNYML-ZRDIBKRKSA-N	4.9		Dupeux et al. (2022)	Q	259

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
lilial $C_{14}H_{20}O$ [80-54-6] SDQFDHOLCGWZPU-UHFFFAOYSA-N	5.7×10^{-1}		Dupeux et al. (2022)	Q	259
hivernal $C_{14}H_{18}O$ [300371-33-9] GEPCDOWRWODJEY-UHFFFAOYSA-N	2.2		Dupeux et al. (2022)	Q	259
silvial $C_{14}H_{20}O$ [6658-48-6] YLIXVKUWWOQREC-UHFFFAOYSA-N	2.9×10^{-1}		Dupeux et al. (2022)	Q	259
mefloral $C_{14}H_{20}O$ [62518-65-4] GLZRHVTZLDNUQP-UHFFFAOYSA-N	3.2×10^{-1}		Dupeux et al. (2022)	Q	259
nympheal $C_{14}H_{20}O$ (3-(4-isobutyl-2-methylphenyl)propanal) [1637294-12-2] UKZXPOJABTXLMK-UHFFFAOYSA-N	8.2×10^{-1}		Dupeux et al. (2022)	Q	259
hexyl cinnamic aldehyde $C_{15}H_{20}O$ [101-86-0] GUUHFMWKWLOQMM-UHFFFAOYSA-N	1.0		Dupeux et al. (2022)	Q	259
α-amyl cinnamaldehyde $C_{14}H_{18}O$ [122-40-7] HMKKIXGYKWDQSV-KAMYIIQDSA-N	1.3		HSDB (2015)	Q	447
MCM:HCOCH2CO3H $C_3H_4O_4$ CFPRXLWZTODTLN-UHFFFAOYSA-N	8.0×10^{4} 3.6×10^{3} 3.2×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:PROPALOOH $C_3H_6O_3$ UTLVMFCPERHVKU-UHFFFAOYSA-N	6.9×10^{3} 8.7×10^{1} 3.6×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:BUTALAOOH $C_4H_8O_3$ UBMPIIYSSVMXGT-UHFFFAOYSA-N	5.5×10^{3} 4.6×10^{1} 1.2×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:BUTALO2H $C_4H_8O_3$ HFNSAVKBHMZYBR-UHFFFAOYSA-N	5.5×10^{3} 2.7×10^{3} 8.7×10^{2}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C3MDIALOOH	3.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_4$	4.7×10^{3}		Wang et al. (2017)	Q	80, 239
WJWKLOFSCXWKQD-UHFFFAOYSA-N	7.3		Wang et al. (2017)	Q	80, 240
MCM:CHOC2CO3H	7.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_4$	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
ZCKJJZIUFVHIST-UHFFFAOYSA-N	1.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:IBUTALBO2H	5.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	3.6×10^{3}		Wang et al. (2017)	Q	80, 239
OSYMKIVGDGNGKG-UHFFFAOYSA-N	5.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:IBUTALO2H	3.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	1.8×10^{1}		Wang et al. (2017)	Q	80, 239
UINKREZTGVLFAU-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MALDALCO3H	2.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_4$	3.5×10^{4}		Wang et al. (2017)	Q	80, 239
QFBRACYMKXGFRM-UHFFFAOYSA-N	3.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PRPAL2CO3H	7.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_4$	2.3×10^{3}		Wang et al. (2017)	Q	80, 239
IGHWWGZEWMXWCB-UHFFFAOYSA-N	8.0		Wang et al. (2017)	Q	80, 240
MCM:C3EDIALOOH	2.7×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	2.1×10^{3}		Wang et al. (2017)	Q	80, 239
IOKXWRCVGKGMQG-UHFFFAOYSA-N	4.9		Wang et al. (2017)	Q	80, 240
MCM:C3M3CHOOOH	3.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	8.7×10^{2}		Wang et al. (2017)	Q	80, 239
FJYKIGXUSFRBER-UHFFFAOYSA-N	3.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C4CHOAOOH	4.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	3.0×10^{1}		Wang et al. (2017)	Q	80, 239
ZCMMOPXACREGKB-UHFFFAOYSA-N	6.3		Wang et al. (2017)	Q	80, 240
MCM:C4CHOBOOH	4.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	1.5×10^{3}		Wang et al. (2017)	Q	80, 239
JELNOURJPXUYRE-UHFFFAOYSA-N	3.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C4CODBCO3H	2.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_4$	4.2×10^{4}		Wang et al. (2017)	Q	80, 239
JLZDPUBRQDSTHL-UHFFFAOYSA-N	6.9×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C514OOH	4.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	2.0×10^{6}		Wang et al. (2017)	Q	80, 239
PUFIIBDSTKVRQR-UHFFFAOYSA-N	6.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C5DIALOOH	1.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_4$	7.3×10^{4}		Wang et al. (2017)	Q	80, 239
MJFLAVCETRHPDB-UHFFFAOYSA-N	3.0×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CHOC4OOH	4.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	5.3×10^{3}		Wang et al. (2017)	Q	80, 239
CTZAXNMAMSERLK-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CO1M22CO3H	4.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	8.0×10^{2}		Wang et al. (2017)	Q	80, 239
HHOOHNHNSGMLRV-UHFFFAOYSA-N	8.9		Wang et al. (2017)	Q	80, 240
MCM:IC4CHOAOOH	5.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	3.8×10^{1}		Wang et al. (2017)	Q	80, 239
MEJCTHPUJKQILI-UHFFFAOYSA-N	8.3		Wang et al. (2017)	Q	80, 240
MCM:MC3ODBCO3H	2.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_4$	3.9×10^{4}		Wang et al. (2017)	Q	80, 239
UTZOYJZISPOIDM-UHFFFAOYSA-N	3.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C522CO3H	1.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	8.0×10^{3}		Wang et al. (2017)	Q	80, 239
NCACXMVSAKPDND-UHFFFAOYSA-N	1.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C615OOH	2.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	2.2×10^{4}		Wang et al. (2017)	Q	80, 239
XHCYBISQWAKVQU-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C6DIALOOH	3.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	1.5×10^{6}		Wang et al. (2017)	Q	80, 239
UGGYJIUZOSPDSO-UHFFFAOYSA-N	5.4×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:CHOC4CO3H	4.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	3.7×10^{3}		Wang et al. (2017)	Q	80, 239
RHHSYYPMFOTTRH-UHFFFAOYSA-N	6.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO1C6OOH	3.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	3.4×10^{3}		Wang et al. (2017)	Q	80, 239
HEPNQRDDKATRCQ-UHFFFAOYSA-N	8.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C615CO3H	3.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	3.4×10^{5}		Wang et al. (2017)	Q	80, 239
DXQJLRIPGQOCBO-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C729OOH	7.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_3$	2.6×10^{3}		Wang et al. (2017)	Q	80, 239
PQESPNYRBXTFKD-UHFFFAOYSA-N	4.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C729CO3H	7.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	1.6×10^{3}		Wang et al. (2017)	Q	80, 239
MJXLYBJUYDBXAC-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C810OOH	1.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_4$	5.5×10^{5}		Wang et al. (2017)	Q	80, 239
YJCLQCSGAKCWEJ-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C822OOH	8.8×10^{3}	11000	Wieser et al. (2023)	Q	437
$C_8H_{14}O_3$	6.0×10^{3}		Wang et al. (2017)	Q	80, 238
XWYULULFGKWPMD-UHFFFAOYSA-N	2.8×10^{3}		Wang et al. (2017)	Q	80, 239
	1.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C830OOH	6.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_3$	4.4×10^{3}		Wang et al. (2017)	Q	80, 239
QPQAMUJVCCDVQB-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C831OOH	1.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_4$	3.0×10^{5}		Wang et al. (2017)	Q	80, 239
IGXVNESWPQHYEP-UHFFFAOYSA-N	3.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C89OOH	6.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_3$	4.4×10^{3}		Wang et al. (2017)	Q	80, 239
TYPKFPBYWMWINI-UHFFFAOYSA-N	8.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C822CO3H	1.7×10^{4}	14000	Wieser et al. (2023)	Q	437
$C_9H_{14}O_4$	7.3×10^{4}		Wang et al. (2017)	Q	80, 238
DRDXOQWGQPPQFG-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 239
	3.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C830CO3H	7.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	2.8×10^{3}		Wang et al. (2017)	Q	80, 239
YIGLTTCQERBPNX-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C89CO3H	7.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	2.9×10^{3}		Wang et al. (2017)	Q	80, 239
QJRQWHYQDGSSTJ-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C126OOH	7.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_3$	4.9×10^{3}		Wang et al. (2017)	Q	80, 239
KEVCPNVRIXMZTI-UHFFFAOYSA-N	1.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C126CO3H	8.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{20}O_4$	1.9×10^{3}		Wang et al. (2017)	Q	80, 239
OZAZBNTYEOZXRC-UHFFFAOYSA-N	2.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C136OOH	5.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_3$	4.3×10^{3}		Wang et al. (2017)	Q	80, 239
MAMVWZJYPZZMSJ-UHFFFAOYSA-N	4.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C136CO3H	6.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_4$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
JKRMUSIUVDAEPW-UHFFFAOYSA-N	7.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HCOCOHCO3H	2.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_3H_4O_5$	1.3×10^{4}		Wang et al. (2017)	Q	80, 239
DIZMXPJJIVKAJT-UHFFFAOYSA-N	6.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HOCHOCOOH	2.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_4$	1.3×10^{5}		Wang et al. (2017)	Q	80, 239
GWWSSJVARZQKFN-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:OCCOHCOOH	1.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_4$	5.9×10^{4}		Wang et al. (2017)	Q	80, 239
UFAXCNDNIIDPQE-UHFFFAOYSA-N	2.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C4OCCOHOOH	1.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	1.2×10^{5}		Wang et al. (2017)	Q	80, 239
JJIHBDXOHFOUDV-UHFFFAOYSA-N	7.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:COCCOHCOOH	2.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	2.0×10^{5}		Wang et al. (2017)	Q	80, 239
XTEYRSCVGRLIOG-UHFFFAOYSA-N	8.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:COHM2CO3H	1.7×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_5$	4.6×10^{3}		Wang et al. (2017)	Q	80, 239
AEAZUHMXWJBPCW-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HMACROOH	3.9×10^{10}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_5$	2.4×10^{8}		Wang et al. (2017)	Q	80, 239
AWITZWJPGUOCMB-UHFFFAOYSA-N	4.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:MACROHOOH	6.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	7.1×10^{4}		Wang et al. (2017)	Q	80, 239
HWQXXVVDRNBYQB-UHFFFAOYSA-N	6.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:MACROOH	1.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	7.6×10^{4}		Wang et al. (2017)	Q	80, 239
MOSGWPXPTZVSII-UHFFFAOYSA-N	5.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MALDIALOOH	1.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_5$	6.2×10^{6}		Wang et al. (2017)	Q	80, 239
MNYHDFHIZDEDLP-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:ALC4DOLOOH	1.6×10^{10}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_5$	3.8×10^{8}		Wang et al. (2017)	Q	80, 239
BTJWWKUWEVGVGA-UHFFFAOYSA-N	5.0×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C4MALOHOOH	5.6×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	6.6×10^{6}		Wang et al. (2017)	Q	80, 239
NJMKFLHNNBFYIH-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C57OOH	1.3×10^{10}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_5$	8.5×10^{7}		Wang et al. (2017)	Q	80, 239
VJGRRPOTERGJKF-UHFFFAOYSA-N	1.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C58OOH	1.9×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_5$	3.7×10^{8}		Wang et al. (2017)	Q	80, 239
MTCQYLXAFMKVMT-UHFFFAOYSA-N	3.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:CHOC4OHOOH	1.5×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	1.4×10^{6}		Wang et al. (2017)	Q	80, 239
LTZYUHWRVSINRM-UHFFFAOYSA-N	1.6×10^{5}		Wang et al. (2017)	Q	80, 240

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HIEB1OOH	3.7×10^{13}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_6$	1.6×10^{11}		Wang et al. (2017)	Q	80, 239
COFCBVJXHDFSHS-UHFFFAOYSA-N	6.5×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:HIEB2OOH	2.4×10^{13}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_6$	1.0×10^{11}		Wang et al. (2017)	Q	80, 239
PKIUCWJPHHVKPZ-UHFFFAOYSA-N	1.2×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:HOC4CHOOOH	1.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	6.9×10^{5}		Wang et al. (2017)	Q	80, 239
LRYOXTYJCQGVIC-UHFFFAOYSA-N	1.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:IEB2OOH	1.3×10^{10}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_5$	3.7×10^{8}		Wang et al. (2017)	Q	80, 239
MCOKLECUTPXNOW-UHFFFAOYSA-N	2.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C1H4C5CO3H	1.6×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	5.9×10^{7}		Wang et al. (2017)	Q	80, 239
DOEHHISPDHWTCR-UHFFFAOYSA-N	2.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C623OOH	2.8×10^{10}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_5$	7.4×10^{8}		Wang et al. (2017)	Q	80, 239
OGBKQGQRAMSXTF-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C67OOH	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	4.2×10^{5}		Wang et al. (2017)	Q	80, 239
ONTGLCVTLGTTQS-UHFFFAOYSA-N	9.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C68OOH	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	4.6×10^{5}		Wang et al. (2017)	Q	80, 239
ITDKDNQPTMKBIM-UHFFFAOYSA-N	3.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CO1H63OOH	1.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	1.8×10^{7}		Wang et al. (2017)	Q	80, 239
KJWILEAANBSBHN-UHFFFAOYSA-N	3.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C728OOH	5.3×10^{10}	18000	Wieser et al. (2023)	Q	437
$C_7H_{14}O_5$	2.1×10^{10}		Wang et al. (2017)	Q	80, 238
WJYXJQPIZCIBJO-UHFFFAOYSA-N	1.7×10^{9}		Wang et al. (2017)	Q	80, 239
	1.4×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C730OOH	6.1×10^{10}	18000	Wieser et al. (2023)	Q	437
$C_7H_{14}O_5$	2.1×10^{10}		Wang et al. (2017)	Q	80, 238
YXKHJQXHKYJCPI-UHFFFAOYSA-N	1.1×10^{10}		Wang et al. (2017)	Q	80, 239
	2.6×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C824OOH	8.4×10^{6}	15000	Wieser et al. (2023)	Q	437
$C_8H_{14}O_4$	1.9×10^{7}		Wang et al. (2017)	Q	80, 238
FGEKWAMEWUMQIL-UHFFFAOYSA-N	6.3×10^{5}		Wang et al. (2017)	Q	80, 239
	6.3×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A3.5: Aldehydes (RCHO) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C826OOH	6.3×10^{9}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_5$	5.1×10^{8}		Wang et al. (2017)	Q	80, 239
MATCTRFTDTXPPO-UHFFFAOYSA-N	1.7×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C127OOH	1.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_4$	1.9×10^{7}		Wang et al. (2017)	Q	80, 239
CZSOPCQUOGQYQQ-UHFFFAOYSA-N	2.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C1311OOH	1.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_4$	1.6×10^{7}		Wang et al. (2017)	Q	80, 239
GNGYVQPBVCXXTM-UHFFFAOYSA-N	1.2×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C1313OOH	6.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_5$	9.1×10^{8}		Wang et al. (2017)	Q	80, 239
ALNYAIDMJTUDIF-UHFFFAOYSA-N	1.9×10^{6}		Wang et al. (2017)	Q	80, 240

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A3.6 Ketones (RCOR)

Table A3.6: Ketones (RCOR)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
propanone	2.7×10^{-1}	5500	Burkholder et al. (2019)	L	
CH_3COCH_3	2.7×10^{-1}	5500	Burkholder et al. (2015)	L	
(acetone)	2.9×10^{-1}	5300	Brockbank (2013)	L	1, 476
[67-64-1]	2.7×10^{-1}	5500	Sander et al. (2011)	L	
CSCPPACGZOOCGX-UHFFFAOYSA-N	3.3×10^{-1}	5300	Poulain et al. (2010)	L	
	2.8×10^{-1}	5100	Sander et al. (2006)	L	
	2.6×10^{-1}	5700	Fogg and Sangster (2003)	L	
	2.8×10^{-1}	4800	Staudinger and Roberts (2001)	L	
	2.7×10^{-1}	5000	Plyasunov and Shock (2001)	L	
	3.0×10^{-1}	4600	Staudinger and Roberts (1996)	L	
	2.9×10^{-1}	5100	Poulain et al. (2010)	M	
	3.3×10^{-1}	4500	O'Farrell and Waghorne (2010)	M	
	2.6×10^{-1}	5400	Ji and Evans (2007)	M	
	2.4×10^{-1}	4200	Falabella et al. (2006)	M	11, 338
	2.6×10^{-1}	6400	Strekowski and George (2005)	M	
	2.4×10^{-1}		Straver and de Loos (2005)	M	
	2.4×10^{-1}	4300	Chai et al. (2005)	M	11
	2.7×10^{-1}		Nozière and Riemer (2003)	M	79
	1.0×10^{-1}		Ayuttaya et al. (2001)	M	340
	9.4×10^{-4}		Ayuttaya et al. (2001)	M	341
	5.3×10^{-1}		Ayuttaya et al. (2001)	M	342
	9.6×10^{-2}		Welke et al. (1998)	M	
	2.7×10^{-1}	5300	Benkelberg et al. (1995)	M	
	2.7×10^{-1}		Hoff et al. (1993)	M	
	1.7×10^{-1}		Yu (1992)	M	12
	3.2×10^{-1}	5800	Betterton (1991)	M	
	3.5×10^{-1}	3800	Zhou and Mopper (1990)	M	456
	1.2×10^{-1}		Guitart et al. (1989)	M	14
	1.4×10^{-1}		Hellmann (1987)	M	87
	2.5×10^{-1}	4800	Snider and Dawson (1985)	M	
	3.2×10^{-1}	5400	Schoene and Steinhanses (1985)	M	
	1.9×10^{-1}		Richon et al. (1985)	M	38
	2.6×10^{-1}	5100	Lichtenbelt and Schram (1985)	M	477
	2.0×10^{-1}	7800	Ioffe et al. (1984)	M	
	1.5×10^{-1}		Sato and Nakajima (1979a)	M	14
	2.5×10^{-1}		Vitenberg et al. (1975)	M	
	2.5×10^{-1}		Vitenberg et al. (1974)	M	
	3.2×10^{-1}		Vitenberg et al. (1974)	M	
	2.5×10^{-1}		Buttery et al. (1969)	M	
	3.1×10^{-1}		Nelson and Hoff (1968)	M	297
	2.8×10^{-1}		Burnett (1963)	M	
	1.8×10^{-2}		Abraham and Acree (2007)	V	
	2.6×10^{-1}		Hwang et al. (1992)	V	
	3.1×10^{-2}	3100	Djerki and Laub (1988)	V	
	2.4×10^{-1}		Rathbun and Tai (1982)	V	

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.1×10^{-2}		Hine and Weimar (1965)	R	
	3.0×10^{-1}		Butler and Ramchandani (1935)	R	
	2.5×10^{-1}	4900	Bagno et al. (1991)	T	473
	2.1×10^{-1}		Yaws (2003)	X	258
	2.2×10^{-1}	5000	Schaffer and Daubert (1969)	X	298
	3.0×10^{-2}	3300	Janini and Quaddora (1986)	X	298
	3.0×10^{-1}		Gaffney and Senum (1984)	X	389
	2.7×10^{-1}		Cabani et al. (1981)	C	
	6.1×10^{-1}		Dupeux et al. (2022)	Q	259
	2.6×10^{-1}		Hayer et al. (2022)	Q	20
	1.2×10^{-1}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	6.6×10^{-2}		Wang et al. (2017)	Q	80, 238
	4.3×10^{-1}		Wang et al. (2017)	Q	80, 239
	7.1×10^{-1}		Wang et al. (2017)	Q	80, 240
	2.5×10^{-1}		Li et al. (2014)	Q	241
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.4×10^{-1}		Hilal et al. (2008)	Q	
	4.0×10^{-1}		Modarresi et al. (2007)	Q	67
		5500	Kühne et al. (2005)	Q	
	2.5×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.5×10^{-1}		English and Carroll (2001)	Q	230, 231
	2.4×10^{-2}		Katritzky et al. (1998)	Q	
	2.1×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.9×10^{-1}		Suzuki et al. (1992)	Q	232
	2.5×10^{-1}		Taft et al. (1985)	Q	
	2.8×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	2.5×10^{-1}		Mackay et al. (2006c)	?	21
		5100	Kühne et al. (2005)	?	
	1.5×10^{-1}		Yaws (1999)	?	21
	1.8×10^{-1}		Yaws et al. (1998)	?	
	1.6×10^{-1}		Abraham and Weathersby (1994)	?	21
	2.3×10^{-1}		Yaws and Yang (1992)	?	21
	2.5×10^{-1}		Abraham et al. (1990)	?	
propanone-2-13C CH_3COCH_3 (acetone-2-13C) [3881-06-9] CSCPPACGZOOCGX-LBPDFUHNSA-N	3.1×10^{-1}	5300	Hiatt (2013)	M	
1-hydroxypropanone CH_3COCH_2OH (hydroxyacetone) [116-09-6] XLSMFKSTNGKWQX-UHFFFAOYSA-N	7.7×10^{1}		Lee and Zhou (1993)	C	87
	8.3		Wang et al. (2017)	Q	80, 238
	1.4×10^{2}		Wang et al. (2017)	Q	80, 239
	1.9×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
butanone	1.8×10^{-1}	5700	Burkholder et al. (2019)	L	
$C_2H_5COCH_3$	1.8×10^{-1}	5700	Burkholder et al. (2015)	L	
(methyl ethyl ketone; MEK)	1.8×10^{-1}	5600	Brockbank (2013)	L	1
[78-93-3]	1.8×10^{-1}	5700	Sander et al. (2011)	L	
ZWEHNKRNPOVVGH-UHFFFAOYSA-N	1.8×10^{-1}	5700	Sander et al. (2006)	L	
	1.9×10^{-1}	4600	Fogg and Sangster (2003)	L	
	1.8×10^{-1}	5400	Staudinger and Roberts (2001)	L	
	1.8×10^{-1}	5500	Plyasunov and Shock (2001)	L	
	2.0×10^{-1}	5000	Staudinger and Roberts (1996)	L	
	1.0×10^{-1}		Kim and Kim (2014)	M	
	9.5×10^{-2}		Helburn et al. (2008)	M	
	2.1×10^{-1}	5200	Ji and Evans (2007)	M	
	1.5×10^{-1}	4400	Falabella et al. (2006)	M	11, 338
	2.7×10^{-2}	12000	Strekowski and George (2005)	M	
	1.7×10^{-1}		Straver and de Loos (2005)	M	
	1.5×10^{-1}	4500	Chai et al. (2005)	M	11
			Cheng et al. (2004)	M	328
			Cheng et al. (2003)	M	328
	1.1×10^{-1}		Karl et al. (2003)	M	
	1.3×10^{-1}	4300	Hovorka et al. (2002)	M	11
	9.9×10^{-2}		van Ruth et al. (2002)	M	14
	1.0×10^{-1}		van Ruth and Villeneuve (2002)	M	14, 361
	9.0×10^{-2}		van Ruth et al. (2001)	M	14
	1.6×10^{-1}		Kim et al. (2000)	M	
	1.6×10^{-1}		Welke et al. (1998)	M	
	1.9×10^{-1}		Chaintreau et al. (1995)	M	
	1.4×10^{-1}	4700	Ettre et al. (1993)	M	11
	1.9×10^{-1}	5000	Zhou and Mopper (1990)	M	456
	6.8×10^{-2}	-5100	Ashworth et al. (1988)	M	33, 278
	1.3×10^{-1}		Hellmann (1987)	M	87
	1.8×10^{-1}		Park et al. (1987)	M	
	1.7×10^{-1}	5700	Snider and Dawson (1985)	M	
	1.4×10^{-1}		Hawthorne et al. (1985)	M	
	1.2×10^{-1}		Richon et al. (1985)	M	38
	3.2×10^{-1}		Ioffe et al. (1984)	M	80
	1.0×10^{-1}		Friant and Suffet (1979)	M	38
	9.8×10^{-2}		Sato and Nakajima (1979a)	M	14
	1.8×10^{-1}		Vitenberg et al. (1975)	M	
	1.1×10^{-1}		Vitenberg et al. (1974)	M	
	1.9×10^{-1}		Rohrschneider (1973)	M	
	2.1×10^{-1}		Buttery et al. (1969)	M	
	1.1×10^{-2}		Abraham and Acree (2007)	V	
	2.8×10^{-1}		Mackay et al. (2006c)	V	
	2.8×10^{-1}		Mackay et al. (1995)	V	
	2.6×10^{-1}		Hwang et al. (1992)	V	
	8.6×10^{-2}	3700	Djerki and Laub (1988)	V	
	1.6×10^{-1}		Rathbun and Tai (1982)	V	

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.1×10^{-2}		Hine and Weimar (1965)	R	
	2.1×10^{-1}	5500	Bagno et al. (1991)	T	473
		5500	Della Gatta et al. (1981)	T	
	7.6×10^{-2}		Yaws (2003)	X	258
	7.6×10^{-2}		Yaws (2003)	X	237
	7.1×10^{-2}	5800	Janini and Quaddora (1986)	X	298
	2.3×10^{-1}		Mackay et al. (1995)	C	
	4.1×10^{-1}		Harrison et al. (1993)	C	
	1.9×10^{-1}		Cabani et al. (1981)	C	
	2.3×10^{-1}		Dupeux et al. (2022)	Q	259
	1.8×10^{-1}		Hayer et al. (2022)	Q	20
	1.6×10^{-1}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	5.1×10^{-2}		Wang et al. (2017)	Q	80, 238
	2.5×10^{-1}		Wang et al. (2017)	Q	80, 239
	3.6×10^{-1}		Wang et al. (2017)	Q	80, 240
	2.1×10^{-1}		Li et al. (2014)	Q	241
	2.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	8.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
	1.3×10^{-1}		Hilal et al. (2008)	Q	
	3.0×10^{-1}		Modarresi et al. (2007)	Q	67
		5900	Kühne et al. (2005)	Q	
	1.7×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	1.4×10^{-1}		English and Carroll (2001)	Q	230, 231
	3.0×10^{-2}		Katritzky et al. (1998)	Q	
	1.6×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.5×10^{-1}		Suzuki et al. (1992)	Q	232
	1.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	1.0×10^{-1}		Mackay et al. (2006c)	?	21
		5300	Kühne et al. (2005)	?	
	3.3×10^{-1}		Yaws (1999)	?	21
	1.5×10^{-1}		Yaws et al. (1998)	?	
	1.0×10^{-1}		Abraham and Weathersby (1994)	?	21
	3.1×10^{-1}		Betterton (1991)	?	
	2.1×10^{-1}		Abraham et al. (1990)	?	
butanone-1,1,1,3,3-d5 $C_2H_5COCH_3$ (methyl ethyl ketone-d5; MEK-d5) [24313-50-6] ZWEHNKRNPOVVGH-PDWRLMEDSA-N	3.7×10^{-1}	8200	Hiatt (2013)	M	

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
2-pentanone	1.3×10^{-1}	6000	Brockbank (2013)	L	1
$C_3H_7COCH_3$	1.3×10^{-1}	5900	Plyasunov and Shock (2001)	L	
[107-87-9]	1.3×10^{-1}	5900	Hovorka et al. (2019)	M	
XNLICIUVMPYHGG-UHFFFAOYSA-N	1.6×10^{-1}	5700	Ji and Evans (2007)	M	
	1.0×10^{-1}	4600	Falabella et al. (2006)	M	11, 338
	8.6×10^{-2}		Straver and de Loos (2005)	M	
	1.0×10^{-1}	4800	Chai et al. (2005)	M	11
	1.1×10^{-1}		Kim et al. (2000)	M	
	1.2×10^{-1}		Shiu and Mackay (1997)	M	
	9.0×10^{-2}		Hawthorne et al. (1985)	M	
	6.4×10^{-2}		Sato and Nakajima (1979a)	M	14
	1.7×10^{-1}		Vitenberg et al. (1974)	M	
	1.1×10^{-1}		Vitenberg et al. (1974)	M	478
	1.6×10^{-1}		Buttery et al. (1969)	M	
	9.2×10^{-2}		Nelson and Hoff (1968)	M	297
	1.5×10^{-1}		Mackay et al. (2006c)	V	
	5.9×10^{-2}		Philippe et al. (2003)	V	14
	1.5×10^{-1}		Shiu and Mackay (1997)	V	
	1.5×10^{-1}		Mackay et al. (1995)	V	
	2.4×10^{-1}	4300	Djerki and Laub (1988)	V	
	2.6×10^{-1}		Rathbun and Tai (1982)	V	
	3.1×10^{-1}		Amoore and Buttery (1978)	V	
		5900	Della Gatta et al. (1981)	T	
	1.4×10^{-1}		Yaws (2003)	X	258
	9.1×10^{-2}	4600	Janini and Quaddora (1986)	X	298
	1.7×10^{-1}		Mackay et al. (1995)	C	
	2.5×10^{-1}		Dupeux et al. (2022)	Q	259
	8.7×10^{-2}		Hayer et al. (2022)	Q	20
	2.2×10^{-1}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	299
	4.3×10^{-2}		Wang et al. (2017)	Q	80, 238
	1.6×10^{-1}		Wang et al. (2017)	Q	80, 239
	1.8×10^{-1}		Wang et al. (2017)	Q	80, 240
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.0×10^{-1}		Hilal et al. (2008)	Q	
	1.7×10^{-1}		Modarresi et al. (2007)	Q	67
		6200	Kühne et al. (2005)	Q	
	1.4×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	1.9×10^{-2}		Katritzky et al. (1998)	Q	
	1.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.2×10^{-1}		Russell et al. (1992)	Q	279
	1.2×10^{-1}		Suzuki et al. (1992)	Q	232
	1.2×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	1.6×10^{-1}		Mackay et al. (2006c)	?	21
		6500	Kühne et al. (2005)	?	

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	1.4×10^{-1}		Yaws (1999)	?	21
	1.3×10^{-1}		Yaws et al. (1998)	?	
	6.7×10^{-2}		Abraham and Weathersby (1994)	?	21
	1.5×10^{-1}		Abraham et al. (1990)	?	
	3.1×10^{-1}		Mackay and Yeun (1983)	?	
3-pentanone	8.9×10^{-2}	5800	Brockbank (2013)	L	1, 479
$C_2H_5COC_2H_5$	1.1×10^{-1}	6000	Plyasunov and Shock (2001)	L	
(diethyl ketone)	1.1×10^{-1}	5900	Hovorka et al. (2019)	M	
[96-22-0]	2.1×10^{-1}		O'Farrell and Waghorne (2010)	M	
FDPIMTJIUBPUKL-UHFFFAOYSA-N	1.6×10^{-1}	5600	Ji and Evans (2007)	M	
	7.0×10^{-2}		Sato and Nakajima (1979a)	M	14
	9.7×10^{-5}		Saylor et al. (1938)	M	38
	8.4×10^{-2}		Mackay et al. (2006c)	V	
	1.2×10^{-1}		Mackay et al. (1995)	V	
	8.4×10^{-2}		Mackay et al. (1995)	V	
	2.8×10^{-1}		Rathbun and Tai (1982)	V	
	1.3×10^{-1}	6000	Bagno et al. (1991)	T	473
		6000	Della Gatta et al. (1981)	T	
	8.2×10^{-2}		Yaws (2003)	X	258
	8.2×10^{-2}		Yaws (2003)	X	237
	2.0×10^{-1}	9200	Janini and Quaddora (1986)	X	298
	1.1×10^{-1}		Howard (1993)	X	412
	1.3×10^{-1}		Cabani et al. (1981)	C	
	8.6×10^{-2}		Dupeux et al. (2022)	Q	259
	2.2×10^{-1}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	4.3×10^{-2}		Wang et al. (2017)	Q	80, 238
	1.3×10^{-1}		Wang et al. (2017)	Q	80, 239
	6.6×10^{-2}		Wang et al. (2017)	Q	80, 240
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	7.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
	9.2×10^{-2}		Hilal et al. (2008)	Q	
	1.9×10^{-1}		Modarresi et al. (2007)	Q	67
		6200	Kühne et al. (2005)	Q	
	1.4×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	4.3×10^{-2}		Yao et al. (2002)	Q	229
	1.1×10^{-1}		English and Carroll (2001)	Q	230, 274
	2.7×10^{-2}		Katritzky et al. (1998)	Q	
	1.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	2.0×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		6800	Kühne et al. (2005)	?	
	8.2×10^{-2}		Yaws (1999)	?	21
	1.2×10^{-1}		Yaws et al. (1998)	?	
	7.3×10^{-2}		Abraham and Weathersby (1994)	?	21
	1.3×10^{-1}		Abraham et al. (1990)	?	

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-cyclopropyl-ethanone	9.5×10^{-1}	5900	Bagno et al. (1991)	T	473
C_5H_8O		5900	Della Gatta et al. (1981)	T	
(cyclopropyl methyl ketone)	2.2×10^{-1}		Keshavarz et al. (2022)	Q	
[765-43-5]	9.9×10^{-2}		Duchowicz et al. (2020)	Q	299
HVCFCNAITDHQFX-UHFFFAOYSA-N	4.8×10^{-1}		Hilal et al. (2008)	Q	
	5.2×10^{-1}		Modarresi et al. (2007)	Q	67
	3.1×10^{-1}		English and Carroll (2001)	Q	230, 274
	6.4×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	9.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
3-methyl-2-butanone	1.1×10^{-1}	5800	Brockbank (2013)	L	1
$C_5H_{10}O$	9.1×10^{-2}	5700	Plyasunov and Shock (2001)	L	
(isopropyl methyl ketone)	9.3×10^{-2}	5600	Hovorka et al. (2019)	M	
[563-80-4]	1.0×10^{-1}		Duchowicz et al. (2020)	V	186
SYBYTAAJFKOIEJ-UHFFFAOYSA-N	8.7×10^{-2}		HSDB (2015)	V	
	9.6×10^{-2}		Cabani et al. (1981)	V	
	9.0×10^{-2}	5700	Bagno et al. (1991)	T	473
		5700	Della Gatta et al. (1981)	T	
	1.3×10^{-2}		Duchowicz et al. (2020)	Q	
	4.9×10^{-2}		Wang et al. (2017)	Q	80, 238
	1.3×10^{-1}		Wang et al. (2017)	Q	80, 239
	2.5×10^{-1}		Wang et al. (2017)	Q	80, 240
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	8.4×10^{-2}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	67
		5300	Kühne et al. (2005)	Q	
	9.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	6.4×10^{-2}		English and Carroll (2001)	Q	230, 231
	2.5×10^{-2}		Katritzky et al. (1998)	Q	
	1.0×10^{-1}		Nirmalakhandan et al. (1997)	Q	
		7200	Kühne et al. (2005)	?	
	1.1×10^{-1}		Yaws (1999)	?	21
	1.1×10^{-1}		Yaws et al. (1998)	?	
	9.7×10^{-2}		Abraham et al. (1990)	?	
cyclopentanone	1.2	5800	Brockbank (2013)	L	1
C_5H_8O	2.8		O'Farrell and Waghorne (2010)	M	
[120-92-3]	8.2×10^{-1}	4900	Hovorka et al. (2002)	M	11
BGTOWKSIORTVQH-UHFFFAOYSA-N	8.2×10^{-1}		Hawthorne et al. (1985)	M	
	7.4×10^{-1}		Keshavarz et al. (2022)	Q	
	2.5×10^{-1}		Duchowicz et al. (2020)	Q	299
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.1		Hilal et al. (2008)	Q	
	4.7×10^{-1}		Modarresi et al. (2007)	Q	67

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
		5800	Kühne et al. (2005)	Q	
	1.0		Yaffe et al. (2003)	Q	248, 249
	7.5×10^{-1}		English and Carroll (2001)	Q	230, 260
	6.9×10^{-2}		Katritzky et al. (1998)	Q	
	7.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	9.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		5600	Kühne et al. (2005)	?	
	1.1		Abraham et al. (1990)	?	
2-hexanone $C_6H_{12}O$ [591-78-6] QQZOPKMRPOGIEB-UHFFFAOYSA-N	1.1×10^{-1}	6500	Brockbank (2013)	L	1
	9.8×10^{-2}	6300	Plyasunov and Shock (2001)	L	
	9.9×10^{-2}	6300	Hovorka et al. (2019)	M	
	1.5×10^{-1}	8600	Hiatt (2013)	M	
	7.9×10^{-2}	4800	Falabella et al. (2006)	M	11, 338
	1.1×10^{-1}		Straver and de Loos (2005)	M	
	8.6×10^{-2}	5100	Chai et al. (2005)	M	11
	4.3×10^{-2}		Sato and Nakajima (1979a)	M	14
	1.1×10^{-1}		Duchowicz et al. (2020)	V	186
	1.1×10^{-1}		HSDB (2015)	V	
	1.1×10^{-1}		Mackay et al. (2006c)	V	
	1.1×10^{-1}		Mackay et al. (1995)	V	
	1.0×10^{-1}		Meylan and Howard (1991)	V	
	6.5×10^{-1}	4900	Djerki and Laub (1988)	V	
	1.0×10^{-1}		Cabani et al. (1981)	V	
		6200	Della Gatta et al. (1981)	T	
	1.2×10^{-1}		Yaws (2003)	X	258
	1.0×10^{-1}		Howard (1993)	X	412
	1.7×10^{-1}		Dupeux et al. (2022)	Q	259
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	3.8×10^{-2}		Wang et al. (2017)	Q	80, 238
	1.1×10^{-1}		Wang et al. (2017)	Q	80, 239
	1.7×10^{-1}		Wang et al. (2017)	Q	80, 240
	8.2×10^{-2}		Hilal et al. (2008)	Q	
	1.5×10^{-1}		Modarresi et al. (2007)	Q	67
		6600	Kühne et al. (2005)	Q	
	7.9×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	8.4×10^{-2}		English and Carroll (2001)	Q	230, 231
	2.4×10^{-2}		Katritzky et al. (1998)	Q	
	9.2×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	8.5×10^{-2}		Meylan and Howard (1991)	Q	
		6200	Kühne et al. (2005)	?	
	1.2×10^{-1}		Yaws (1999)	?	21
	1.2×10^{-1}		Yaws et al. (1998)	?	
	4.5×10^{-2}		Abraham and Weathersby (1994)	?	21
	1.0×10^{-1}		Abraham et al. (1990)	?	

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-hexanone-1,1,1,3,3-d5 $C_6H_{12}O$ [4840-82-8] QQZOPKMRPOGIEB-ZTIZGVCASA-N	1.7×10^{-1}	9000	Hiatt (2013)	M	
3-hexanone $C_6H_{12}O$ [589-38-8] PFCHFHIRKBAQGU-UHFFFAOYSA-N	7.9×10^{-2}	7100	Brockbank (2013)	L	1
	7.5×10^{-2}		Plyasunov and Shock (2001)	L	
	7.6×10^{-2}	6400	Hovorka et al. (2019)	M	
			Dewulf et al. (1999)	M	362
	7.9×10^{-2}		Duchowicz et al. (2020)	V	186
	8.0×10^{-2}		Yaws (2003)	X	237
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	3.8×10^{-2}		Wang et al. (2017)	Q	80, 238
	8.9×10^{-2}		Wang et al. (2017)	Q	80, 239
	1.5×10^{-1}		Wang et al. (2017)	Q	80, 240
	6.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
	6.9×10^{-2}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Modarresi et al. (2007)	Q	67
		6600	Kühne et al. (2005)	Q	
	7.9×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.1×10^{-2}		Katritzky et al. (1998)	Q	
		5800	Kühne et al. (2005)	?	
	8.0×10^{-2}		Yaws (1999)	?	21
	8.0×10^{-2}		Yaws et al. (1998)	?	
3-methyl-2-pentanone $C_6H_{12}O$ [565-61-7] UIHCLUNTQKBZGK-UHFFFAOYSA-N	8.4×10^{-2}		Plyasunov and Shock (2001)	L	
	7.9×10^{-2}	6000	Hovorka et al. (2019)	M	
	1.3×10^{-1}		Duchowicz et al. (2020)	V	186
	1.3×10^{-2}		Duchowicz et al. (2020)	Q	
	4.0×10^{-2}		Wang et al. (2017)	Q	80, 238
	1.1×10^{-1}		Wang et al. (2017)	Q	80, 239
	1.8×10^{-1}		Wang et al. (2017)	Q	80, 240
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	7.3×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-1}		Modarresi et al. (2007)	Q	67
	9.6×10^{-2}		Yaws et al. (1998)	?	
4-methyl-2-pentanone $(CH_3)_2CHCH_2COCH_3$ (methyl isobutyl ketone; MIBK) [108-10-1] NTIZESTWPVYFNL-UHFFFAOYSA-N	6.9×10^{-2}	6200	Brockbank (2013)	L	1
	6.9×10^{-2}	6000	Plyasunov and Shock (2001)	L	
	6.5×10^{-2}	6000	Hovorka et al. (2019)	M	
	3.9×10^{-2}		Kim and Kim (2014)	M	
	1.0×10^{-1}	8700	Hiatt (2013)	M	
	3.9×10^{-2}		Kim et al. (2000)	M	
	4.7×10^{-2}		Welke et al. (1998)	M	
	4.3×10^{-2}	4600	Kolb et al. (1992)	M	277
	2.2×10^{-2}	110	Ashworth et al. (1988)	M	42, 278
	6.5×10^{-2}		Hellmann (1987)	M	87

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.1×10^{-2}		Sato and Nakajima (1979a)	M	14
	7.2×10^{-2}		Duchowicz et al. (2020)	V	186
	7.0×10^{-2}		HSDB (2015)	V	
	6.5×10^{-2}		Mackay et al. (2006c)	V	
	6.5×10^{-2}		Mackay et al. (1995)	V	
	7.2×10^{-2}		Hwang et al. (1992)	V	
	1.4×10^{-1}		Rathbun and Tai (1982)	V	
	7.1×10^{-2}		Cabani et al. (1981)	V	
	7.3×10^{-2}		Yaws (2003)	X	258
	1.1×10^{-1}		Howard (1990)	X	412
	1.4×10^{-1}		Dupeux et al. (2022)	Q	259
	1.3×10^{-2}		Duchowicz et al. (2020)	Q	
	4.0×10^{-2}		Wang et al. (2017)	Q	80, 238
	1.3×10^{-1}		Wang et al. (2017)	Q	80, 239
	2.1×10^{-1}		Wang et al. (2017)	Q	80, 240
	8.8×10^{-2}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Modarresi et al. (2007)	Q	67
		6600	Kühne et al. (2005)	Q	
	7.3×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	5.1×10^{-2}		English and Carroll (2001)	Q	230, 260
	1.7×10^{-2}		Katritzky et al. (1998)	Q	
	7.9×10^{-2}		Nirmalakhandan et al. (1997)	Q	
		5700	Kühne et al. (2005)	?	
	7.3×10^{-2}		Yaws (1999)	?	21
	7.2×10^{-2}		Yaws et al. (1998)	?	
	3.2×10^{-2}		Abraham and Weathersby (1994)	?	21
	3.0×10^{-1}		Betterton (1991)	?	
	7.0×10^{-2}		Abraham et al. (1990)	?	
2-methyl-3-pentanone	5.3×10^{-2}		Plyasunov and Shock (2001)	L	
$C_6H_{12}O$	5.2×10^{-2}	6100	Hovorka et al. (2019)	M	
[565-69-5]	6.4×10^{-2}		Duchowicz et al. (2020)	V	186
HYTRYEXINDDXJK-UHFFFAOYSA-N	1.3×10^{-2}		Duchowicz et al. (2020)	Q	
	4.0×10^{-2}		Wang et al. (2017)	Q	80, 238
	9.3×10^{-2}		Wang et al. (2017)	Q	80, 239
	1.1×10^{-1}		Wang et al. (2017)	Q	80, 240
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.5×10^{-2}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Modarresi et al. (2007)	Q	67
	9.7×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	2.3×10^{-2}		Katritzky et al. (1998)	Q	
	6.4×10^{-2}		Yaws et al. (1998)	?	

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3-dimethyl-2-butanone	4.3×10^{-2}	5800	Brockbank (2013)	L	1
$C_6H_{12}O$	4.5×10^{-2}	5700	Plyasunov and Shock (2001)	L	
(*tert*-butyl methyl ketone)	4.3×10^{-2}	5700	Hovorka et al. (2019)	M	
[75-97-8]	4.5×10^{-2}		Duchowicz et al. (2020)	V	186
PJGSXYOJTGTZAV-UHFFFAOYSA-N	4.5×10^{-2}		HSDB (2015)	V	
	7.6×10^{-2}	6000	Bagno et al. (1991)	T	473
		6000	Della Gatta et al. (1981)	T	
	5.5×10^{-3}		Duchowicz et al. (2020)	Q	
	2.8×10^{-2}		Wang et al. (2017)	Q	80, 238
	7.1×10^{-2}		Wang et al. (2017)	Q	80, 239
	1.8×10^{-1}		Wang et al. (2017)	Q	80, 240
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.7×10^{-2}		Hilal et al. (2008)	Q	
	2.8×10^{-1}		Modarresi et al. (2007)	Q	67
		5700	Kühne et al. (2005)	Q	
	7.9×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	4.5×10^{-2}		English and Carroll (2001)	Q	230, 231
	2.7×10^{-2}		Katritzky et al. (1998)	Q	
	7.9×10^{-2}		Nirmalakhandan et al. (1997)	Q	
		5400	Kühne et al. (2005)	?	
	6.4×10^{-2}		Yaws et al. (1998)	?	
cyclohexanone	1.5	6400	Brockbank (2013)	L	1
$C_6H_{10}O$	8.6×10^{-1}	5100	Hovorka et al. (2002)	M	11
[108-94-1]	8.2×10^{-1}		Hawthorne et al. (1985)	M	
JHIVVAPYMSGYDF-UHFFFAOYSA-N	1.1		HSDB (2015)	V	
	3.8×10^{-1}		Mackay et al. (2006c)	V	
	3.8×10^{-1}		Mackay et al. (1995)	V	
	4.4×10^{-1}		Meylan and Howard (1991)	V	
	2.2		Yaws (2003)	X	258
	2.6		Dupeux et al. (2022)	Q	259
	1.0		Keshavarz et al. (2022)	Q	
	2.5×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.0×10^{-1}		Wang et al. (2017)	Q	80, 238
	2.0		Wang et al. (2017)	Q	80, 239
	5.9		Wang et al. (2017)	Q	80, 240
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.0		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	67
		6200	Kühne et al. (2005)	Q	
	1.2		Yaffe et al. (2003)	Q	248, 249
	9.0×10^{-1}		English and Carroll (2001)	Q	230, 231
	6.2×10^{-2}		Katritzky et al. (1998)	Q	
	5.6×10^{-1}		Nirmalakhandan et al. (1997)	Q	

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	1.9×10^{-1}		Meylan and Howard (1991)	Q	
	1.1		Duchowicz et al. (2020)	?	185, 21
		6300	Kühne et al. (2005)	?	
	1.8		Yaws (1999)	?	21
	1.6		Abraham et al. (1990)	?	
2-heptanone	6.8×10^{-2}	6800	Brockbank (2013)	L	1
$C_7H_{14}O$	7.2×10^{-2}	6800	Plyasunov and Shock (2001)	L	
[110-43-0]	5.9×10^{-2}	5300	Falabella et al. (2006)	M	11, 338
CATSNJVOTSVZJV-UHFFFAOYSA-N	6.8×10^{-2}	5700	Chai et al. (2005)	M	11
	3.9×10^{-2}		van Ruth et al. (2002)	M	14
	4.1×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 361
	2.5×10^{-2}		van Ruth et al. (2001)	M	14
	6.2×10^{-2}		Kim et al. (2000)	M	
	5.8×10^{-2}		Shiu and Mackay (1997)	M	
	3.7×10^{-2}		Sato and Nakajima (1979a)	M	14
	6.8×10^{-2}		Buttery et al. (1969)	M	
	7.5×10^{-2}		Mackay et al. (2006c)	V	
	7.5×10^{-2}		Shiu and Mackay (1997)	V	
	7.5×10^{-2}		Mackay et al. (1995)	V	
	1.8	5600	Djerki and Laub (1988)	V	
	1.7×10^{-1}		Rathbun and Tai (1982)	V	
	7.5×10^{-2}		Yaws (2003)	X	258
	7.4×10^{-2}		Yaws (2003)	X	237
	3.5×10^{-1}	4500	Janini and Quaddora (1986)	X	298
	1.5×10^{-1}		Dupeux et al. (2022)	Q	259
	5.3×10^{-2}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	184
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	5.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
	6.2×10^{-2}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	67
		6900	Kühne et al. (2005)	Q	
	1.2×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	6.5×10^{-2}		English and Carroll (2001)	Q	230, 274
	2.3×10^{-2}		Katritzky et al. (1998)	Q	
	7.2×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	6.2×10^{-2}		Russell et al. (1992)	Q	279
	6.9×10^{-2}		Suzuki et al. (1992)	Q	232
	5.8×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	6.8×10^{-2}		Mackay et al. (2006c)	?	21
		6900	Kühne et al. (2005)	?	
	7.5×10^{-2}		Yaws (1999)	?	21
	7.5×10^{-2}		Yaws et al. (1998)	?	
	3.9×10^{-2}		Abraham and Weathersby (1994)	?	21
	6.9×10^{-2}		Abraham et al. (1990)	?	

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^{-1}		Mackay and Yeun (1983)	?	
3-heptanone	7.2×10^{-2}	7000	Brockbank (2013)	L	1
$C_7H_{14}O$	1.1×10^{-1}		HSDB (2015)	V	
[106-35-4]	4.9×10^{-2}		Yaws (2003)	X	258
NGAZZOYFWWSOGK-UHFFFAOYSA-N	5.0×10^{-2}		Yaws (2003)	X	237
	7.3×10^{-2}		Dupeux et al. (2022)	Q	259
	3.1×10^{-2}		Wang et al. (2017)	Q	80, 238
	6.0×10^{-2}		Wang et al. (2017)	Q	80, 239
	1.4×10^{-1}		Wang et al. (2017)	Q	80, 240
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	5.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
	1.3×10^{-1}		Modarresi et al. (2007)	Q	67
		6900	Kühne et al. (2005)	Q	
	1.2×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	1.4×10^{-2}		Katritzky et al. (1998)	Q	
		6000	Kühne et al. (2005)	?	
	2.4×10^{-2}		Yaws et al. (1998)	?	
4-heptanone	5.1×10^{-2}	6800	Brockbank (2013)	L	1, 480
$C_7H_{14}O$	6.1×10^{-2}	7000	Plyasunov and Shock (2001)	L	
[123-19-3]	1.8×10^{-1}		Duchowicz et al. (2020)	V	186
HCFAJYNVAYBARA-UHFFFAOYSA-N	4.1×10^{-2}		HSDB (2015)	V	
	5.6×10^{-2}		Cabani et al. (1981)	V	
	3.3×10^{-2}		Yaws (2003)	X	258
	3.3×10^{-2}		Yaws (2003)	X	237
	3.8×10^{-2}		Dupeux et al. (2022)	Q	259
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	5.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
	4.8×10^{-2}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	67
		6900	Kühne et al. (2005)	Q	
	5.8×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	6.5×10^{-2}		English and Carroll (2001)	Q	230, 231
	1.8×10^{-2}		Katritzky et al. (1998)	Q	
	7.7×10^{-2}		Nirmalakhandan et al. (1997)	Q	
		7800	Kühne et al. (2005)	?	
	2.3×10^{-2}		Yaws et al. (1998)	?	38
	5.6×10^{-2}		Abraham et al. (1990)	?	

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methyl-2-hexanone	2.8×10^{-2}		Yaws (2003)	X	237
$C_7H_{14}O$	4.0×10^{-3}		Gharagheizi et al. (2012)	Q	
[2550-21-2]	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
GYWYASONLSQZBB-UHFFFAOYSA-N	3.2×10^{-2}		Yaws et al. (1998)	?	
4-methyl-2-hexanone	4.9×10^{-2}		Yaws (2003)	X	237
$C_7H_{14}O$	3.6×10^{-2}		Wang et al. (2017)	Q	80, 238
[105-42-0]	9.3×10^{-2}		Wang et al. (2017)	Q	80, 239
XUPXMIAWKPTZLZ-UHFFFAOYSA-N	2.1×10^{-1}		Wang et al. (2017)	Q	80, 240
	4.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
	3.3×10^{-2}		Yaws et al. (1998)	?	
5-methyl-2-hexanone	6.4×10^{-2}	6800	Brockbank (2013)	L	1
$C_7H_{14}O$	6.2×10^{-2}		Duchowicz et al. (2020)	V	186
[110-12-3]	6.2×10^{-2}		HSDB (2015)	V	
FFWSICBKRCICMR-UHFFFAOYSA-N	4.1×10^{-2}		Yaws (2003)	X	237
	1.3×10^{-2}		Duchowicz et al. (2020)	Q	
	3.6×10^{-2}		Wang et al. (2017)	Q	80, 238
	1.1×10^{-1}		Wang et al. (2017)	Q	80, 239
	3.8×10^{-1}		Wang et al. (2017)	Q	80, 240
	4.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
	7.7×10^{-2}		Hilal et al. (2008)	Q	
	1.1×10^{-1}		Modarresi et al. (2007)	Q	67
		6900	Kühne et al. (2005)	Q	
	7.3×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.2×10^{-2}		Katritzky et al. (1998)	Q	
		7600	Kühne et al. (2005)	?	
	2.7×10^{-2}		Yaws et al. (1998)	?	
2-methyl-3-hexanone	4.9×10^{-2}		Yaws (2003)	X	237
$C_7H_{14}O$	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
[7379-12-6]	4.1×10^{-2}		Yaws et al. (1998)	?	
HIGGFWFRAWSMBR-UHFFFAOYSA-N					
4-methyl-3-hexanone	3.1×10^{-2}		Yaws (2003)	X	237
$C_7H_{14}O$	3.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
[17042-16-9]	3.7×10^{-2}		Yaws et al. (1998)	?	
ULPMRIXXHGUZFA-UHFFFAOYSA-N					
5-methyl-3-hexanone	3.1×10^{-2}		Yaws (2003)	X	237
$C_7H_{14}O$	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
[623-56-3]	3.7×10^{-2}		Yaws et al. (1998)	?	
DXVYLFHTJZWTRF-UHFFFAOYSA-N					
3-ethyl-2-pentanone	2.9×10^{-2}		Yaws (2003)	X	237
$C_7H_{14}O$	3.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
[6137-03-7]	3.4×10^{-2}		Yaws et al. (1998)	?	
GSNKRSKIWFBWEG-UHFFFAOYSA-N					

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3-dimethyl-2-pentanone	3.1×10^{-2}		Yaws (2003)	X	237
$C_7H_{14}O$	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
[20669-04-9]	4.5×10^{-2}		Yaws et al. (1998)	?	
QSHJLBQLQVSEFV-UHFFFAOYSA-N					
3,4-dimethyl-2-pentanone	3.2×10^{-2}		Yaws (2003)	X	237
$C_7H_{14}O$	3.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
[565-78-6]	4.3×10^{-2}		Yaws et al. (1998)	?	
QXHRQZNDMYRDPA-UHFFFAOYSA-N					
4,4-dimethyl-2-pentanone	3.6×10^{-2}		Yaws (2003)	X	237
$C_7H_{14}O$	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
[590-50-1]	5.5×10^{-2}		Yaws et al. (1998)	?	
AZASWMGVGQEVCS-UHFFFAOYSA-N					
2,2-dimethyl-3-pentanone	3.6×10^{-2}		Yaws (2003)	X	237
$C_7H_{14}O$	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
[564-04-5]	5.5×10^{-2}		Yaws et al. (1998)	?	
VLNUTKMHYLQCQB-UHFFFAOYSA-N					
2,4-dimethyl-3-pentanone	2.3×10^{-2}	6100	Brockbank (2013)	L	1
$C_7H_{14}O$	2.4×10^{-2}	6500	Plyasunov and Shock (2001)	L	
(diisopropyl ketone)	2.8×10^{-2}		Duchowicz et al. (2020)	V	186
[565-80-0]	4.1×10^{-2}		Cabani et al. (1981)	V	
HXVNBWAKAOHACI-UHFFFAOYSA-N	9.5×10^{-1}	6400	Bagno et al. (1991)	T	473
		6400	Della Gatta et al. (1981)	T	
	2.8×10^{-2}		Yaws (2003)	X	237
	4.9×10^{-3}		Duchowicz et al. (2020)	Q	
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
	3.5×10^{-2}		Hilal et al. (2008)	Q	
	1.5×10^{-1}		Modarresi et al. (2007)	Q	67
		6000	Kühne et al. (2005)	Q	
	2.8×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.4×10^{-2}		Yao et al. (2002)	Q	229
	1.4×10^{-2}		English and Carroll (2001)	Q	230, 231
	1.3×10^{-2}		Katritzky et al. (1998)	Q	
	6.0×10^{-2}		Nirmalakhandan et al. (1997)	Q	
		4900	Kühne et al. (2005)	?	
	2.8×10^{-2}		Yaws (1999)	?	21
	2.8×10^{-2}		Yaws et al. (1998)	?	
cycloheptanone	7.0×10^{-1}		Hilal et al. (2008)	Q	
$C_7H_{12}O$					
[502-42-1]					
CGZZMOTZOONQIA-UHFFFAOYSA-N					

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methylcyclohexanone $C_7H_{12}O$ [583-60-8] LFSAPCRASZRSKS-UHFFFAOYSA-N		5600 4600	Kühne et al. (2005) Kühne et al. (2005)	Q ?	
3-methylcyclohexanone $C_7H_{12}O$ [591-24-2] UJBOOUHRTQVGRU-UHFFFAOYSA-N	6.7×10^{-2} 9.9×10^{-2}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
4-methylcyclohexanone $C_7H_{12}O$ [589-92-4] VGVHNLRUAMRIEW-UHFFFAOYSA-N		6500 6100	Kühne et al. (2005) Kühne et al. (2005)	Q ?	
dicyclopropylmethanone $C_7H_{10}O$ (dicyclopropyl ketone) [1121-37-5] BIPUHAHGLJKIPK-UHFFFAOYSA-N	3.1	7300 7300	Bagno et al. (1991) Della Gatta et al. (1981)	T T	473
2-octanone $C_6H_{13}COCH_3$ [111-13-7] ZPVFWPFBNIEHGJ-UHFFFAOYSA-N	5.0×10^{-2} 5.8×10^{-2} 2.9×10^{-2} 3.1×10^{-2} 1.8×10^{-2} 5.2×10^{-2} 4.9×10^{-2} 4.9×10^{-2} 5.5×10^{-2} 7.1×10^{-2} 3.2×10^{-2} 6.2×10^{-2} 3.9×10^{-2} 4.9×10^{-2} 5.1×10^{-2} 1.2×10^{-1} 5.2×10^{-2} 5.1×10^{-2} 2.0×10^{-2} 5.7×10^{-2} 3.3×10^{-2} 5.3×10^{-2} 5.2×10^{-2} 5.2×10^{-2} 9.6×10^{-2} 1.5×10^{-1}	7500 7300 	Brockbank (2013) Plyasunov and Shock (2001) van Ruth et al. (2002) van Ruth and Villeneuve (2002) van Ruth et al. (2001) Buttery et al. (1969) Mackay et al. (2006c) Mackay et al. (1995) Rathbun and Tai (1982) Keshavarz et al. (2022) Duchowicz et al. (2020) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Kühne et al. (2005) Yaffe et al. (2003) English and Carroll (2001) Katritzky et al. (1998) Nirmalakhandan et al. (1997) Russell et al. (1992) Suzuki et al. (1992) Duchowicz et al. (2020) Mackay et al. (2006c) Kühne et al. (2005) Yaws (1999) Yaws et al. (1998)	L L M M M M V V V Q Q Q Q Q Q Q Q Q Q Q Q Q Q Q ? ? ? ?	1, 481 14 14, 361 14 184 271, 243 244 245 67 248, 249 230, 231 279 232 185, 21 21 21, 12 12

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.2×10^{-2}		Abraham et al. (1990)	?	
3-octanone	4.3×10^{-2}	6900	Brockbank (2013)	L	1
$C_8H_{16}O$	2.9×10^{-2}	5800	Wu et al. (2022a)	M	482
[106-68-3]	7.6×10^{-2}		HSDB (2015)	V	
RHLVCLIPMVJYKS-UHFFFAOYSA-N	2.5×10^{-2}		Wang et al. (2017)	Q	80, 238
	4.2×10^{-2}		Wang et al. (2017)	Q	80, 239
	1.3×10^{-1}		Wang et al. (2017)	Q	80, 240
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.1×10^{-1}		Modarresi et al. (2007)	Q	67
4-octanone	3.6×10^{-2}		Hilal et al. (2008)	Q	
$C_8H_{16}O$					
[589-63-9]					
YWXLSHOWXZUMSR-UHFFFAOYSA-N					
5-methyl-3-heptanone	5.0×10^{-2}		Ebert et al. (2023)	?	316
$C_8H_{16}O$					
[541-85-5]					
PSBKJPTZCVYXSD-UHFFFAOYSA-N					
6-methyl-3-heptanone	3.7×10^{-2}		HSDB (2015)	Q	99
$C_8H_{16}O$					
[624-42-0]					
CCCIYAQYQZQDIZ-UHFFFAOYSA-N					
cyclohexyl methyl ketone	2.9×10^{-1}	7200	Bagno et al. (1991)	T	473
$C_6H_{11}COCH_3$	7.1×10^{-2}		Keshavarz et al. (2022)	Q	
[823-76-7]	9.9×10^{-2}		Duchowicz et al. (2020)	Q	184
RIFKADJTWUGDOV-UHFFFAOYSA-N	4.1×10^{-1}		Hilal et al. (2008)	Q	
	4.2×10^{-1}		Modarresi et al. (2007)	Q	67
	2.3×10^{-1}		English and Carroll (2001)	Q	230, 231
	3.1×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	2.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2-nonanone	3.2×10^{-2}	7400	Brockbank (2013)	L	1, 483
$C_9H_{18}O$	3.7×10^{-2}	7500	Plyasunov and Shock (2001)	L	
[821-55-6]	4.1×10^{-2}		Li and Carr (1993)	M	
VKCYHJWLYTUGCC-UHFFFAOYSA-N	2.7×10^{-2}		Buttery et al. (1969)	M	
		7600	Abraham (1984)	V	
	2.1×10^{-2}		Yaws (2003)	X	258
	1.1×10^{-1}		Dupeux et al. (2022)	Q	259
	9.6×10^{-2}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	299
	4.1×10^{-3}		Ghargheizi et al. (2012)	Q	
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.1×10^{-2}		Hilal et al. (2008)	Q	
	1.0×10^{-1}		Modarresi et al. (2007)	Q	67
		7600	Kühne et al. (2005)	Q	
	2.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	3.9×10^{-2}		English and Carroll (2001)	Q	230, 231
	1.3×10^{-2}		Katritzky et al. (1998)	Q	
	4.4×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	4.0×10^{-2}		Suzuki et al. (1992)	Q	232
	2.7×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		8100	Kühne et al. (2005)	?	
	2.9×10^{-2}		Yaws et al. (1998)	?	
	2.7×10^{-2}		Abraham et al. (1990)	?	
3-nonanone	5.1×10^{-2}	6600	Brockbank (2013)	L	1
$C_9H_{18}O$	2.2×10^{-2}		Wang et al. (2017)	Q	80, 238
[925-78-0]	3.2×10^{-2}		Wang et al. (2017)	Q	80, 239
IYTXKIXETAELAV-UHFFFAOYSA-N	1.2×10^{-1}		Wang et al. (2017)	Q	80, 240
5-nonanone	4.0×10^{-2}	8000	Brockbank (2013)	L	1
$C_9H_{18}O$	3.5×10^{-2}		Duchowicz et al. (2020)	V	186
(dibutyl ketone)	3.5×10^{-2}		HSDB (2015)	V	
[502-56-7]	3.4×10^{-2}		Meylan and Howard (1991)	V	
WSGCRAOTEDLMFQ-UHFFFAOYSA-N	3.7×10^{-2}		Cabani et al. (1981)	V	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	2.7×10^{-2}		Hilal et al. (2008)	Q	
	9.0×10^{-2}		Modarresi et al. (2007)	Q	67
		7600	Kühne et al. (2005)	Q	
	2.7×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	3.9×10^{-2}		English and Carroll (2001)	Q	230, 231
	4.7×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	3.6×10^{-2}		Meylan and Howard (1991)	Q	
		7900	Kühne et al. (2005)	?	
	3.4×10^{-2}		Yaws et al. (1998)	?	38
	3.5×10^{-2}		Abraham et al. (1990)	?	
2,6-dimethyl-4-heptanone	1.3×10^{-2}	7500	Brockbank (2013)	L	1
$C_9H_{18}O$	1.3×10^{-2}		Plyasunov and Shock (2001)	L	
(diisobutyl ketone)	8.4×10^{-2}		Duchowicz et al. (2020)	V	186
[108-83-8]	8.2×10^{-2}		HSDB (2015)	V	
PTTPXKJBFFKCEK-UHFFFAOYSA-N	4.9×10^{-3}		Duchowicz et al. (2020)	Q	
	3.1×10^{-2}		Hilal et al. (2008)	Q	
	1.1×10^{-1}		Modarresi et al. (2007)	Q	67
		7600	Kühne et al. (2005)	Q	
	8.6×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
		5500	Kühne et al. (2005)	?	
	8.3×10^{-2}		Yaws (1999)	?	21, 79
	9.2×10^{-2}		Yaws et al. (1998)	?	79

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,4,4-tetramethyl-3-pentanone $C_9H_{18}O$ (di-(*tert*-butyl) ketone) [815-24-7] UIQGEWJEWJMQSL-UHFFFAOYSA-N	2.3×10^{-2}		Bagno et al. (1991)	T	473
2-decanone $C_8H_{17}COCH_3$ [693-54-9] ZAJNGDIORYACQU-UHFFFAOYSA-N	1.8×10^{-2}		van Ruth et al. (2002)	M	14
	1.5×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 361
	1.5×10^{-2}		van Ruth et al. (2001)	M	14
	2.1×10^{-2}		Abraham (1984)	V	
	1.7×10^{-2}		Yaws (2003)	X	258
	9.2×10^{-2}		Dupeux et al. (2022)	Q	259
	4.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.4×10^{-2}		Hilal et al. (2008)	Q	
	8.0×10^{-2}		Modarresi et al. (2007)	Q	67
	2.7×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	3.1×10^{-2}		English and Carroll (2001)	Q	230, 260
	1.4×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.4×10^{-2}		Yaws et al. (1998)	?	
	2.1×10^{-2}		Abraham et al. (1990)	?	
2-undecanone $C_9H_{19}COCH_3$ [112-12-9] KYWIYKKSMDLRDC-UHFFFAOYSA-N	1.9×10^{-2}		Plyasunov and Shock (2001)	L	
	1.6×10^{-2}		Buttery et al. (1969)	M	
	1.8×10^{-2}		Yaws (2003)	X	258
	1.7×10^{-2}		Yaws (2003)	X	237
	7.6×10^{-2}		Dupeux et al. (2022)	Q	259
	1.8×10^{-1}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	299
	1.5×10^{-2}		Li et al. (2014)	Q	241
	4.1×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.7×10^{-2}		Hilal et al. (2008)	Q	
	6.3×10^{-2}		Modarresi et al. (2007)	Q	67
	1.6×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.3×10^{-2}		English and Carroll (2001)	Q	230, 231
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
	2.8×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	2.4×10^{-2}		Suzuki et al. (1992)	Q	232
	1.6×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	5.8×10^{-3}		Yaws et al. (1998)	?	
	1.5×10^{-2}		Abraham et al. (1990)	?	

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
6-undecanone $C_{11}H_{22}O$ [927-49-1] ZPQAKYPOZRXKFA-UHFFFAOYSA-N	1.5×10^{-2} 6.9×10^{-2}		Hilal et al. (2008) Modarresi et al. (2007)	Q Q	 67
2-dodecanone $C_{12}H_{24}O$ [6175-49-1] LSKONYYRONEBKA-UHFFFAOYSA-N	4.6×10^{-3} 2.1×10^{-3}		Gharagheizi et al. (2012) Yaws et al. (1998)	Q ?	
2,6,8-trimethyl-4-nonanone $C_{12}H_{24}O$ [123-18-2] GFWVDQCGGDBTBS-UHFFFAOYSA-N			Brockbank (2013)	W	484
2-tridecanone $C_{13}H_{26}O$ [593-08-8] CYIFVRUOHKNECG-UHFFFAOYSA-N	4.6×10^{-3} 6.7×10^{-4}		Gharagheizi et al. (2012) Yaws et al. (1998)	Q ?	
2-tetradecanone $C_{14}H_{28}O$ [2345-27-9] POQLVOYRGNFGRM-UHFFFAOYSA-N	4.7×10^{-3} 2.1×10^{-4}		Gharagheizi et al. (2012) Yaws et al. (1998)	Q ?	
2-pentadecanone $C_{15}H_{30}O$ [2345-28-0] CJPNOLIZCWDHJK-UHFFFAOYSA-N	5.4×10^{-5}		Yaws et al. (1998)	?	
2-hexadecanone $C_{16}H_{32}O$ [18787-63-8] XCXKZBWAKKPFCJ-UHFFFAOYSA-N	1.7×10^{-5}		Yaws et al. (1998)	?	
2-heptadecanone $C_{17}H_{34}O$ [2922-51-2] TVTCXPXLRKTHAU-UHFFFAOYSA-N	3.9×10^{-6}		Yaws et al. (1998)	?	
menthone $C_{10}H_{18}O$ [89-80-5] NFLGAXVYCFJBMK-UHFFFAOYSA-N	5.7×10^{-2} 5.0×10^{-2} 6.2×10^{-2} 5.8×10^{-2}		Marin et al. (1999) Marin et al. (1999) HSDB (2015) Marin et al. (1999)	M V Q Q	 99
tricyclo[3.3.1.1(3,7)]decanone $C_{10}H_{14}O$ (2-adamantanone) [700-58-3] IYKFYARMMIESOX-UHFFFAOYSA-N	1.4 7.5×10^{-1}	5800	van Roon et al. (2005) Cabani et al. (1981)	V V	

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl cedryl ketone $C_{17}H_{26}O$ [32388-55-9] YBUIAJZFOGJGLJ-SWRJLBSHSA-N	6.1		Dupeux et al. (2022)	Q	259
3-buten-2-one	4.0×10^{-1}		Burkholder et al. (2019)	L	
C_4H_6O	4.0×10^{-1}		Burkholder et al. (2015)	L	
(methyl vinyl ketone; MVK)	2.6×10^{-1}	4800	Ji and Evans (2007)	M	
[78-94-4]	4.0×10^{-1}		Iraci et al. (1999)	M	
FUSUHKVFWTUUBE-UHFFFAOYSA-N	2.1×10^{-1}	7800	Allen et al. (1998)	M	
	1.6×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.5×10^{-1}		Wang et al. (2017)	Q	80, 238
	3.1×10^{-1}		Wang et al. (2017)	Q	80, 239
	7.8×10^{-1}		Wang et al. (2017)	Q	80, 240
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	7.1×10^{-1}		Modarresi et al. (2007)	Q	67
		6000	Kühne et al. (2005)	Q	
	2.1×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		7800	Kühne et al. (2005)	?	
	4.3×10^{-1}		Betterton (1991)	?	
methyl isopropenyl ketone	9.8×10^{-2}		Yaws (2003)	X	237
C_5H_8O	3.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[814-78-8]	9.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
ZGHFDIIVVIFNPS-UHFFFAOYSA-N	5.2×10^{-2}		Yao et al. (2002)	Q	229
	9.8×10^{-2}		Yaws (1999)	?	21
4-methyl-3-penten-2-one	2.7×10^{-1}		HSDB (2015)	V	
$C_6H_{10}O$	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
(mesityl oxide)	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	244
[141-79-7]	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	245
SHOJXDKTYKFBRD-UHFFFAOYSA-N	1.8×10^{-1}		Hilal et al. (2008)	Q	
	2.5×10^{-1}		Modarresi et al. (2007)	Q	67
	2.0×10^{-1}		Yaws (1999)	?	21, 12
1-phenylethanone	1.1	7900	Brockbank (2013)	L	1
$C_6H_5COCH_3$	1.1	7700	Staudinger and Roberts (2001)	L	
(acetophenone)	9.7×10^{-1}	6800	Hiatt (2013)	M	
[98-86-2]	1.2	7800	Ji et al. (2008)	M	
KWOLFJPFCHCOCG-UHFFFAOYSA-N	9.7×10^{-1}	12000	Allen et al. (1998)	M	
	9.3×10^{-1}		Shiu and Mackay (1997)	M	
	1.1	6000	Betterton (1991)	M	
	1.0		Mackay et al. (2006c)	V	
	1.0		Shiu and Mackay (1997)	V	
	1.0		Mackay et al. (1995)	V	

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Table A3.6: Ketones (RCOR) (. . . continued)

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	9.2×10^{-1}		Hine and Mookerjee (1975)	V	
	9.5×10^{-1}	6400	Bagno et al. (1991)	T	473
	1.1		Yaws (2003)	X	258
	9.3×10^{-1}		Schüürmann (2000)	C	21
	1.8		Dupeux et al. (2022)	Q	259
	7.1×10^{-2}		Keshavarz et al. (2022)	Q	
	2.2×10^{-1}		Duchowicz et al. (2020)	Q	184
	2.0		Wang et al. (2017)	Q	80, 238
	2.0		Wang et al. (2017)	Q	80, 239
	4.6		Wang et al. (2017)	Q	80, 240
	9.2×10^{-1}		Li et al. (2014)	Q	241
	1.2		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.1		Hilal et al. (2008)	Q	
	2.9		Modarresi et al. (2007)	Q	67
		6100	Kühne et al. (2005)	Q	
	1.0		Yaffe et al. (2003)	Q	248, 249
	1.1		English and Carroll (2001)	Q	230, 231
	1.9×10^{-1}		Katritzky et al. (1998)	Q	
	5.3×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	9.2×10^{-1}		Suzuki et al. (1992)	Q	232
	9.5×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		6700	Kühne et al. (2005)	?	
	1.1		Yaws (1999)	?	21
	9.2×10^{-1}		Abraham et al. (1990)	?	
1-phenylethanone-d5 $C_6D_5COCH_3$ (acetophenone-d5) [28077-64-7] KWOLFJPFCHCOCG-VIQYUKPQSA-N	2.3	10000	Hiatt (2013)	M	
4-methoxy-4-methyl-2-pentanone $C_7H_{14}O_2$ [107-70-0] KOKPBCHLPVDQTK-UHFFFAOYSA-N	5.1		Duchowicz et al. (2020)	V	186
	5.1		HSDB (2015)	V	
	2.2×10^{-1}		Duchowicz et al. (2020)	Q	
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	2.0		Raventos-Duran et al. (2010)	Q	244
	7.8		Raventos-Duran et al. (2010)	Q	245
	1.8		Hilal et al. (2008)	Q	
	2.4		Modarresi et al. (2007)	Q	67
2′-hydroxyacetophenone $C_8H_8O_2$ [118-93-4] JECYUBVRTQDVAT-UHFFFAOYSA-N	1.0	8400	Ji et al. (2008)	M	

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
6-methyl-5-hepten-2-one $C_8H_{14}O$ [110-93-0] UHEPJGULSIKKTP-UHFFFAOYSA-N	1.2×10^{-1} 2.5×10^{-1}	6200	Wu et al. (2022b) Dupeux et al. (2022)	M Q	 259
phenyl ethyl ketone $C_9H_{10}O$ (propiophenone) [93-55-0] KRIOVPPHQSLHCZ-UHFFFAOYSA-N	9.9×10^{-1} 6.6×10^{-1} 7.6×10^{-2} 2.2×10^{-1} 1.9 1.4 9.1×10^{-1} 7.5×10^{-1} 7.2×10^{-1} 1.6 9.7×10^{-1} 8.6×10^{-1} 8.0×10^{-1} 7.9×10^{-2} 2.9×10^{-1} 	7900 6400 7700	Ji et al. (2008) Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Kühne et al. (2005) Yaffe et al. (2003) Katritzky et al. (1998) Kühne et al. (2005)	M V V Q Q Q Q Q Q Q Q Q Q Q Q Q ?	 186 80, 238 80, 239 80, 240 287, 288 287, 289 287, 290 287, 291 67 248, 249
2′-methylacetophenone $C_9H_{10}O$ [577-16-2] YXWWHNCQZBVZPV-UHFFFAOYSA-N	7.6×10^{-1} 1.2 2.4 1.3	7600	Ji et al. (2008) Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	M Q Q Q	 80, 238 80, 239 80, 240
3′-methylacetophenone $C_9H_{10}O$ [585-74-0] FSPSELPMWGWDRY-UHFFFAOYSA-N	1.5	7600	Ji et al. (2008)	M	
4'-methylacetophenone $C_9H_{10}O$ [122-00-9] GNKZMNRKLCTJAY-UHFFFAOYSA-N	1.8 1.1 4.3 1.2 1.2 9.5×10^{-1} 3.8×10^{-1}	8400	Ji et al. (2008) Abraham et al. (1994a) Abney (2021) Hilal et al. (2008) Yaffe et al. (2003) English and Carroll (2001) Nirmalakhandan et al. (1997)	M R Q Q Q Q Q	 399 248, 249 230, 260
2′-methoxyacetophenone $C_9H_{10}O_2$ (2-methoxyphenyl methyl ketone) [579-74-8] DWPLEOPKBWNPQV-UHFFFAOYSA-N	1.7×10^{1}	9500	Ji et al. (2008)	M	

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3′-methoxyacetophenone $C_9H_{10}O_2$ (3-methoxyphenyl methyl ketone) [586-37-8] BAYUSCHCCGXLAY-UHFFFAOYSA-N	1.9×10^{1}	9400	Ji et al. (2008)	M	
4′-methoxyacetophenone	6.8×10^{-1}		Bagno et al. (1991)	T	473
$C_9H_{10}O_2$	6.9		Hilal et al. (2008)	Q	
(4-methoxyphenyl methyl ketone)	1.4		English and Carroll (2001)	Q	230, 231
[100-06-1]	1.3		Nirmalakhandan et al. (1997)	Q	
NTPLXRHDUXRPNE-UHFFFAOYSA-N					
2-methyl-5-(1-methylethenyl)-2-cyclohexen-1-one	4.9×10^{-1}		Amoore and Buttery (1978)	M	
$C_{10}H_{14}O$	5.5×10^{-1}		Amoore and Buttery (1978)	V	
(carvone)	8.0×10^{-1}		Hilal et al. (2008)	Q	
[6485-40-1]					
ULDHMXUKGWMISQ-SECBINFHSA-N					
benzophenone	1.7×10^{1}		Mackay et al. (2006c)	V	
$C_{13}H_{10}O$	6.1	9400	Bagno et al. (1991)	T	473
(diphenyl ketone)	1.7		Yaws (2003)	X	258
[119-61-9]	9.6		Dupeux et al. (2022)	Q	259
RWCCWEUUXYIKHB-UHFFFAOYSA-N	5.2		HSDB (2015)	Q	99
	5.1		Zhang et al. (2010)	Q	287, 288
	2.9		Zhang et al. (2010)	Q	287, 289
	3.6×10^{1}		Zhang et al. (2010)	Q	287, 290
	3.4×10^{1}		Zhang et al. (2010)	Q	287, 291
	1.7		Yaws (1999)	?	21
2,4-dihydroxybenzophenone $C_{13}H_{10}O_3$ [131-56-6] ZXDDPOHVAMWLBH-UHFFFAOYSA-N	4.6×10^{5}		Abraham et al. (2019)	Q	
3,5,5-trimethyl-2-cyclohexen-1-one	1.5		Duchowicz et al. (2020)	V	186
$C_9H_{14}O$	1.5		HSDB (2015)	V	
(isophorone)	1.7		Mackay et al. (2006d)	V	
[78-59-1]	1.7		Hwang et al. (1992)	V	
HJOVHMDZYOCNQW-UHFFFAOYSA-N	1.7		Suntio et al. (1988)	V	12
	1.7	3900	Goldstein (1982)	X	298
	1.8		Suntio et al. (1988)	C	12
	1.7×10^{-2}		Duchowicz et al. (2020)	Q	
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	6.9×10^{-1}		Hilal et al. (2008)	Q	
	1.3		Modarresi et al. (2007)	Q	67
		7300	Kühne et al. (2005)	Q	

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.5		Yaffe et al. (2003)	Q	248, 249
	1.2×10^{-1}		Katritzky et al. (1998)	Q	
		7400	Kühne et al. (2005)	?	
	1.5		Yaws (1999)	?	21
bicyclo[2.2.1]heptan-2-one $C_7H_{10}O$ (norcamphor; 2-norbornanone) [497-38-1] KPMKEVXVVHNIEY-UHFFFAOYSA-N	4.3×10^{-1}	5100	van Roon et al. (2005)	V	
4-methyl-1-(1-methylethyl)-bicyclo[3.1.0]hexan-3-one $C_{10}H_{16}O$ (thujone) [1125-12-8] USMNOWBWPHYOEA-UHFFFAOYSA-N	1.0×10^{-1}	4700	van Roon et al. (2005)	V	
isopropyl phenyl ketone $C_{10}H_{12}O$ [611-70-1] BSMGLVDZZMBWQB-UHFFFAOYSA-N	5.7×10^{-1}		Zhang et al. (2010)	Q	287, 288
	3.9×10^{-1}		Zhang et al. (2010)	Q	287, 289
	1.7		Zhang et al. (2010)	Q	287, 290
	8.2×10^{-1}		Zhang et al. (2010)	Q	287, 291
carvone $C_{10}H_{14}O$ [99-49-0] ULDHMXUKGWMISQ-UHFFFAOYSA-N	1.3×10^{-1}		HSDB (2015)	Q	99
thujone $C_{10}H_{16}O$ [76231-76-0] USMNOWBWPHYOEA-VWHDNNRLSA-N	6.2×10^{-1}		HSDB (2015)	Q	99
cis-jasmone $C_{11}H_{16}O$ [488-10-8] XMLSXPIVAXONDL-PLNGDYQASA-N	5.2		Dupeux et al. (2022)	Q	259
α-damascone $C_{13}H_{20}O$ [24720-09-0] CRIGTVCBMUKRSL-FNORWQNLSA-N	2.1×10^{1}		Abney (2021)	Q	399
(E)-β-damascenone $C_{13}H_{18}O$ [23726-93-4] POIARNZEYGURDG-FNORWQNLSA-N	3.2×10^{-1}	4600	Wieland et al. (2015)	M	485

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
9H-fluoren-9-one	6.4		Abraham et al. (2019)	Q	
$C_{13}H_8O$	1.5×10^{1}		HSDB (2015)	Q	99
[486-25-9]	2.3×10^{1}		Parnis et al. (2015)	Q	369
YLQWCDOCJODRMT-UHFFFAOYSA-N					
anthrone	1.2×10^{1}		HSDB (2015)	Q	99
$C_{14}H_{10}O$					
[90-44-8]					
RJGDLRCDCYRQOQ-UHFFFAOYSA-N					
1,2,3,5,6,7-hexahydro-1,1,2,3,3-pentamethyl-4H-inden-4-one	7.0×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{14}H_{22}O$	6.7×10^{-3}		Zhang et al. (2010)	Q	287, 289
[33704-61-9]	2.0×10^{1}		Zhang et al. (2010)	Q	287, 290
MIZGSAALSYARKU-UHFFFAOYSA-N	4.8×10^{-2}		Zhang et al. (2010)	Q	287, 291
benzoin	2.2×10^{5}		Abraham et al. (2019)	Q	
$C_{14}H_{12}O_2$					
[119-53-9]					
ISAOCJYIOMOJEB-UHFFFAOYSA-N					
methyl-alpha-ionone	1.2		Dupeux et al. (2022)	Q	259
$C_{14}H_{22}O$					
[93302-56-8]					
VPKMGDRERYMTJX-XEHSLEBBSA-N					
iso-e super	5.5×10^{-1}		Dupeux et al. (2022)	Q	259
$C_{16}H_{26}O$					
[54464-57-2]					
FVUGZKDGWGKCFE-UHFFFAOYSA-N					
2,4,6-trimethylbenzophenone	3.8		Zhang et al. (2010)	Q	287, 288
$C_{16}H_{16}O$	3.8		Zhang et al. (2010)	Q	287, 289
[954-16-5]	1.5×10^{1}		Zhang et al. (2010)	Q	287, 290
HPAFOABSQZMTHE-UHFFFAOYSA-N	6.0		Zhang et al. (2010)	Q	287, 291
1-(1,2,3,5,6,7,8,8a-octahydro-2,3,8,8-tetramethyl-2-naphthyl)ethan-1-one	2.5×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{16}H_{26}O$	3.0×10^{-1}		Zhang et al. (2010)	Q	287, 289
[68155-66-8]	1.1×10^{1}		Zhang et al. (2010)	Q	287, 290
NOMWSTMYQKABST-UHFFFAOYSA-N	4.0×10^{-2}		Zhang et al. (2010)	Q	287, 291
civetone	3.0		Dupeux et al. (2022)	Q	259
$C_{17}H_{30}O$					
[542-46-1]					
ZKVZSBSZTMPBQR-UPHRSURJSA-N					

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-(2,3-dihydro-1,1,2,3,3,6-hexamethyl-1H-inden-5-yl)ethanone	3.1×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_{17}H_{24}O$	2.0		Zhang et al. (2010)	Q	287, 289
[15323-35-0]	5.2		Zhang et al. (2010)	Q	287, 290
VDBHOHJWUDKDRW-UHFFFAOYSA-N	9.9×10^{-2}		Zhang et al. (2010)	Q	287, 291
celestolide	3.1×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_{17}H_{24}O$	2.4		Zhang et al. (2010)	Q	287, 289
[13171-00-1]	3.1		Zhang et al. (2010)	Q	287, 290
IKTHMQYJOWTSJO-UHFFFAOYSA-N	8.8×10^{-2}		Zhang et al. (2010)	Q	287, 291
7H-benz[*de*]anthracen-7-one	1.5×10^{2}		HSDB (2015)	Q	99
$C_{17}H_{10}O$	8.0×10^{2}		Parnis et al. (2015)	Q	369
(benzanthrone)					
[82-05-3]					
HUKPVYBUJRAUAG-UHFFFAOYSA-N					
11H-benzo[*a*]fluoren-11-one	7.2×10^{1}		Parnis et al. (2015)	Q	369
$C_{17}H_{10}O$					
[479-79-8]					
RNICURKFVSAHLQ-UHFFFAOYSA-N					
11H-benzo[*b*]fluoren-11-one	5.4×10^{4}		Parnis et al. (2015)	Q	369
$C_{17}H_{10}O$					
[3074-03-1]					
MLMNDNOSVOKYMT-UHFFFAOYSA-N					
benz[*a*]anthracene-7,12-dione	4.2×10^{2}		Parnis et al. (2015)	Q	369
$C_{18}H_{10}O_2$					
[2498-66-0]					
LHMRXAIRPKSGDE-UHFFFAOYSA-N					
1-[2,3-dihydro-1,1,2,6-tetramethyl-3-(1-methylethyl)-1H-inden-5-yl]ethanone	2.3×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_{18}H_{26}O$	3.2		Zhang et al. (2010)	Q	287, 289
[68140-48-7]	4.4		Zhang et al. (2010)	Q	287, 290
IMRYETFJNLKUHK-UHFFFAOYSA-N	1.3×10^{-1}		Zhang et al. (2010)	Q	287, 291
tonalide	7.0×10^{-2}		HSDB (2015)	V	
$C_{18}H_{26}O$	2.3×10^{-1}		Zhang et al. (2010)	Q	287, 288
[21145-77-7]	2.4		Zhang et al. (2010)	Q	287, 289
DNRJTBAOUJJKDY-UHFFFAOYSA-N	7.9		Zhang et al. (2010)	Q	287, 290
	7.9×10^{-2}		Zhang et al. (2010)	Q	287, 291

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
2,3-butanedione	7.3×10^{-1}	5700	Burkholder et al. (2019)	L	
$CH_3COCOCH_3$	7.3×10^{-1}	5700	Burkholder et al. (2015)	L	
(diacetyl; dimethylglyoxal)	7.3×10^{-1}	5700	Sander et al. (2011)	L	
[431-03-8]	1.4×10^{-1}	4900	Wu et al. (2022b)	M	
QSJXEFYPDANLFS-UHFFFAOYSA-N	4.2×10^{-1}	7200	Wieland et al. (2015)	M	486
	5.6×10^{-1}	6700	Strekowski and George (2005)	M	
	5.6×10^{-1}		Straver and de Loos (2005)	M	
	2.1×10^{-1}		van Ruth et al. (2002)	M	14
	2.0×10^{-1}		van Ruth and Villeneuve (2002)	M	14, 361
	2.0×10^{-1}		van Ruth et al. (2001)	M	14
	1.0		Marin et al. (1999)	M	
	3.7×10^{-1}		Roberts and Pollien (1997)	M	
	9.1×10^{-1}		Landy et al. (1995)	M	
	7.3×10^{-1}	5700	Betterton (1991)	M	
	5.7×10^{-1}		Snider and Dawson (1985)	M	
	6.1×10^{-1}		Marin et al. (1999)	V	
	1.9		Gaffney and Senum (1984)	X	446
	1.9		Gaffney and Senum (1984)	X	389
	1.6×10^{-1}		Keshavarz et al. (2022)	Q	
	2.2		Duchowicz et al. (2020)	Q	299
	3.6×10^{1}		Wang et al. (2017)	Q	80, 238
	9.1		Wang et al. (2017)	Q	80, 239
	1.9×10^{-1}		Wang et al. (2017)	Q	80, 240
	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	271, 243
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	3.8		Hilal et al. (2008)	Q	
	1.4×10^{1}		Modarresi et al. (2007)	Q	67
		6500	Kühne et al. (2005)	Q	
	7.1×10^{-1}		Marin et al. (1999)	Q	
	7.4×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		6000	Kühne et al. (2005)	?	
2,3-pentanedione	1.3×10^{-1}	6200	Wu et al. (2022b)	M	
$C_5H_8O_2$	3.2×10^{1}		Wang et al. (2017)	Q	80, 238
[600-14-6]	8.7		Wang et al. (2017)	Q	80, 239
TZMFJUDUGYTVRY-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	80, 240
2,4-pentanedione	8.5×10^{-1}	3800	Brockbank (2013)	L	1
$C_5H_8O_2$	1.5		Nozière and Riemer (2003)	M	79
(acetylacetone)	9.9×10^{-1}	4400	Hovorka et al. (2002)	M	11
[123-54-6]	1.7		Hellmann (1987)	M	87
YRKCREAYFQTBPV-UHFFFAOYSA-N	4.3		HSDB (2015)	V	
	3.0		Yaws (2003)	X	237, 12
	3.2×10^{1}		Wang et al. (2017)	Q	80, 238
	4.5×10^{1}		Wang et al. (2017)	Q	80, 239
	2.5×10^{1}		Wang et al. (2017)	Q	80, 240
	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{2}		Raventos-Duran et al. (2010)	Q	245
	3.2		Gharagheizi et al. (2010)	Q	246
	1.7×10^{1}		Hilal et al. (2008)	Q	
	1.1×10^{1}		Modarresi et al. (2007)	Q	67
		7300	Kühne et al. (2005)	Q	
	1.1×10^{1}		Yao et al. (2002)	Q	229
		4400	Kühne et al. (2005)	?	
	2.2		Yaws (1999)	?	21, 12
1,2-naphthalenedione $C_{10}H_6O_2$ [524-42-5] KETQAJRQOHHATG-UHFFFAOYSA-N	2.3×10^{3}		HSDB (2015)	Q	99
1,4-naphthalenedione $C_{10}H_6O_2$ (1,4-naphthoquinone) [130-15-4] FRASJONUBLZVQX-UHFFFAOYSA-N	5.0×10^{3} 1.6×10^{2}		HSDB (2015) Parnis et al. (2015)	Q Q	99 369
menadione $C_{11}H_8O_2$ [58-27-5] MJVAVZPDRWSRRC-UHFFFAOYSA-N	3.2×10^{3}		HSDB (2015)	Q	99
2,6-di-*tert*-butyl-*p*-benzoquinone $C_{14}H_{20}O_2$ [719-22-2] RDQSIADLBQFVMY-UHFFFAOYSA-N	6.2×10^{2}		HSDB (2015)	Q	99
9,10-phenanthrenedione $C_{14}H_8O_2$ [84-11-7] YYVYAPXYZVYDHN-UHFFFAOYSA-N	3.7×10^{3}		HSDB (2015)	Q	447
9,10-anthracenedione $C_{14}H_8O_2$ [84-65-1] RZVHIXYEVGDQDX-UHFFFAOYSA-N	4.2×10^{2} 4.2×10^{2} 1.1×10^{-1} 4.9×10^{2} 1.6×10^{2} 3.1×10^{3} 5.6×10^{2} 1.7×10^{2} 2.5×10^{4} 1.1×10^{-1}		Duchowicz et al. (2020) HSDB (2015) Yaws (2003) Duchowicz et al. (2020) Parnis et al. (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Gharagheizi et al. (2010)	V V X Q Q Q Q Q Q Q	186 237 369 287, 288 287, 289 287, 290 287, 291 246

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
2-hydroxy-9,10-anthracenedione $C_{14}H_8O_3$ [605-32-3] GCDBEYOJCZLKMC-UHFFFAOYSA-N	5.4×10^5 2.8×10^6		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
1,4-dihydroxy-9,10-anthracenedione $C_{14}H_8O_4$ [81-64-1] GUEIZVNYDFNHJU-UHFFFAOYSA-N	1.2×10^2 1.4×10^4		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
benzil $C_{14}H_{10}O_2$ [134-81-6] WURBFLDFSFBTLW-UHFFFAOYSA-N	3.0×10^1		Abraham et al. (2019)	Q	
dibenzoylmethane $C_{15}H_{12}O_2$ [120-46-7] NZZIMKJIVMHWJC-UHFFFAOYSA-N	7.5×10^3 8.0×10^2 6.9×10^4 1.3×10^4		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
2-methyl-9,10-anthracenedione $C_{15}H_{10}O_2$ [84-54-8] NJWGQARXZDRHCD-UHFFFAOYSA-N	2.4×10^2		Parnis et al. (2015)	Q	369
2-ethyl-9,10-anthracenedione $C_{16}H_{12}O_2$ [84-51-5] SJEBAWHUJDUKQK-UHFFFAOYSA-N	2.6×10^1 2.1×10^3 4.2×10^2 1.6×10^2 1.1×10^4		Abraham et al. (2019) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	 287, 288 287, 289 287, 290 287, 291
diphenadione $C_{23}H_{16}O_3$ [82-66-6] JYGLAHSAISAEAL-UHFFFAOYSA-N	6.4×10^4 2.9×10^4		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
MCM:CH3COCO3H $C_3H_4O_4$ BXASKOSTAOGNPV-UHFFFAOYSA-N	6.6×10^4 4.7×10^2 4.5×10^1		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:HYPERACET $C_3H_6O_3$ LSIGHSKIPNHVEN-UHFFFAOYSA-N	5.0×10^3 2.1×10^2 1.4×10^2		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:BIACETOOH $C_4H_6O_4$ JYWVDPVJSGSFMT-UHFFFAOYSA-N	2.6×10^6 1.2×10^4 5.6×10^1		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:CO2C3CO3H $C_4H_6O_4$ SJOPHMGAZWPERQ-UHFFFAOYSA-N	5.1×10^4 6.2×10^3 2.8×10^2		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MEKAOOH	4.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	6.3×10^{3}		Wang et al. (2017)	Q	80, 239
VEPDQRPXKSSVPR-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:MEKBOOH	4.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	7.4×10^{1}		Wang et al. (2017)	Q	80, 239
ISENHDUDKGYVAU-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MEKCOOH	4.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	1.0×10^{2}		Wang et al. (2017)	Q	80, 239
PSPWSCBXMKHAFW-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MVKOOH	1.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_3$	2.6×10^{2}		Wang et al. (2017)	Q	80, 239
PRFKYXWFQJOCGY-UHFFFAOYSA-N	9.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C41CO3H	4.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	2.0×10^{3}		Wang et al. (2017)	Q	80, 239
FAYQBJFLFGEPOW-UHFFFAOYSA-N	3.3		Wang et al. (2017)	Q	80, 240
MCM:C5CO14OOH	2.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_4$	7.8×10^{4}		Wang et al. (2017)	Q	80, 239
FKGAAIITVQJZMS-UHFFFAOYSA-N	4.4		Wang et al. (2017)	Q	80, 240
MCM:C5CO234	2.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_3$	2.2×10^{3}		Wang et al. (2017)	Q	80, 239
MVDYEFQVZNBPPH-UHFFFAOYSA-N	2.5×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C5CO234OOH	1.6×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_5$	3.0×10^{6}		Wang et al. (2017)	Q	80, 239
XNGUZQHZGCMOHY-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C5CO23OOH	2.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	5.3×10^{3}		Wang et al. (2017)	Q	80, 239
BRUGMCFWMGXRAP-UHFFFAOYSA-N	3.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO23C4CO3H	3.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_5$	4.5×10^{5}		Wang et al. (2017)	Q	80, 239
BRGQKBIYWSYIOL-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO23C54OOH	2.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	4.0×10^{3}		Wang et al. (2017)	Q	80, 239
QASRSSCEZIIDDC-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO24C53OOH	2.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	2.1×10^{4}		Wang et al. (2017)	Q	80, 239
AULGAHCEUUOLTF-UHFFFAOYSA-N	8.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO2C4CO3H	1.9×10^{4}	12000	Wieser et al. (2023)	Q	437
$C_5H_8O_4$	4.8×10^{4}		Wang et al. (2017)	Q	80, 238
COVHHGSUFOHLBW-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	80, 239
	7.1×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CO3C4CO3H	4.8×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	2.5×10^3		Wang et al. (2017)	Q	80, 239
HMOQHHYQXPCOJD-UHFFFAOYSA-N	1.6×10^1		Wang et al. (2017)	Q	80, 240
MCM:DIEKAOOH	3.7×10^3		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	3.6×10^1		Wang et al. (2017)	Q	80, 239
GVIFMISHBUBLQF-UHFFFAOYSA-N	1.0×10^2		Wang et al. (2017)	Q	80, 240
MCM:DIEKBOOH	3.2×10^3		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	3.4×10^3		Wang et al. (2017)	Q	80, 239
PNIUWVGTVWVIRO-UHFFFAOYSA-N	3.0×10^3		Wang et al. (2017)	Q	80, 240
MCM:MIPKAOOH	2.6×10^3		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	1.6×10^1		Wang et al. (2017)	Q	80, 239
UWVYZAHMDOAIIN-UHFFFAOYSA-N	9.3×10^1		Wang et al. (2017)	Q	80, 240
MCM:MIPKBOOH	3.7×10^3		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	3.2×10^3		Wang et al. (2017)	Q	80, 239
OWEKNVKRJSTQCB-UHFFFAOYSA-N	6.8×10^2		Wang et al. (2017)	Q	80, 240
MCM:MPRKAOOH	3.7×10^3		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	4.0×10^1		Wang et al. (2017)	Q	80, 239
RFXMBEJILJIJHO-UHFFFAOYSA-N	8.9×10^1		Wang et al. (2017)	Q	80, 240
MCM:MPRKBOOH	3.7×10^3		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	2.3×10^3		Wang et al. (2017)	Q	80, 239
BOKMIGXVNYNOOE-UHFFFAOYSA-N	8.5×10^2		Wang et al. (2017)	Q	80, 240
MCM:PE2ONE1OOH	3.2×10^3		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	5.8×10^1		Wang et al. (2017)	Q	80, 239
NFPIZNOAHNBIPJ-UHFFFAOYSA-N	3.9×10^1		Wang et al. (2017)	Q	80, 240
MCM:C23C54CO3H	3.0×10^7		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	1.7×10^5		Wang et al. (2017)	Q	80, 239
FOQTZZGGVXWRDJ-UHFFFAOYSA-N	2.0×10^1		Wang et al. (2017)	Q	80, 240
MCM:C3COCCO3H	3.7×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	1.4×10^3		Wang et al. (2017)	Q	80, 239
NQEGAXBMSWAEEJ-UHFFFAOYSA-N	2.6×10^1		Wang et al. (2017)	Q	80, 240
MCM:C4DBDIKET	1.0×10^2		Wang et al. (2017)	Q	80, 238
$C_6H_8O_2$	1.8×10^3		Wang et al. (2017)	Q	80, 239
OTSKZNVDZOOHRX-UHFFFAOYSA-N	2.6×10^2		Wang et al. (2017)	Q	80, 240
MCM:C51CO3H	4.5×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	3.7×10^3		Wang et al. (2017)	Q	80, 239
JNOOBNCRVAKFDO-UHFFFAOYSA-N	2.5×10^1		Wang et al. (2017)	Q	80, 240
MCM:C5CODBCO3H	1.3×10^5		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	5.6×10^4		Wang et al. (2017)	Q	80, 239
DSQMAYIDJPXZOY-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C5DBCOCO3H	1.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	5.4×10^{4}		Wang et al. (2017)	Q	80, 239
NVTHKHSWEWVMOZ-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	80, 240
MCM:C611OOH	1.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	3.1×10^{3}		Wang et al. (2017)	Q	80, 239
YTLUYDMGHZZGIK-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C619OOH	6.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	3.0×10^{6}		Wang et al. (2017)	Q	80, 239
CLPCTPYJHZPKKC-UHFFFAOYSA-N	1.9×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C627OOH	1.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	2.3×10^{5}		Wang et al. (2017)	Q	80, 239
BKNNHKNGGIDPKB-UHFFFAOYSA-N	5.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C62OOH	1.5×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	1.4×10^{6}		Wang et al. (2017)	Q	80, 239
NRJLAAIGKSDANL-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C6CO134OOH	2.5×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	2.3×10^{5}		Wang et al. (2017)	Q	80, 239
KXHHBNOARBHHNQ-UHFFFAOYSA-N	3.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C6CO34	2.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_2$	5.4		Wang et al. (2017)	Q	80, 239
KVFQMAZOBTXCAZ-UHFFFAOYSA-N	1.1×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C6CO34OOH	2.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	2.0×10^{3}		Wang et al. (2017)	Q	80, 239
GOPKJUXJYMJAQC-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C6CYTONOOH	4.8×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_5$	2.1×10^{9}		Wang et al. (2017)	Q	80, 239
JAWAIWJCDBIXQU-UHFFFAOYSA-N	2.6×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C6DCRBBOOH	1.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	2.9×10^{4}		Wang et al. (2017)	Q	80, 239
JRENYXREJDINFO-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	80, 240
MCM:CO234C6	1.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	1.1×10^{3}		Wang et al. (2017)	Q	80, 239
FYLKBSXPBXZFJV-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:CO234C6OOH	1.5×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
RXZSKHWIVPRCNE-UHFFFAOYSA-N	4.9		Wang et al. (2017)	Q	80, 240
MCM:CO235C6	1.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	3.1×10^{3}		Wang et al. (2017)	Q	80, 239
POASQEFMMPWSLD-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CO235C6OOH	1.3×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	2.9×10^{6}		Wang et al. (2017)	Q	80, 239
OFEOQWJKJVUBKA-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CO23C65OOH	2.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	9.6×10^{4}		Wang et al. (2017)	Q	80, 239
QKJDOFMXAZMTSN-UHFFFAOYSA-N	3.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CO23C6	2.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_2$	6.0		Wang et al. (2017)	Q	80, 239
MWVFCEVNXHTDNF-UHFFFAOYSA-N	7.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:CO24C63OOH	2.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	9.1×10^{3}		Wang et al. (2017)	Q	80, 239
BCTNDVKHSPOTQH-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO24C6	2.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_2$	3.5×10^{1}		Wang et al. (2017)	Q	80, 239
NDOGLIPWGGRQCO-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO24C6OOH	2.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	1.3×10^{4}		Wang et al. (2017)	Q	80, 239
SLWLMHWJPVVUSV-UHFFFAOYSA-N	5.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO24M3C5	3.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_2$	2.1×10^{1}		Wang et al. (2017)	Q	80, 239
GSOHKPVFCOWKPU-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO25C6	2.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_2$	4.9×10^{2}		Wang et al. (2017)	Q	80, 239
OJVAMHKKJGICOG-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CO25C6OOH	2.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	6.6×10^{4}		Wang et al. (2017)	Q	80, 239
JXALTZPWVLRWQW-UHFFFAOYSA-N	6.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:CO2C54CO3H	4.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	3.8×10^{3}		Wang et al. (2017)	Q	80, 239
CNZIZHTUCKWXKF-UHFFFAOYSA-N	4.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO2M33CO3H	2.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	7.1×10^{2}		Wang et al. (2017)	Q	80, 239
NINAOMADVJMMOS-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	80, 240
MCM:CO3C54CO3H	4.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	8.7×10^{2}		Wang et al. (2017)	Q	80, 239
VXADHVSNPNTBLA-UHFFFAOYSA-N	1.8		Wang et al. (2017)	Q	80, 240
MCM:CO3C5CO3H	3.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	5.3×10^{3}		Wang et al. (2017)	Q	80, 239
NEAYDZAAQZUWAX-UHFFFAOYSA-N	3.3×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:CY6COCOOOH	6.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	1.1×10^{8}		Wang et al. (2017)	Q	80, 239
PCNCBCRTMCKUHD-UHFFFAOYSA-N	4.5×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:CY6DIONOOH	6.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	2.2×10^{7}		Wang et al. (2017)	Q	80, 239
WZMMYHNHRXLTAA-UHFFFAOYSA-N	5.8×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:CYC613DION	8.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_2$	2.5×10^{3}		Wang et al. (2017)	Q	80, 239
HJSLFCCWAKVHIW-UHFFFAOYSA-N	2.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:CYC6DIONE	8.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_2$	6.5×10^{2}		Wang et al. (2017)	Q	80, 239
OILAIQUEIWYQPH-UHFFFAOYSA-N	8.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CYHXONAOOH	9.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	4.8×10^{4}		Wang et al. (2017)	Q	80, 239
YLRYKXGGQIKRPE-UHFFFAOYSA-N	5.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:ECO3CO3H	2.0×10^{10}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_6$	2.6×10^{7}		Wang et al. (2017)	Q	80, 239
LOIDTPBEOYVNRI-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:EIPKAOOH	2.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	8.9		Wang et al. (2017)	Q	80, 239
UUAGRKYHKVSONO-UHFFFAOYSA-N	4.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:EIPKBOOH	2.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.7×10^{3}		Wang et al. (2017)	Q	80, 239
GSVDUVPILFIVQC-UHFFFAOYSA-N	5.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HEX2ONAOOH	2.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
BPODHSIMBCVMGL-UHFFFAOYSA-N	2.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HEX2ONBOOH	2.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	3.5×10^{3}		Wang et al. (2017)	Q	80, 239
XXENGSKOCXRCDY-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HEX2ONCOOH	2.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	2.8×10^{1}		Wang et al. (2017)	Q	80, 239
UIIPZQPVNWMUDI-UHFFFAOYSA-N	4.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HEX3ONAOOH	2.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.3×10^{3}		Wang et al. (2017)	Q	80, 239
ZKBVMKAKXKAOJC-UHFFFAOYSA-N	6.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HEX3ONBOOH	2.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	2.2×10^{1}		Wang et al. (2017)	Q	80, 239
CFZVDJFTDOASSJ-UHFFFAOYSA-N	9.1×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:HEX3ONCOOH	2.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	2.3×10^{1}		Wang et al. (2017)	Q	80, 239
RCWXBCITQMXQRJ-UHFFFAOYSA-N	5.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HEX3ONDOOH	2.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	2.2×10^{3}		Wang et al. (2017)	Q	80, 239
GTTLVNDFVPDHBU-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:M2BKAOOH	3.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.6×10^{3}		Wang et al. (2017)	Q	80, 239
UYZBTKCJJDJNOE-UHFFFAOYSA-N	8.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:M2BKBOOH	2.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.1×10^{1}		Wang et al. (2017)	Q	80, 239
HXTZBJMRLHBTDT-UHFFFAOYSA-N	3.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MIBK3CO	3.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_2$	5.1		Wang et al. (2017)	Q	80, 239
JENYBWHRLYZSSZ-UHFFFAOYSA-N	5.9×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:MIBK3COOOH	1.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	8.9×10^{2}		Wang et al. (2017)	Q	80, 239
REESTLWXXTVHDK-UHFFFAOYSA-N	6.8		Wang et al. (2017)	Q	80, 240
MCM:MIBKAOOH	2.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	8.5×10^{2}		Wang et al. (2017)	Q	80, 239
TVLYPTZVJFAYSU-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MIBKBOOH	3.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	3.2×10^{1}		Wang et al. (2017)	Q	80, 239
NTAUGUQNNYBRPR-UHFFFAOYSA-N	3.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MTBKOOH	2.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.6×10^{3}		Wang et al. (2017)	Q	80, 239
FSDVGLADHCPPED-UHFFFAOYSA-N	5.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C235C6CO3H	1.6×10^{10}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_6$	4.4×10^{7}		Wang et al. (2017)	Q	80, 239
MCULIRAVDBAPRO-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C710OOH	1.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_3$	5.1×10^{2}		Wang et al. (2017)	Q	80, 239
WMYMHSKADBIKCY-UHFFFAOYSA-N	6.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C713OOH	1.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	1.2×10^{4}		Wang et al. (2017)	Q	80, 239
BVAIBJLRLSWCNT-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C714OOH	2.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	3.0×10^{4}		Wang et al. (2017)	Q	80, 239
FQLJODGQMVISEK-UHFFFAOYSA-N	2.1×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C715OOH	8.3×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	2.5×10^{5}		Wang et al. (2017)	Q	80, 239
IFAJGMRYFBSYLP-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C7236CO	6.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_3$	6.8×10^{4}		Wang et al. (2017)	Q	80, 239
ZXGNNLLPQXKXPQ-UHFFFAOYSA-N	8.7		Wang et al. (2017)	Q	80, 240
MCM:C726CO5OOH	7.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	1.0×10^{5}		Wang et al. (2017)	Q	80, 239
DRGOPDAWFSWANX-UHFFFAOYSA-N	6.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C727CO	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	5.6×10^{3}		Wang et al. (2017)	Q	80, 239
XDJAUXXWCBLXGT-UHFFFAOYSA-N	6.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C727OOH	2.0×10^{5}	13000	Wieser et al. (2023)	Q	437
$C_7H_{12}O_4$	1.8×10^{6}		Wang et al. (2017)	Q	80, 238
IMCLYNFQESJQRO-UHFFFAOYSA-N	4.3×10^{4}		Wang et al. (2017)	Q	80, 239
	9.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C73OOH	1.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
QFXLTANEYKLVBH-UHFFFAOYSA-N	7.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C74OOH	1.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	1.4×10^{6}		Wang et al. (2017)	Q	80, 239
ZLQFKUKGFNRBMM-UHFFFAOYSA-N	4.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C75OOH	2.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_3$	8.9×10^{2}		Wang et al. (2017)	Q	80, 239
YNKFHYFADYHYPZ-UHFFFAOYSA-N	1.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C7ADCCO3H	8.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	6.5×10^{4}		Wang et al. (2017)	Q	80, 239
KFHCVBUEDOHUEG-UHFFFAOYSA-N	5.0		Wang et al. (2017)	Q	80, 240
MCM:C7BDICARB	6.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_2$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
SGWFXGZCQBUONH-UHFFFAOYSA-N	3.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C7DCCO3H	1.4×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	1.5×10^{4}		Wang et al. (2017)	Q	80, 239
VBFDFNFUMYAFQG-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	80, 240
MCM:C7DDCCO3H	1.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	2.2×10^{4}		Wang et al. (2017)	Q	80, 239
ITRURPAVBUVUCD-UHFFFAOYSA-N	5.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C7EDICARB	9.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_2$	1.1×10^{3}		Wang et al. (2017)	Q	80, 239
YTVSAHBJOWKZHT-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C821OOH	1.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	2.6×10^{6}		Wang et al. (2017)	Q	80, 239
VNKKTGYQOPWEKF-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CO235C7	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	9.6×10^{2}		Wang et al. (2017)	Q	80, 239
PLNIROICNOROEN-UHFFFAOYSA-N	9.6		Wang et al. (2017)	Q	80, 240
MCM:CO245C7	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	9.6×10^{2}		Wang et al. (2017)	Q	80, 239
SOSHREJUCDQQIR-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO25C6CO3H	2.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	4.6×10^{6}		Wang et al. (2017)	Q	80, 239
NZAOVWOYFADSGM-UHFFFAOYSA-N	7.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:CO25C73OOH	1.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	2.8×10^{4}		Wang et al. (2017)	Q	80, 239
NWTMJMDPQCUZCE-UHFFFAOYSA-N	9.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CO25C74OOH	1.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	2.8×10^{4}		Wang et al. (2017)	Q	80, 239
VDRXHYKLZSMLBZ-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:CO25C7	2.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_2$	2.6×10^{2}		Wang et al. (2017)	Q	80, 239
HGRGPAAXHOTBAM-UHFFFAOYSA-N	8.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO3C75OOH	2.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_3$	8.0×10^{2}		Wang et al. (2017)	Q	80, 239
TVVPPVSOZMPRIM-UHFFFAOYSA-N	4.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:IC7DCCO3H	1.4×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	1.6×10^{4}		Wang et al. (2017)	Q	80, 239
JFPQYVJBAXIOAT-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:M3CO245C6	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	6.3×10^{2}		Wang et al. (2017)	Q	80, 239
FMABCBYNHKBBEH-UHFFFAOYSA-N	8.5		Wang et al. (2017)	Q	80, 240
MCM:M3CO25C6	2.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_2$	1.8×10^{2}		Wang et al. (2017)	Q	80, 239
NLLILAUVOOREKR-UHFFFAOYSA-N	8.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C5DBECO3H	6.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_5$	1.5×10^{6}		Wang et al. (2017)	Q	80, 239
QHSWUEYXPZRIAH-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:C5EDBCO3H	6.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_5$	1.6×10^{6}		Wang et al. (2017)	Q	80, 239
YXJCVNQUVAHMKT-UHFFFAOYSA-N	6.9×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C727CO3H	2.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	9.6×10^{5}		Wang et al. (2017)	Q	80, 239
FJTLPXSURBYIDW-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C7CO2M5OOH	4.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
GOMWBXPFFZKXIF-UHFFFAOYSA-N	2.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C7M2CO5OOH	4.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	7.6×10^{4}		Wang et al. (2017)	Q	80, 239
BVDWDBGMQXZSJX-UHFFFAOYSA-N	4.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C7M3CO	4.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_3$	8.1×10^{4}		Wang et al. (2017)	Q	80, 239
WFGYJTNUNWJHJN-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C7ODLBCO3H	8.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	1.2×10^{4}		Wang et al. (2017)	Q	80, 239
NMESNSUDSMNPLZ-UHFFFAOYSA-N	3.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C816CO	3.1×10^{2}	10000	Wieser et al. (2023)	Q	437
$C_8H_{12}O_2$	3.8×10^{1}		Wang et al. (2017)	Q	80, 238
FXXXYZSMIIVJDG-UHFFFAOYSA-N	3.0×10^{2}		Wang et al. (2017)	Q	80, 239
	6.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C816OOH	4.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_3$	2.0×10^{3}		Wang et al. (2017)	Q	80, 239
GWYFGLCLLKWWIQ-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C817OOH	1.2×10^{6}	13000	Wieser et al. (2023)	Q	437
$C_8H_{14}O_4$	1.5×10^{6}		Wang et al. (2017)	Q	80, 238
WQMXPSRLZZCZTO-UHFFFAOYSA-N	1.5×10^{6}		Wang et al. (2017)	Q	80, 239
	1.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C8236CO	4.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_3$	6.0×10^{4}		Wang et al. (2017)	Q	80, 239
IOHUPZZTKNTURH-UHFFFAOYSA-N	4.8		Wang et al. (2017)	Q	80, 240
MCM:C826CO3OOH	6.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	4.4×10^{4}		Wang et al. (2017)	Q	80, 239
JGDMXPACXAYITG-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C827OOH	9.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_4$	1.5×10^{4}		Wang et al. (2017)	Q	80, 239
MYZHYUNBFYQPIX-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C828OOH	6.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	3.1×10^{5}		Wang et al. (2017)	Q	80, 239
IPIPKWBUGMDLTO-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C83OOH	1.1×10^{9}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	3.6×10^{5}		Wang et al. (2017)	Q	80, 239
MTDHYROWVQXAOV-UHFFFAOYSA-N	5.6		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C84OOH	1.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_4$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
HQUQRVBRCVTTSE-UHFFFAOYSA-N	7.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C85OOH	5.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_3$	5.5×10^{3}		Wang et al. (2017)	Q	80, 239
MGHQHHXZPXRHRQ-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C88CO	2.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_3$	7.4×10^{4}		Wang et al. (2017)	Q	80, 239
KYJUTSWXKQCOOZ-UHFFFAOYSA-N	3.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C88OOH	3.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	6.9×10^{5}		Wang et al. (2017)	Q	80, 239
LSPOECQNSUKNPK-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C8BCCO	2.0×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O$	9.6×10^{-1}		Wang et al. (2017)	Q	80, 239
BYOKRVKHSHTAOM-UHFFFAOYSA-N	3.7		Wang et al. (2017)	Q	80, 240
MCM:CO346C8	1.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_3$	1.1×10^{3}		Wang et al. (2017)	Q	80, 239
YUHNMHTZZXLCQZ-UHFFFAOYSA-N	7.3		Wang et al. (2017)	Q	80, 240
MCM:CO36C8	1.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_2$	1.5×10^{2}		Wang et al. (2017)	Q	80, 239
CVZGUJMLZZTPKH-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO3C85OOH	2.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{16}O_3$	5.9×10^{2}		Wang et al. (2017)	Q	80, 239
RPACFUNWVVDXHA-UHFFFAOYSA-N	3.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MXYQONE	2.1		Wang et al. (2017)	Q	80, 238
$C_8H_8O_2$	5.3×10^{3}		Wang et al. (2017)	Q	80, 239
SENUUPBBLQWHMF-UHFFFAOYSA-N	1.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:OXYQONE	2.1		Wang et al. (2017)	Q	80, 238
$C_8H_8O_2$	5.3×10^{3}		Wang et al. (2017)	Q	80, 239
AIACLXROWHONEE-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PEBQONE	2.7		Wang et al. (2017)	Q	80, 238
$C_8H_8O_2$	4.7×10^{3}		Wang et al. (2017)	Q	80, 239
IGRSQEOIAAGSGS-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PXYQONE	2.1		Wang et al. (2017)	Q	80, 238
$C_8H_8O_2$	5.3×10^{3}		Wang et al. (2017)	Q	80, 239
MYKLQMNSFPAPLZ-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C816CO3H	5.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	1.5×10^{3}		Wang et al. (2017)	Q	80, 239
IXOBJDNIWKDFSA-UHFFFAOYSA-N	3.9×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:C817CO3H	3.4×10^{7}	16000	Wieser et al. (2023)	Q	437
$C_9H_{14}O_5$	1.7×10^{7}		Wang et al. (2017)	Q	80, 238
NVOUBBWYYUIRJW-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	80, 239
	2.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C827CO3H	1.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	6.0×10^{5}		Wang et al. (2017)	Q	80, 239
DZJUGPICXPPSEN-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C828CO3H	7.8×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_6$	2.0×10^{7}		Wang et al. (2017)	Q	80, 239
XCCOWFUPSKLDCA-UHFFFAOYSA-N	8.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C85CO3H	5.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	3.8×10^{3}		Wang et al. (2017)	Q	80, 239
DAYKQISVSRMABH-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C88CO3H	3.7×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	2.0×10^{7}		Wang et al. (2017)	Q	80, 239
KOEDWBONHQRVNE-UHFFFAOYSA-N	4.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C8M2CO6OOH	3.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	3.3×10^{4}		Wang et al. (2017)	Q	80, 239
LMHVWEUXUKAUEE-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C8M3CO	3.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	6.0×10^{4}		Wang et al. (2017)	Q	80, 239
VNKKGGMTAOGJCS-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C917OOH	2.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	1.2×10^{7}		Wang et al. (2017)	Q	80, 239
USPARXGTYFQAAO-UHFFFAOYSA-N	1.2×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C91OOH	1.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{18}O_3$	4.9×10^{2}		Wang et al. (2017)	Q	80, 239
LTHHCRGMHVQJHW-UHFFFAOYSA-N	4.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C923OOH	1.1×10^{4}	12000	Wieser et al. (2023)	Q	437
$C_9H_{16}O_3$	4.1×10^{3}		Wang et al. (2017)	Q	80, 238
ZSCOJLRNNZZYOH-UHFFFAOYSA-N	2.2×10^{3}		Wang et al. (2017)	Q	80, 239
	2.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C928OOH	8.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_4$	1.4×10^{6}		Wang et al. (2017)	Q	80, 239
NVMDAOHKHIQTQS-UHFFFAOYSA-N	1.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C94OOH	1.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_4$	9.3×10^{3}		Wang et al. (2017)	Q	80, 239
ZEMHBLLRPWJDGD-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C95OOH	8.7×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	2.3×10^{5}		Wang et al. (2017)	Q	80, 239
OKPNQXXXVOPUSS-UHFFFAOYSA-N	5.4		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C96OOH	4.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_3$	6.9×10^{3}		Wang et al. (2017)	Q	80, 239
UOSOYGOFRNBVGT-UHFFFAOYSA-N	4.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C9DC	1.2×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	2.3×10^{3}		Wang et al. (2017)	Q	80, 239
MRLMBLCAGJIZHM-UHFFFAOYSA-N	4.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C9DCCO	9.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_3$	7.6×10^{5}		Wang et al. (2017)	Q	80, 239
CNGBBXSWKSNDLL-UHFFFAOYSA-N	2.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C9DCOOH	1.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	8.3×10^{7}		Wang et al. (2017)	Q	80, 239
LVYPIBNFNZWAIN-UHFFFAOYSA-N	2.8×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:CO356C9	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_3$	1.1×10^{3}		Wang et al. (2017)	Q	80, 239
UAWDJSGDSYOWDW-UHFFFAOYSA-N	5.3		Wang et al. (2017)	Q	80, 240
MCM:CO36C9	1.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_2$	1.0×10^{2}		Wang et al. (2017)	Q	80, 239
NTESOQURXNMSRF-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:IPRBQONE	2.5		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_2$	2.4×10^{3}		Wang et al. (2017)	Q	80, 239
XLTSBDOZTUSCMX-UHFFFAOYSA-N	8.7		Wang et al. (2017)	Q	80, 240
MCM:LIMKET	6.4×10^{-1}	8000	Wieser et al. (2023)	Q	437
$C_9H_{14}O$	2.4×10^{-1}		Wang et al. (2017)	Q	80, 238
HOBBEYSRFFJETF-UHFFFAOYSA-N	9.8×10^{-1}		Wang et al. (2017)	Q	80, 239
	3.2		Wang et al. (2017)	Q	80, 240
MCM:METLQONE	1.8		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_2$	3.7×10^{3}		Wang et al. (2017)	Q	80, 239
FBVFNJVAQSWLOP-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NOPINAOOH	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_3$	2.9×10^{4}		Wang et al. (2017)	Q	80, 239
AGOGLNHOAIUZEO-UHFFFAOYSA-N	8.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NOPINBCO	1.2×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	2.2×10^{3}		Wang et al. (2017)	Q	80, 239
AQDJLLQBBRXMBZ-UHFFFAOYSA-N	4.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NOPINBOOH	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_3$	4.0×10^{4}		Wang et al. (2017)	Q	80, 239
ICIAOEDGJQUKIV-UHFFFAOYSA-N	9.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NOPINCOOH	8.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_3$	1.3×10^{4}		Wang et al. (2017)	Q	80, 239
YDBPVAMAGOPNKC-UHFFFAOYSA-N	7.1×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NOPINDCO	1.2×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_2$	5.0×10^{2}		Wang et al. (2017)	Q	80, 239
QEZVNLZLSDOZRT-UHFFFAOYSA-N	8.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NOPINDOOH	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_3$	5.4×10^{2}		Wang et al. (2017)	Q	80, 239
MUTHAEIFCDWSQQ-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NOPINONE	1.8×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O$	1.0		Wang et al. (2017)	Q	80, 239
XZFDKWMYCUEKSS-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:OETLQONE	1.8		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_2$	3.7×10^{3}		Wang et al. (2017)	Q	80, 239
CMBANAGVBLPIPT-UHFFFAOYSA-N	8.1		Wang et al. (2017)	Q	80, 240
MCM:PETLQONE	1.8		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_2$	3.7×10^{3}		Wang et al. (2017)	Q	80, 239
JUIQOKRNPGGIPV-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PPRBQONE	2.2		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_2$	3.0×10^{3}		Wang et al. (2017)	Q	80, 239
NBHAZVWKRHTWRW-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:TM124QONE	1.4		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_2$	4.1×10^{3}		Wang et al. (2017)	Q	80, 239
QIXDHVDGPXBRRD-UHFFFAOYSA-N	7.3		Wang et al. (2017)	Q	80, 240
MCM:C1011CO	3.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_2$	3.3×10^{2}		Wang et al. (2017)	Q	80, 239
HCTKOTXYXFZDNL-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C1011OOH	3.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_3$	4.3×10^{3}		Wang et al. (2017)	Q	80, 239
SNMQVMGNQAVOQP-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C101OOH	1.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{20}O_3$	4.4×10^{2}		Wang et al. (2017)	Q	80, 239
SFSDJTUNVGVIHA-UHFFFAOYSA-N	3.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C104OOH	1.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_4$	6.9×10^{3}		Wang et al. (2017)	Q	80, 239
NAKDXHBWPFMZPE-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C105OOH	7.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_5$	1.7×10^{5}		Wang et al. (2017)	Q	80, 239
SMUSKFONQIUMCM-UHFFFAOYSA-N	2.9		Wang et al. (2017)	Q	80, 240
MCM:C923CO3H	2.2×10^{4}	15000	Wieser et al. (2023)	Q	437
$C_{10}H_{16}O_4$	4.7×10^{4}		Wang et al. (2017)	Q	80, 238
JSHGCXGTVADTAK-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	80, 239
	3.1×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C928CO3H	9.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_5$	1.5×10^{6}		Wang et al. (2017)	Q	80, 239
LCMHUZKVXFPENZ-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C9M2CO6OOH	3.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_4$	1.9×10^{4}		Wang et al. (2017)	Q	80, 239
ACPAJMUJFSDSAX-UHFFFAOYSA-N	9.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C9M3CO	3.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{14}O_3$	3.5×10^{4}		Wang et al. (2017)	Q	80, 239
DYAPBQRZCBYWEA-UHFFFAOYSA-N	9.3		Wang et al. (2017)	Q	80, 240
MCM:CO356C10	8.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_3$	9.1×10^{2}		Wang et al. (2017)	Q	80, 239
OKXFSYMNZFSQOL-UHFFFAOYSA-N	4.7		Wang et al. (2017)	Q	80, 240
MCM:CO36C10	1.2×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_2$	8.0×10^{1}		Wang et al. (2017)	Q	80, 239
WYDYPTCJLWEFAY-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DEC3ONE	1.8×10^{-2}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{20}O$	2.6×10^{-2}		Wang et al. (2017)	Q	80, 239
XJLDYKIEURAVBW-UHFFFAOYSA-N	1.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:PERPINONIC	5.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_4$	3.0×10^{3}		Wang et al. (2017)	Q	80, 239
VFMYUIAYOIIENK-UHFFFAOYSA-N	5.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C1011CO3H	4.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_4$	2.5×10^{3}		Wang et al. (2017)	Q	80, 239
MDKPIQZZHUIYJQ-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C111OOH	1.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{22}O_3$	3.6×10^{2}		Wang et al. (2017)	Q	80, 239
AMIJEMPORNLGBW-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C114OOH	8.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{20}O_4$	5.4×10^{3}		Wang et al. (2017)	Q	80, 239
YQNGKLISCMALPY-UHFFFAOYSA-N	4.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C115OOH	6.3×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_5$	1.3×10^{5}		Wang et al. (2017)	Q	80, 239
VPBZYPGTLQIJKG-UHFFFAOYSA-N	6.0		Wang et al. (2017)	Q	80, 240
MCM:CO356C11	7.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_3$	7.8×10^{2}		Wang et al. (2017)	Q	80, 239
YADKKYWEPSBFCL-UHFFFAOYSA-N	4.9		Wang et al. (2017)	Q	80, 240
MCM:CO36C11	1.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{20}O_2$	6.5×10^{1}		Wang et al. (2017)	Q	80, 239
KWHQQLQVDJMZTG-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:UDEC3ONE	1.4×10^{-2}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{22}O$	2.1×10^{-2}		Wang et al. (2017)	Q	80, 239
YNMZZHPSYMOGCI-UHFFFAOYSA-N	1.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C121OOH	9.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{24}O_3$	2.8×10^{2}		Wang et al. (2017)	Q	80, 239
NWJGDRGQGOZUDJ-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C124OOH	6.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{22}O_4$	4.8×10^{3}		Wang et al. (2017)	Q	80, 239
DCPRRPHGFZBUMW-UHFFFAOYSA-N	9.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C125OOH	4.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_5$	1.1×10^{5}		Wang et al. (2017)	Q	80, 239
FTFXETPWXOMYNK-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO356C12	5.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_3$	7.3×10^{2}		Wang et al. (2017)	Q	80, 239
FQYVJQVZHPFSKC-UHFFFAOYSA-N	3.9		Wang et al. (2017)	Q	80, 240
MCM:CO36C12	8.5		Wang et al. (2017)	Q	80, 238
$C_{12}H_{22}O_2$	5.8×10^{1}		Wang et al. (2017)	Q	80, 239
RUTQSYKISNASLK-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DDEC3ONE	1.1×10^{-2}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{24}O$	1.7×10^{-2}		Wang et al. (2017)	Q	80, 239
PERIHWAPLOBAJM-UHFFFAOYSA-N	9.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C131OOH	1.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_4$	2.0×10^{6}		Wang et al. (2017)	Q	80, 239
HPZPYFVEAXAGHY-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:BCKET	2.3×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O$	2.6		Wang et al. (2017)	Q	80, 239
MBZBBVTYLUNZPJ-UHFFFAOYSA-N	2.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C131CO3H	1.7×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_5$	2.1×10^{6}		Wang et al. (2017)	Q	80, 239
LLSRBTGTUZNRQT-UHFFFAOYSA-N	8.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C141OOH	3.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{24}O_3$	4.9×10^{3}		Wang et al. (2017)	Q	80, 239
HKWHMEKBBPOBSQ-UHFFFAOYSA-N	7.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C141CO3H	4.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{24}O_4$	1.8×10^{3}		Wang et al. (2017)	Q	80, 239
ADRMPTUALHKSOU-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C619CO	5.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_3$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
NGHVTTBOPYXCFB-UHFFFAOYSA-N	1.1×10^{5}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:CY6TRION	5.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_3$	4.6×10^{6}		Wang et al. (2017)	Q	80, 239
GKSCYYCYSPXQFY-UHFFFAOYSA-N	1.9×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PHCOMEOOH	1.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_8O_3$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
BXVCLOREWFXMNM-UHFFFAOYSA-N	3.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MPHCOMEOOH	9.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_3$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
NJDRUBYBGCJLGU-UHFFFAOYSA-N	3.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PHCOCOCOOH	9.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_8O_4$	4.7×10^{4}		Wang et al. (2017)	Q	80, 239
XMJMKOZGMVOAIC-UHFFFAOYSA-N	5.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PHCOCOME	1.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_8O_2$	9.1×10^{1}		Wang et al. (2017)	Q	80, 239
BVQVLAIMHVDZEL-UHFFFAOYSA-N	6.9		Wang et al. (2017)	Q	80, 240
MCM:PHCOETOOH	1.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_3$	6.0×10^{2}		Wang et al. (2017)	Q	80, 239
RYQHVKZCKUBIFL-UHFFFAOYSA-N	3.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DMPHCOME	7.4×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{12}O$	1.5		Wang et al. (2017)	Q	80, 239
BKIHFZLJJUNKMZ-UHFFFAOYSA-N	5.4		Wang et al. (2017)	Q	80, 240
MCM:DMPHCOMOOH	5.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{12}O_3$	8.5×10^{2}		Wang et al. (2017)	Q	80, 239
SEDWELDPOZYWLL-UHFFFAOYSA-N	3.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:EMPHCOME	6.5×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{14}O$	1.2		Wang et al. (2017)	Q	80, 239
CZNQKVDFQIGBEW-UHFFFAOYSA-N	5.0		Wang et al. (2017)	Q	80, 240
MCM:EMPHCOMOOH	5.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{14}O_3$	5.0×10^{2}		Wang et al. (2017)	Q	80, 239
OJNDCDHAKIGFTB-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:BIACETOH	5.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_3$	4.3×10^{3}		Wang et al. (2017)	Q	80, 239
NXIVQSJQXMAXJR-UHFFFAOYSA-N	3.7		Wang et al. (2017)	Q	80, 240
MCM:CO2H3CO3H	2.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_5$	1.7×10^{4}		Wang et al. (2017)	Q	80, 239
WNDCXKJVOGKFRM-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:H13CO2CO3H	1.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_6$	4.0×10^{5}		Wang et al. (2017)	Q	80, 239
RXVYYLAFXUAZCR-UHFFFAOYSA-N	1.7×10^{5}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:H14CO23C4	2.1×10^{6}	17000	Wieser et al. (2023)	Q	437
$C_4H_6O_4$	6.5×10^{5}		Wang et al. (2017)	Q	80, 238
GJCZUCLKDGABDS-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	80, 239
	1.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:H1C23C4OOH	3.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_5$	6.0×10^{7}		Wang et al. (2017)	Q	80, 239
FQXHRCVOGVCTSR-UHFFFAOYSA-N	3.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HMVKAOOH	8.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	7.8×10^{4}		Wang et al. (2017)	Q	80, 239
XTELZFGIGJBUGR-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HMVKBOOH	1.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	2.0×10^{5}		Wang et al. (2017)	Q	80, 239
NGLQGLCPXKPDMS-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO12CO3C4	9.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	3.7×10^{4}		Wang et al. (2017)	Q	80, 239
SEYLPRWNVFCVRQ-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO14CO2C4	1.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	9.8×10^{5}		Wang et al. (2017)	Q	80, 239
XBJODPUPYBBDEM-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HOCO3C4OOH	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	1.9×10^{6}		Wang et al. (2017)	Q	80, 239
GQXQZBROPOTXJQ-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:MEKAOH	1.5×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_2$	1.2×10^{3}		Wang et al. (2017)	Q	80, 239
LVSQXDHWDCMMRJ-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MEKCOH	7.8		Wang et al. (2017)	Q	80, 238
$C_4H_8O_2$	7.8×10^{1}		Wang et al. (2017)	Q	80, 239
GFAZHVHNLUBROE-UHFFFAOYSA-N	8.3		Wang et al. (2017)	Q	80, 240
MCM:MVKOHAOH	6.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	3.7×10^{6}		Wang et al. (2017)	Q	80, 239
UQPHVQVXLPRNCX-UHFFFAOYSA-N	8.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:MVKOHAOOH	4.6×10^{8}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_5$	2.2×10^{7}		Wang et al. (2017)	Q	80, 239
MOVXURHCNUWOQO-UHFFFAOYSA-N	1.8×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:MVKOHBOOH	2.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_5$	2.7×10^{8}		Wang et al. (2017)	Q	80, 239
WSMWIMXDHMPHIN-UHFFFAOYSA-N	5.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:MVKOH	2.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_2$	2.3×10^{2}		Wang et al. (2017)	Q	80, 239
LHBQGXZUVXFJRH-UHFFFAOYSA-N	4.9		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C517OH	3.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	1.6×10^{6}		Wang et al. (2017)	Q	80, 239
NQMZUMSFJBKHAU-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C517OOH	1.1×10^{6}	13000	Wieser et al. (2023)	Q	437
$C_5H_{10}O_4$	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
OAFCGFSFCVGKSH-UHFFFAOYSA-N	4.9×10^{5}		Wang et al. (2017)	Q	80, 239
	1.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C519OOH	1.7×10^{5}	13000	Wieser et al. (2023)	Q	437
$C_5H_{10}O_4$	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
RDSFTYTWLRHJGZ-UHFFFAOYSA-N	4.0×10^{5}		Wang et al. (2017)	Q	80, 239
	8.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C51OH2CO	6.0		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	4.2×10^{1}		Wang et al. (2017)	Q	80, 239
WOVLKKLXYZJMSN-UHFFFAOYSA-N	9.6		Wang et al. (2017)	Q	80, 240
MCM:C51OH	1.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	2.1×10^{5}		Wang et al. (2017)	Q	80, 239
NJUQBPDKVORANW-UHFFFAOYSA-N	4.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C51OOH	1.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	2.1×10^{6}		Wang et al. (2017)	Q	80, 239
IZBMMNKBXWVQLB-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C521OH	1.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	4.8×10^{7}		Wang et al. (2017)	Q	80, 239
UOGQGBWLBZOULD-UHFFFAOYSA-N	9.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C521OOH	6.5×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	1.9×10^{7}		Wang et al. (2017)	Q	80, 239
INSNYERMNWOCIO-UHFFFAOYSA-N	2.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C524CO	3.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	1.9×10^{5}		Wang et al. (2017)	Q	80, 239
JVFYSLPFISVGRS-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C525OOH	3.8×10^{12}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_6$	2.0×10^{11}		Wang et al. (2017)	Q	80, 239
KYXSOONCNSTMJK-UHFFFAOYSA-N	3.1×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C53OH	1.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
PLVCXNLHUHTLCR-UHFFFAOYSA-N	6.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C53OOH	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	1.8×10^{6}		Wang et al. (2017)	Q	80, 239
VCGFNBZCPLQTJR-UHFFFAOYSA-N	6.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C55OOH	3.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	1.3×10^{6}		Wang et al. (2017)	Q	80, 239
IEXMEMALQGQSKE-UHFFFAOYSA-N	2.8×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C59OOH	1.1×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_5$	1.6×10^{8}		Wang et al. (2017)	Q	80, 239
JWNCLQLBUYGJMN-UHFFFAOYSA-N	3.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C5CO243OH	1.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
SLKPFOVYRYRNBA-UHFFFAOYSA-N	9.8		Wang et al. (2017)	Q	80, 240
MCM:C5OHCO4OOH	4.7×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	1.6×10^{6}		Wang et al. (2017)	Q	80, 239
DSLVXKSJLFFUGE-UHFFFAOYSA-N	4.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:CO2C5OH	3.6×10^{3}	9800	Wieser et al. (2023)	Q	437
$C_5H_{10}O_2$	1.2×10^{2}		Wang et al. (2017)	Q	80, 238
JSHPTIGHEWEXRW-UHFFFAOYSA-N	2.6×10^{3}		Wang et al. (2017)	Q	80, 239
	1.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:CO2H3MCO3H	1.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	3.2×10^{3}		Wang et al. (2017)	Q	80, 239
LZACDMRRAOGIBF-UHFFFAOYSA-N	3.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO3H4CO3H	1.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	1.0×10^{4}		Wang et al. (2017)	Q	80, 239
LAOPLCWFGWEKGR-UHFFFAOYSA-N	1.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DIEKAOH	7.3		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	6.8×10^{1}		Wang et al. (2017)	Q	80, 239
QMXCHEVUAIPIRM-UHFFFAOYSA-N	7.6		Wang et al. (2017)	Q	80, 240
MCM:H3C2C4CO3H	6.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	3.0×10^{6}		Wang et al. (2017)	Q	80, 239
NYZNEBYYPQANOB-UHFFFAOYSA-N	6.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HC23C4CO3H	4.5×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_6$	1.1×10^{8}		Wang et al. (2017)	Q	80, 239
UQNPRLJBDVQJQC-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HCOC5	1.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_2$	1.4×10^{2}		Wang et al. (2017)	Q	80, 239
LSMLKPXBSFFBNR-UHFFFAOYSA-N	3.4		Wang et al. (2017)	Q	80, 240
MCM:HMVKBCO3H	1.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	5.8×10^{6}		Wang et al. (2017)	Q	80, 239
VFNFGUWSZFHBRW-UHFFFAOYSA-N	2.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO13CO4C5	1.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	2.6×10^{5}		Wang et al. (2017)	Q	80, 239
CGPIPFJOMJUWGK-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO14CO2C5	1.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	1.5×10^{6}		Wang et al. (2017)	Q	80, 239
XLDKDOKPMNKVMP-UHFFFAOYSA-N	4.2×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HO14CO3C5	1.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	1.6×10^{6}		Wang et al. (2017)	Q	80, 239
YMIRTILUDYUWGY-UHFFFAOYSA-N	4.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO1CO24C5	4.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	3.2×10^{4}		Wang et al. (2017)	Q	80, 239
VBUBLWCIADYRMB-UHFFFAOYSA-N	4.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO1CO34C5	7.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	4.7×10^{4}		Wang et al. (2017)	Q	80, 239
LKLKMCUVBQDYFU-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO1CO3C5	1.2×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	4.6×10^{2}		Wang et al. (2017)	Q	80, 239
TYXULUBCBKMSSK-UHFFFAOYSA-N	6.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HO2CO4C5	1.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	1.3×10^{3}		Wang et al. (2017)	Q	80, 239
PCYZZYAEGNVNMH-UHFFFAOYSA-N	9.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HOCO3C5OOH	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	1.3×10^{6}		Wang et al. (2017)	Q	80, 239
ZLPJDXTYGYNOQK-UHFFFAOYSA-N	4.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HOCO4C5OOH	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	1.9×10^{6}		Wang et al. (2017)	Q	80, 239
MYGJVQXASPJPCS-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:MBOACO	2.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	9.8×10^{2}		Wang et al. (2017)	Q	80, 239
FEIUXLCYYBVUGD-UHFFFAOYSA-N	6.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:ME3CO2BUOL	7.3		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	4.6×10^{1}		Wang et al. (2017)	Q	80, 239
NBEGXSQMVJTIAR-UHFFFAOYSA-N	6.8		Wang et al. (2017)	Q	80, 240
MCM:MIPKAOH	4.5		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	4.4×10^{1}		Wang et al. (2017)	Q	80, 239
BNDRWEVUODOUDW-UHFFFAOYSA-N	7.6		Wang et al. (2017)	Q	80, 240
MCM:MIPKBOH	1.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	6.3×10^{2}		Wang et al. (2017)	Q	80, 239
VVSRECWZBBJOTG-UHFFFAOYSA-N	6.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MPRKAOH	7.3		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	8.5×10^{1}		Wang et al. (2017)	Q	80, 239
HDKKRASBPHFULQ-UHFFFAOYSA-N	4.9		Wang et al. (2017)	Q	80, 240
MCM:BZOBIPEROH	6.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_4$	3.6×10^{3}		Wang et al. (2017)	Q	80, 239
OGRXSIBGKCRBOL-UHFFFAOYSA-N	1.7×10^{7}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:C4COMEOH	5.0		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	2.7×10^{1}		Wang et al. (2017)	Q	80, 239
FDJJNIXWMAWMBP-UHFFFAOYSA-N	8.0		Wang et al. (2017)	Q	80, 240
MCM:C4COMOH3OH	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	7.6×10^{5}		Wang et al. (2017)	Q	80, 239
NCEURKGQTPCVEC-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C4COMOHOOH	4.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	8.9×10^{5}		Wang et al. (2017)	Q	80, 239
JZGTXIGKACACHL-UHFFFAOYSA-N	3.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C4MOHOCO3H	1.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	5.4×10^{3}		Wang et al. (2017)	Q	80, 239
BJXKNHIKUQDPQL-UHFFFAOYSA-N	8.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C517CO3H	1.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	1.1×10^{7}		Wang et al. (2017)	Q	80, 239
HTNOTPIWPYZOLN-UHFFFAOYSA-N	7.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C519CO3H	1.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	1.6×10^{7}		Wang et al. (2017)	Q	80, 239
OBKQTPZEBCGGJT-UHFFFAOYSA-N	5.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C5COHOCO3H	5.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_6$	2.3×10^{5}		Wang et al. (2017)	Q	80, 239
BPYCYKKOURHNJX-UHFFFAOYSA-N	8.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C5O5OHCO3H	1.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	4.8×10^{3}		Wang et al. (2017)	Q	80, 239
GCQMJNYHSPBFDA-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C610OH	1.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	2.4×10^{5}		Wang et al. (2017)	Q	80, 239
YFEDHAOQJOZUIL-UHFFFAOYSA-N	2.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C610OOH	1.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	2.0×10^{6}		Wang et al. (2017)	Q	80, 239
VBEFRWQFSDXQDV-UHFFFAOYSA-N	6.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C611OH	5.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	3.0×10^{3}		Wang et al. (2017)	Q	80, 239
PYRMISJRKRVNPG-UHFFFAOYSA-N	3.5		Wang et al. (2017)	Q	80, 240
MCM:C612OH	9.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	6.0×10^{5}		Wang et al. (2017)	Q	80, 239
VCLSUNMNDIKRMY-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C612OOH	5.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	9.3×10^{5}		Wang et al. (2017)	Q	80, 239
OANIXDZJWBEQCD-UHFFFAOYSA-N	5.5×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C613OOH	1.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_5$	2.0×10^{8}		Wang et al. (2017)	Q	80, 239
MBLADDFAKVGAFO-UHFFFAOYSA-N	1.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C614CO	2.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	1.4×10^{6}		Wang et al. (2017)	Q	80, 239
DFWHGSVPVJPYJZ-UHFFFAOYSA-N	8.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C614OH	9.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	9.1×10^{6}		Wang et al. (2017)	Q	80, 239
WLPHOQAEOJPJID-UHFFFAOYSA-N	8.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C614OOH	7.8×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	8.3×10^{7}		Wang et al. (2017)	Q	80, 239
AZSLPKKGLPCKMI-UHFFFAOYSA-N	4.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C619OH	1.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	2.5×10^{6}		Wang et al. (2017)	Q	80, 239
WEYIBABPZCYASX-UHFFFAOYSA-N	4.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C61CO	3.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	2.2×10^{4}		Wang et al. (2017)	Q	80, 239
MGEAAKFVOQZVFH-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C61OH	1.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	3.6×10^{5}		Wang et al. (2017)	Q	80, 239
JOVKXRBMZIPRBZ-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C61OOH	1.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	1.7×10^{6}		Wang et al. (2017)	Q	80, 239
ZUQHNOSGBJLTRH-UHFFFAOYSA-N	3.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C621OOH	9.8×10^{11}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_6$	2.7×10^{10}		Wang et al. (2017)	Q	80, 239
OMSKVAAPFLCUBC-UHFFFAOYSA-N	3.5×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C624CO	2.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_2$	6.3×10^{2}		Wang et al. (2017)	Q	80, 239
SAJQFIMRYKQCMA-UHFFFAOYSA-N	5.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C625OH	1.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	3.9×10^{8}		Wang et al. (2017)	Q	80, 239
UHZLCNNVPSWLBR-UHFFFAOYSA-N	2.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C625OOH	2.0×10^{10}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_5$	7.8×10^{8}		Wang et al. (2017)	Q	80, 239
RLEQEEKQTRHVBK-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C627OH	3.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	1.9×10^{5}		Wang et al. (2017)	Q	80, 239
YXADPHVQSSNJLB-UHFFFAOYSA-N	5.0×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C630OH	2.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	1.7×10^{6}		Wang et al. (2017)	Q	80, 239
LTOZVYXSZHIEKZ-UHFFFAOYSA-N	2.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C630OOH	1.8×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	2.2×10^{6}		Wang et al. (2017)	Q	80, 239
FPSNWVZQINIJKM-UHFFFAOYSA-N	1.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C63OH	1.4×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.2×10^{5}		Wang et al. (2017)	Q	80, 239
YEHSOHVSOJHCML-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C63OOH	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
RYUSCYCDUHZJRL-UHFFFAOYSA-N	1.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C64OH	8.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	2.2×10^{5}		Wang et al. (2017)	Q	80, 239
DWHFPVYPGLVOER-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C64OOH	7.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
WKWKMZOJIHCBFC-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C66CO	7.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	2.9×10^{4}		Wang et al. (2017)	Q	80, 239
PQXOVUFKUOIXAY-UHFFFAOYSA-N	4.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C66OH	1.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	9.3×10^{5}		Wang et al. (2017)	Q	80, 239
YKCRSYHGTATDJD-UHFFFAOYSA-N	6.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C66OOH	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	7.4×10^{5}		Wang et al. (2017)	Q	80, 239
ZIMKSIUZUDHWGV-UHFFFAOYSA-N	9.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C67CO3H	3.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	6.6×10^{5}		Wang et al. (2017)	Q	80, 239
BGZGHPIMJSIBNB-UHFFFAOYSA-N	3.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C69OH	1.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	8.9×10^{5}		Wang et al. (2017)	Q	80, 239
UAFCVHAXODPLTF-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C69OOH	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	1.3×10^{6}		Wang et al. (2017)	Q	80, 239
IBTXITPBBCYNLS-UHFFFAOYSA-N	6.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C6CO23HO5	7.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	2.6×10^{4}		Wang et al. (2017)	Q	80, 239
ZFXUWHPHUNDYBV-UHFFFAOYSA-N	5.6×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:C6CO243OH	8.5×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	6.6×10^{3}		Wang et al. (2017)	Q	80, 239
YZRCADLLOAXRLD-UHFFFAOYSA-N	5.0		Wang et al. (2017)	Q	80, 240
MCM:C6CO34HO1	7.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	2.0×10^{4}		Wang et al. (2017)	Q	80, 239
LBGWMVXVPMPEID-UHFFFAOYSA-N	9.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C6CO3HO14	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	9.1×10^{5}		Wang et al. (2017)	Q	80, 239
AEYYIRCLAOJEMX-UHFFFAOYSA-N	9.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C6CO3HO25	1.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
AQJAHIKLRWQRAX-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C6CO3HO4	5.6		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	4.6×10^{1}		Wang et al. (2017)	Q	80, 239
SKCYVGUCBRYGTE-UHFFFAOYSA-N	6.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C6CO3OHOOH	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	6.3×10^{5}		Wang et al. (2017)	Q	80, 239
VJHRZIUXRMRGDC-UHFFFAOYSA-N	6.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C6HOCOOOH	9.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	7.4×10^{5}		Wang et al. (2017)	Q	80, 239
DEHZHOWOLMWYLS-UHFFFAOYSA-N	8.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:CO24M3C5OH	3.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
JUTFYFRULBWUNH-UHFFFAOYSA-N	2.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CO25C6OH	3.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	1.6×10^{5}		Wang et al. (2017)	Q	80, 239
MXGSILCFPNVDMX-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:CO2HO3C6	5.6		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	5.8×10^{1}		Wang et al. (2017)	Q	80, 239
UHSBCAJZDUQTHH-UHFFFAOYSA-N	4.1		Wang et al. (2017)	Q	80, 240
MCM:CO2HO4C6	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	7.8×10^{2}		Wang et al. (2017)	Q	80, 239
ODWYTDVNWFBCLV-UHFFFAOYSA-N	3.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO2HOC6OOH	9.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	1.0×10^{6}		Wang et al. (2017)	Q	80, 239
DONIGPAOCGSEHJ-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:CO2M3C5OH	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	1.7×10^{3}		Wang et al. (2017)	Q	80, 239
YJCMJVMCCJIPRV-UHFFFAOYSA-N	4.6×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:CO2MC5OH	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	1.9×10^{3}		Wang et al. (2017)	Q	80, 239
NZBRXFKHZBOFBW-UHFFFAOYSA-N	5.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CY6DIONOH	2.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	6.5×10^{7}		Wang et al. (2017)	Q	80, 239
ACRUCDPQQCIOID-UHFFFAOYSA-N	2.9×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:CYHXOLACO	1.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_2$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
ODZTXUXIYGJLMC-UHFFFAOYSA-N	6.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CYHXONAOH	3.5×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_2$	3.5×10^{4}		Wang et al. (2017)	Q	80, 239
TWEVQGUWCLBRMJ-UHFFFAOYSA-N	8.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:DMK2OH	2.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	4.2×10^{6}		Wang et al. (2017)	Q	80, 239
RQDWELNLPMBYMA-UHFFFAOYSA-N	2.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DMKCOOH	6.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	3.2×10^{5}		Wang et al. (2017)	Q	80, 239
OKDWWGVTKQPUTM-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DMKOHOOH	4.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	7.3×10^{6}		Wang et al. (2017)	Q	80, 239
WAHPQVAXIMVNLL-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:EIPKAOH	3.9		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	3.3×10^{1}		Wang et al. (2017)	Q	80, 239
SYAVYWAMVZKGTF-UHFFFAOYSA-N	4.5		Wang et al. (2017)	Q	80, 240
MCM:EIPKBOH	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	3.1×10^{2}		Wang et al. (2017)	Q	80, 239
JYEMLYGXHDIVRA-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:H13M3CO4C5	9.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.7×10^{5}		Wang et al. (2017)	Q	80, 239
NBNMOYHUQSLZCQ-UHFFFAOYSA-N	3.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:H3C25C6OH	5.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	4.8×10^{7}		Wang et al. (2017)	Q	80, 239
XLUGOLRJPRATMY-UHFFFAOYSA-N	3.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:H3C25C6OOH	2.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	5.0×10^{7}		Wang et al. (2017)	Q	80, 239
XIJKANBCMKWKRM-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HEX3ONAOH	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	6.5×10^{2}		Wang et al. (2017)	Q	80, 239
XHYXKWWFNRBCGE-UHFFFAOYSA-N	4.2×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:HEX3ONCOH	5.6		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	4.2×10^{1}		Wang et al. (2017)	Q	80, 239
ZWBUSAWJHMPOEJ-UHFFFAOYSA-N	3.5		Wang et al. (2017)	Q	80, 240
MCM:HEX3ONDOH	9.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	2.6×10^{2}		Wang et al. (2017)	Q	80, 239
ITHSWIXXHGKFJW-UHFFFAOYSA-N	5.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HO1CO24C6	3.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
NUDMYLMVZRZHHU-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO1CO4C6	9.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
APQMHEQLBDXGMP-UHFFFAOYSA-N	4.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO2CO5C6	2.8×10^{3}	10000	Wieser et al. (2023)	Q	437
$C_6H_{12}O_2$	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
ZSDLLTJVENEIDW-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	80, 239
	6.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:M2BKAOH	1.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	6.9×10^{2}		Wang et al. (2017)	Q	80, 239
ZXZUCILLTLHIBZ-UHFFFAOYSA-N	4.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:M2BKBOH	3.9		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	4.4×10^{1}		Wang et al. (2017)	Q	80, 239
KHCUSEDRQWYNDS-UHFFFAOYSA-N	3.6		Wang et al. (2017)	Q	80, 240
MCM:MBKCOOHOOH	2.5×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	2.1×10^{6}		Wang et al. (2017)	Q	80, 239
VGLNQNYMXFMHPV-UHFFFAOYSA-N	4.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MIBKAOH3CO	2.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	4.6×10^{2}		Wang et al. (2017)	Q	80, 239
NARMPYMUEZMSEV-UHFFFAOYSA-N	2.4		Wang et al. (2017)	Q	80, 240
MCM:MIBKBOH	6.5		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	6.3×10^{1}		Wang et al. (2017)	Q	80, 239
IGPIDYBTABPKQT-UHFFFAOYSA-N	2.6		Wang et al. (2017)	Q	80, 240
MCM:MIBKHO14	9.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	8.1×10^{5}		Wang et al. (2017)	Q	80, 239
UZSRJTNVDUYOLE-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:MIBKHO4OOH	5.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
FGHCAVJLMYVGOV-UHFFFAOYSA-N	1.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:MIBKOH34	5.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	4.1×10^{4}		Wang et al. (2017)	Q	80, 239
OSPIOFUQWMUWOI-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MIBKOHAOOH	8.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	1.8×10^{5}		Wang et al. (2017)	Q	80, 239
WIXFQYMFSUQGGT-UHFFFAOYSA-N	4.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MIBKOHBOOH	7.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	2.9×10^{5}		Wang et al. (2017)	Q	80, 239
NCKNZQNPSVRYAP-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:MTBKOH	7.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	3.8×10^{2}		Wang et al. (2017)	Q	80, 239
DYAWMXSWDGPGOI-UHFFFAOYSA-N	3.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PBZQCO	8.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_4O_4$	3.6×10^{9}		Wang et al. (2017)	Q	80, 239
LTWQMQDFZHUKCN-UHFFFAOYSA-N	3.4×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PBZQOH	3.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_4$	5.0×10^{8}		Wang et al. (2017)	Q	80, 239
KGAUAKJVBKFEJK-UHFFFAOYSA-N	1.5×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PBZQOOH	5.3×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_5$	1.9×10^{9}		Wang et al. (2017)	Q	80, 239
GWWKDNIKIVTFLV-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C61CO3H	7.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_6$	4.6×10^{5}		Wang et al. (2017)	Q	80, 239
LNQZNTUCDYUQNY-UHFFFAOYSA-N	4.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C62CO3H	8.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_6$	5.1×10^{5}		Wang et al. (2017)	Q	80, 239
OTMFEIRKQNFPTO-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C711OOH	5.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_4$	7.4×10^{5}		Wang et al. (2017)	Q	80, 239
CHMPWQJFRSDBMP-UHFFFAOYSA-N	5.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C712OH	8.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_3$	3.6×10^{5}		Wang et al. (2017)	Q	80, 239
XKQDJNZCXUTPAB-UHFFFAOYSA-N	5.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C712OOH	6.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_4$	7.6×10^{5}		Wang et al. (2017)	Q	80, 239
ISDXEEIPAJYQKS-UHFFFAOYSA-N	8.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C713OH	2.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_3$	4.0×10^{4}		Wang et al. (2017)	Q	80, 239
KKMPMNHIJNYFMY-UHFFFAOYSA-N	2.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C714OH	3.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_3$	6.8×10^{4}		Wang et al. (2017)	Q	80, 239
BDJIDAHXOAZMLT-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C719OH	5.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	7.1×10^{10}		Wang et al. (2017)	Q	80, 239
SNLGDBZBHBGDGF-UHFFFAOYSA-N	2.3×10^{8}		Wang et al. (2017)	Q	80, 240
MCM:C719OOH	7.1×10^{10}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	5.8×10^{11}		Wang et al. (2017)	Q	80, 239
RIQZESWBZQGTOF-UHFFFAOYSA-N	2.0×10^{9}		Wang et al. (2017)	Q	80, 240
MCM:C71OOH	8.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_4$	4.1×10^{5}		Wang et al. (2017)	Q	80, 239
NBQALOYIKVIATH-UHFFFAOYSA-N	3.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C726CO3OH	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	9.1×10^{4}		Wang et al. (2017)	Q	80, 239
KXKCGTAVIRFZLI-UHFFFAOYSA-N	6.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C72OH	1.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_3$	1.9×10^{5}		Wang et al. (2017)	Q	80, 239
NSVUCXUEJIZYCX-UHFFFAOYSA-N	8.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C72OOH	9.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_4$	9.3×10^{5}		Wang et al. (2017)	Q	80, 239
HOCRXLJRXJDOAI-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C76OOH	8.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_4$	8.0×10^{5}		Wang et al. (2017)	Q	80, 239
RNKPJWWQPAQZAU-UHFFFAOYSA-N	1.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C77CO	2.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_3$	8.1×10^{3}		Wang et al. (2017)	Q	80, 239
LRWMVVHMPWURQP-UHFFFAOYSA-N	7.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C77OH	8.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_3$	3.2×10^{5}		Wang et al. (2017)	Q	80, 239
BWFQHNYIFKCYIN-UHFFFAOYSA-N	8.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C77OOH	6.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_4$	6.5×10^{5}		Wang et al. (2017)	Q	80, 239
VLZZBCPZVYCEGU-UHFFFAOYSA-N	4.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C78CO	4.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_3$	1.8×10^{4}		Wang et al. (2017)	Q	80, 239
XZDSUXRHWGXGLP-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C78OH	9.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_3$	3.0×10^{5}		Wang et al. (2017)	Q	80, 239
RHPFPSWJNNLJIH-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C78OOH	5.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_4$	3.7×10^{5}		Wang et al. (2017)	Q	80, 239
CHSMMMZNDOATLZ-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:C79OOH	2.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	1.0×10^{7}		Wang et al. (2017)	Q	80, 239
PAASZTKJDWJXEO-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C7BDCOH	1.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	3.6×10^{6}		Wang et al. (2017)	Q	80, 239
IQLAANIUQOXZGT-UHFFFAOYSA-N	7.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C7BDCOOH	2.3×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	2.5×10^{6}		Wang et al. (2017)	Q	80, 239
YSGKLAZJXASOJQ-UHFFFAOYSA-N	2.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C7EDCCO	5.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	2.2×10^{5}		Wang et al. (2017)	Q	80, 239
ZZJOBVIMQADRSG-UHFFFAOYSA-N	8.7		Wang et al. (2017)	Q	80, 240
MCM:C7EDCOH	2.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	2.7×10^{6}		Wang et al. (2017)	Q	80, 239
ILHMXLYATWSMQV-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C7EDCOOH	3.7×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	4.6×10^{6}		Wang et al. (2017)	Q	80, 239
GFYCWCYSZRNKIC-UHFFFAOYSA-N	4.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:CO25C73OH	3.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_3$	8.3×10^{4}		Wang et al. (2017)	Q	80, 239
SUAOXERUOLNODJ-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:CO25C74OH	3.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_3$	8.5×10^{4}		Wang et al. (2017)	Q	80, 239
WVDVIEDFZYMNAI-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:H2M2CO5C6	6.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_2$	1.5×10^{3}		Wang et al. (2017)	Q	80, 239
GNNBSAPGFGNCCT-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:H2M3CO5C6	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_2$	1.7×10^{3}		Wang et al. (2017)	Q	80, 239
JXXNGUYHZPNXHL-UHFFFAOYSA-N	2.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:H2M4CO5C6	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_2$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
ZIVAMUMQDXZFCR-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:H3C25CCO3H	3.3×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_6$	9.8×10^{8}		Wang et al. (2017)	Q	80, 239
ARDZNQBCJILRHG-UHFFFAOYSA-N	6.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HCC7CO	9.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_2$	4.6×10^{4}		Wang et al. (2017)	Q	80, 239
WVMVYBISUAVCBD-UHFFFAOYSA-N	1.9×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:HO2CO35C7	3.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_3$	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
LULWLYVLBHVZLB-UHFFFAOYSA-N	5.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HO2CO5C7	8.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_2$	1.3×10^{3}		Wang et al. (2017)	Q	80, 239
DWMNUVZLRBCGOL-UHFFFAOYSA-N	2.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO3CO6C7	2.1×10^{3}	11000	Wieser et al. (2023)	Q	437
$C_7H_{14}O_2$	8.7×10^{1}		Wang et al. (2017)	Q	80, 238
MQRALIJAASQPNT-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	80, 239
	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PTLQCO	5.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_6O_4$	6.2×10^{9}		Wang et al. (2017)	Q	80, 239
QCLUMLMJJNMFFX-UHFFFAOYSA-N	6.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PTLQOH	2.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_4$	5.1×10^{8}		Wang et al. (2017)	Q	80, 239
FWCZASAULMADEU-UHFFFAOYSA-N	1.2×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PTLQOOH	3.6×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_5$	1.8×10^{9}		Wang et al. (2017)	Q	80, 239
ULCYCDVSDDOIBS-UHFFFAOYSA-N	3.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:TLCOBIPEOH	3.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_4$	7.3×10^{2}		Wang et al. (2017)	Q	80, 239
BTRXIMYXFXXDNL-UHFFFAOYSA-N	2.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:TLOBIPEROH	3.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_4$	1.3×10^{3}		Wang et al. (2017)	Q	80, 239
OGIZZGFCOPEREO-UHFFFAOYSA-N	1.1×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C6MOCOCO3H	2.1×10^{9}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_6$	1.7×10^{9}		Wang et al. (2017)	Q	80, 239
UAMJQIWVNIVSAA-UHFFFAOYSA-N	4.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C7CO2M5OH	7.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_3$	2.0×10^{4}		Wang et al. (2017)	Q	80, 239
VIGCXZSBZQABDL-UHFFFAOYSA-N	2.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C7CO2OCO3H	2.1×10^{9}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_6$	2.0×10^{9}		Wang et al. (2017)	Q	80, 239
PYNUJNZYCLWJPS-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C7M2CO5OH	9.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_3$	8.5×10^{4}		Wang et al. (2017)	Q	80, 239
IWFVDGADKJRMAI-UHFFFAOYSA-N	2.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C817OH	5.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_3$	4.9×10^{5}		Wang et al. (2017)	Q	80, 239
HXKXVESDDNIBIQ-UHFFFAOYSA-N	2.5×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:C818CO	6.5×10^{6}	16000	Wieser et al. (2023)	Q	437
$C_8H_{12}O_4$	3.6×10^{7}		Wang et al. (2017)	Q	80, 238
CRQAGKNTHDNGEW-UHFFFAOYSA-N	1.7×10^{7}		Wang et al. (2017)	Q	80, 239
	1.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C818OH	8.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_4$	2.9×10^{8}		Wang et al. (2017)	Q	80, 239
GYBDPSWJEGVQPC-UHFFFAOYSA-N	7.4×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C818OOH	5.7×10^{8}	17000	Wieser et al. (2023)	Q	437
$C_8H_{14}O_5$	5.0×10^{9}		Wang et al. (2017)	Q	80, 238
DLMBPALZQHFDOH-UHFFFAOYSA-N	1.0×10^{8}		Wang et al. (2017)	Q	80, 239
	9.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C819OOH	2.1×10^{7}	17000	Wieser et al. (2023)	Q	437
$C_8H_{14}O_5$	3.5×10^{9}		Wang et al. (2017)	Q	80, 238
JRXMSSDNDAZISI-UHFFFAOYSA-N	6.3×10^{7}		Wang et al. (2017)	Q	80, 239
	6.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C81OOH	6.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{16}O_4$	3.3×10^{5}		Wang et al. (2017)	Q	80, 239
SFFBCYBCCUXGLX-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C820OOH	2.3×10^{12}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_6$	1.4×10^{9}		Wang et al. (2017)	Q	80, 239
MPCACGHSMGOFNV-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C826CO3OH	1.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_3$	5.6×10^{4}		Wang et al. (2017)	Q	80, 239
GGSZUEZFMJTLBX-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C827OH	1.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_3$	5.4×10^{4}		Wang et al. (2017)	Q	80, 239
VYHQZXLAUHJBAB-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C829OH	1.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_4$	1.0×10^{8}		Wang et al. (2017)	Q	80, 239
ZFRREEXTYBESJX-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C829OOH	2.8×10^{9}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_5$	8.0×10^{7}		Wang et al. (2017)	Q	80, 239
PFFZQAOPEABNHW-UHFFFAOYSA-N	9.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C82OOH	8.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{16}O_4$	6.8×10^{5}		Wang et al. (2017)	Q	80, 239
AQECYOJQUIJAFS-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C84OH	2.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_3$	4.1×10^{4}		Wang et al. (2017)	Q	80, 239
HXKSWDLNZPICFQ-UHFFFAOYSA-N	5.0×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C88OH	6.0×10^3		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_3$	1.1×10^6		Wang et al. (2017)	Q	80, 239
DCTATDQRTQNXHW-UHFFFAOYSA-N	3.9×10^3		Wang et al. (2017)	Q	80, 240
MCM:EBZOBPEROH	2.8×10^6		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_4$	8.3×10^2		Wang et al. (2017)	Q	80, 239
YDVGTQTYIBCIQC-UHFFFAOYSA-N	6.0×10^5		Wang et al. (2017)	Q	80, 240
MCM:HO34CO6C8	1.0×10^5		Wang et al. (2017)	Q	80, 238
$C_8H_{16}O_3$	1.7×10^5		Wang et al. (2017)	Q	80, 239
GQDVWZAGWHUXKX-UHFFFAOYSA-N	3.3×10^2		Wang et al. (2017)	Q	80, 240
MCM:HO3CO46C8	2.8×10^3		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_3$	8.3×10^3		Wang et al. (2017)	Q	80, 239
LLYUJOAMIUBKSA-UHFFFAOYSA-N	3.0×10^1		Wang et al. (2017)	Q	80, 240
MCM:HO3CO6C8	8.0×10^1		Wang et al. (2017)	Q	80, 238
$C_8H_{16}O_2$	9.6×10^2		Wang et al. (2017)	Q	80, 239
VJDZJBNTVLGPEM-UHFFFAOYSA-N	8.7×10^1		Wang et al. (2017)	Q	80, 240
MCM:MXYOBPEROH	1.9×10^6		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_4$	3.0×10^2		Wang et al. (2017)	Q	80, 239
BQJOHFWATKFGAQ-UHFFFAOYSA-N	4.5×10^4		Wang et al. (2017)	Q	80, 240
MCM:MXYQOH	1.3×10^6		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_4$	3.0×10^8		Wang et al. (2017)	Q	80, 239
DNSXSYZLXRHYTM-UHFFFAOYSA-N	3.5×10^4		Wang et al. (2017)	Q	80, 240
MCM:MXYQOOH	1.9×10^9		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_5$	3.0×10^8		Wang et al. (2017)	Q	80, 239
UAWVAAITGKOKNW-UHFFFAOYSA-N	5.9×10^7		Wang et al. (2017)	Q	80, 240
MCM:OXYQCO	3.4×10^6		Wang et al. (2017)	Q	80, 238
$C_8H_8O_4$	6.2×10^9		Wang et al. (2017)	Q	80, 239
QSCBEAAIZXLBQA-UHFFFAOYSA-N	1.8×10^5		Wang et al. (2017)	Q	80, 240
MCM:OXYQOH	1.6×10^6		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_4$	3.5×10^8		Wang et al. (2017)	Q	80, 239
LJMMKZLQFVIDLQ-UHFFFAOYSA-N	7.6×10^4		Wang et al. (2017)	Q	80, 240
MCM:OXYQOOH	2.3×10^9		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_5$	1.2×10^9		Wang et al. (2017)	Q	80, 239
NOWQTCYBLCRAEJ-UHFFFAOYSA-N	1.4×10^5		Wang et al. (2017)	Q	80, 240
MCM:PXYQOH	1.3×10^6		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_4$	3.0×10^8		Wang et al. (2017)	Q	80, 239
RORXCXPFLRGHQV-UHFFFAOYSA-N	5.8×10^4		Wang et al. (2017)	Q	80, 240
MCM:PXYQOOH	1.9×10^9		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_5$	4.2×10^8		Wang et al. (2017)	Q	80, 239
FYDHRLZPZZTRLJ-UHFFFAOYSA-N	2.4×10^6		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C6EO2HCO3H	1.7×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_6$	1.6×10^{9}		Wang et al. (2017)	Q	80, 239
KMUWHHLOUXRZEC-UHFFFAOYSA-N	3.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C7MJPCO3H	1.7×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_6$	1.2×10^{9}		Wang et al. (2017)	Q	80, 239
HVGFJXMJLWNDQT-UHFFFAOYSA-N	6.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C7MOCOCO3H	1.4×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_6$	2.3×10^{9}		Wang et al. (2017)	Q	80, 239
UXMGGYROBLVMKA-UHFFFAOYSA-N	9.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C8M2CO6OH	7.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_3$	4.8×10^{4}		Wang et al. (2017)	Q	80, 239
AUYUFIFJEJTOMG-UHFFFAOYSA-N	8.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C917OH	9.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_3$	4.3×10^{6}		Wang et al. (2017)	Q	80, 239
DVAQWOBQFULNSX-UHFFFAOYSA-N	3.1×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C920OOH	6.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_4$	1.6×10^{6}		Wang et al. (2017)	Q	80, 239
CXKZGZZGALDRTB-UHFFFAOYSA-N	6.9×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C921OOH	1.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_5$	3.2×10^{9}		Wang et al. (2017)	Q	80, 239
MIFQELLQXZRDIQ-UHFFFAOYSA-N	7.1×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C922OOH	3.6×10^{11}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_6$	7.8×10^{9}		Wang et al. (2017)	Q	80, 239
IOTRHTNOHNKLJT-UHFFFAOYSA-N	6.6×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C923OH	5.3×10^{3}	12000	Wieser et al. (2023)	Q	437
$C_9H_{16}O_2$	1.5×10^{2}		Wang et al. (2017)	Q	80, 238
VZYSLJNPEGILSI-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 239
	7.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C924CO	1.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_3$	5.6×10^{4}		Wang et al. (2017)	Q	80, 239
IEIWFPIZSBHOOD-UHFFFAOYSA-N	4.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C924OH	3.8×10^{5}	16000	Wieser et al. (2023)	Q	437
$C_9H_{16}O_3$	2.2×10^{4}		Wang et al. (2017)	Q	80, 238
OXSRPARPRXNCEH-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	80, 239
	2.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C924OOH	3.0×10^{6}	16000	Wieser et al. (2023)	Q	437
$C_9H_{16}O_4$	1.2×10^{7}		Wang et al. (2017)	Q	80, 238
BVODBOGLMHSHGK-UHFFFAOYSA-N	3.1×10^{5}		Wang et al. (2017)	Q	80, 239
	5.0×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:C925OOH	9.1×10^{12}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_6$	5.0×10^{10}		Wang et al. (2017)	Q	80, 239
BGVLBDREANINMN-UHFFFAOYSA-N	1.6×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C927OH	2.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_3$	1.2×10^{7}		Wang et al. (2017)	Q	80, 239
JILOVKBSEAXPMT-UHFFFAOYSA-N	9.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C927OOH	7.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_4$	8.9×10^{6}		Wang et al. (2017)	Q	80, 239
UVVCFFCMOUIWEJ-UHFFFAOYSA-N	6.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C928OH	2.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_3$	3.8×10^{5}		Wang et al. (2017)	Q	80, 239
QGCNXROUFNWXOO-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C929CO	2.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	5.4×10^{6}		Wang et al. (2017)	Q	80, 239
BWILLNTUIBCKIM-UHFFFAOYSA-N	3.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C929OH	4.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_4$	5.9×10^{8}		Wang et al. (2017)	Q	80, 239
PMWQIXWFMSCXRH-UHFFFAOYSA-N	6.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C929OOH	2.9×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_5$	3.3×10^{8}		Wang et al. (2017)	Q	80, 239
IKUORCWWMOEDGL-UHFFFAOYSA-N	1.2×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C92OOH	5.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{18}O_4$	2.9×10^{5}		Wang et al. (2017)	Q	80, 239
MOTPUWPPGZYDTM-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C93CO	2.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_3$	6.6×10^{3}		Wang et al. (2017)	Q	80, 239
NCWLHDSPZIENNF-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C93OH	8.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{18}O_3$	1.5×10^{5}		Wang et al. (2017)	Q	80, 239
XOZZRVPGLURXSY-UHFFFAOYSA-N	2.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C93OOH	6.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{18}O_4$	3.3×10^{5}		Wang et al. (2017)	Q	80, 239
DSWUVSMVGXSNEV-UHFFFAOYSA-N	8.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C94OH	2.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_3$	2.6×10^{4}		Wang et al. (2017)	Q	80, 239
RCWXDPYULCSTKX-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C96OH	1.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_2$	3.3×10^{3}		Wang et al. (2017)	Q	80, 239
RRFQMYCDTHUGSU-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:C97OH	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_3$	1.2×10^{6}		Wang et al. (2017)	Q	80, 239
QWYKJUJQBVIHQW-UHFFFAOYSA-N	8.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C97OOH	8.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_4$	3.9×10^{5}		Wang et al. (2017)	Q	80, 239
AXRJNDGSGFVBSX-UHFFFAOYSA-N	1.9×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C98OH	9.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_4$	1.0×10^{8}		Wang et al. (2017)	Q	80, 239
BWKWRXKCGJAJAO-UHFFFAOYSA-N	4.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C98OOH	2.9×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_5$	3.3×10^{7}		Wang et al. (2017)	Q	80, 239
MEUGYCLQCHCPCY-UHFFFAOYSA-N	1.1×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C9DCOH	4.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	1.9×10^{7}		Wang et al. (2017)	Q	80, 239
DIFRJFLUSYQBJM-UHFFFAOYSA-N	4.9×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:HO4CO7C9	6.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{18}O_2$	8.3×10^{2}		Wang et al. (2017)	Q	80, 239
BPRAKHMXALGYKO-UHFFFAOYSA-N	7.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:IPBZOBPROH	2.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	7.1×10^{2}		Wang et al. (2017)	Q	80, 239
WRQNGVASMLSOGA-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:IPRBQCO	4.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_4$	2.6×10^{9}		Wang et al. (2017)	Q	80, 239
UYSSVGYDANWBFJ-UHFFFAOYSA-N	1.2×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:IPRBQOH	1.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	1.7×10^{8}		Wang et al. (2017)	Q	80, 239
BQKYQBQGKYWJSQ-UHFFFAOYSA-N	7.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:IPRBQOOH	2.9×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	6.9×10^{8}		Wang et al. (2017)	Q	80, 239
CCPBRYDTGCPJNX-UHFFFAOYSA-N	1.2×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:LMKAOH	2.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_3$	6.2×10^{6}		Wang et al. (2017)	Q	80, 239
RDFFVUMNEKCADL-UHFFFAOYSA-N	1.2×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:LMKAOOH	1.5×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_4$	2.7×10^{7}		Wang et al. (2017)	Q	80, 239
ZYSXBTHWQDNLBX-UHFFFAOYSA-N	3.6×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:LMKBCO	5.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_3$	3.7×10^{5}		Wang et al. (2017)	Q	80, 239
QJYRJOZGIVJKQK-UHFFFAOYSA-N	2.9×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:LMKBOOH	1.5×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_4$	2.6×10^{7}		Wang et al. (2017)	Q	80, 239
PMLHMEIQMSUJKR-UHFFFAOYSA-N	8.9×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:METLOBPROH	1.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	1.8×10^{2}		Wang et al. (2017)	Q	80, 239
ZSTYNOBMCJBFRA-UHFFFAOYSA-N	2.5×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:METLQOH	1.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	2.0×10^{8}		Wang et al. (2017)	Q	80, 239
YIUSRNITCRMQJW-UHFFFAOYSA-N	2.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:METLQOOH	1.7×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	1.3×10^{8}		Wang et al. (2017)	Q	80, 239
JBNOKZJMGKNXDA-UHFFFAOYSA-N	5.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NOPINAOH	5.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_2$	2.5×10^{4}		Wang et al. (2017)	Q	80, 239
CVWGOJDPALGYKB-UHFFFAOYSA-N	4.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NOPINBOH	5.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_2$	3.2×10^{4}		Wang et al. (2017)	Q	80, 239
FPBMXOVOMRHDTB-UHFFFAOYSA-N	2.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NOPINCOH	3.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_2$	9.3×10^{3}		Wang et al. (2017)	Q	80, 239
OXRZVROAQQDWAA-UHFFFAOYSA-N	3.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NOPINDOH	2.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_2$	7.3×10^{2}		Wang et al. (2017)	Q	80, 239
MLOBETUCFXAOOL-UHFFFAOYSA-N	8.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:OETLQCO	3.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_4$	4.7×10^{9}		Wang et al. (2017)	Q	80, 239
WOEKXHYIEUECKR-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:OETLQOH	1.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	2.0×10^{8}		Wang et al. (2017)	Q	80, 239
DZHQWTGZQAKVBN-UHFFFAOYSA-N	5.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:OETLQOOH	1.9×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	8.0×10^{8}		Wang et al. (2017)	Q	80, 239
KKWSBZSFLIKUTL-UHFFFAOYSA-N	2.1×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PBZOBPEROH	2.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	5.5×10^{2}		Wang et al. (2017)	Q	80, 239
JGNLEXNHGWFGHL-UHFFFAOYSA-N	5.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:PETLQOH	1.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	2.2×10^{8}		Wang et al. (2017)	Q	80, 239
KZOAJFYPECZGSC-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PETLQOOH	1.7×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	2.0×10^{8}		Wang et al. (2017)	Q	80, 239
BJRXYYOXPIRVAX-UHFFFAOYSA-N	2.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:TM123OBPOH	1.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	1.7×10^{2}		Wang et al. (2017)	Q	80, 239
WQSRSICCLTUNRX-UHFFFAOYSA-N	4.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:TM124QOH	8.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	1.7×10^{8}		Wang et al. (2017)	Q	80, 239
GVKLCWOTVYVOTB-UHFFFAOYSA-N	2.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:TM124QOOH	1.3×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	2.6×10^{8}		Wang et al. (2017)	Q	80, 239
SLEWHRYFRSXVOQ-UHFFFAOYSA-N	3.2×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:TM135OBPOH	1.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	1.9×10^{2}		Wang et al. (2017)	Q	80, 239
MWFXWFJYOSXFGA-UHFFFAOYSA-N	4.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:APINBCO	1.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_2$	4.4×10^{2}		Wang et al. (2017)	Q	80, 239
VZRRCQOUNSHSGB-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C1011OH	1.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_2$	2.1×10^{3}		Wang et al. (2017)	Q	80, 239
FSFKNSSBELMLGT-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C102OOH	4.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{20}O_4$	2.6×10^{5}		Wang et al. (2017)	Q	80, 239
QHLMVJFPSLBXKZ-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C103CO	2.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_3$	5.4×10^{3}		Wang et al. (2017)	Q	80, 239
QIIAZEBRWZSMOM-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C103OH	7.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{20}O_3$	1.3×10^{5}		Wang et al. (2017)	Q	80, 239
SXEGIXJYQPFAQK-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C103OOH	5.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{20}O_4$	3.0×10^{5}		Wang et al. (2017)	Q	80, 239
DOFXWCNTKGZWNU-UHFFFAOYSA-N	1.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C104OH	2.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_3$	1.9×10^{4}		Wang et al. (2017)	Q	80, 239
FHITZQAABUJLCH-UHFFFAOYSA-N	4.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C920CO3H	6.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_5$	9.1×10^{5}		Wang et al. (2017)	Q	80, 239
OFVMBWQGLFFRLM-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C9M2CO6OH	5.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_3$	2.4×10^{4}		Wang et al. (2017)	Q	80, 239
SLPXKTFAPIGCFF-UHFFFAOYSA-N	4.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DMEOBPROH	1.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{14}O_4$	1.3×10^{2}		Wang et al. (2017)	Q	80, 239
ZCTKJUASOMJGQC-UHFFFAOYSA-N	9.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO5CO8C10	5.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{20}O_2$	7.4×10^{2}		Wang et al. (2017)	Q	80, 239
GDOWVFFRHQHNBZ-UHFFFAOYSA-N	8.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:LIMBCO	1.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_2$	3.5×10^{2}		Wang et al. (2017)	Q	80, 239
JEQLRDRDFLXSHY-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C112OOH	3.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{22}O_4$	2.4×10^{5}		Wang et al. (2017)	Q	80, 239
IFXOTQISYXBGBQ-UHFFFAOYSA-N	5.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C113CO	1.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{20}O_3$	4.5×10^{3}		Wang et al. (2017)	Q	80, 239
VJVDGYIYRBYKOQ-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C113OH	5.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{22}O_3$	1.1×10^{5}		Wang et al. (2017)	Q	80, 239
IBMABDXBRFZEGO-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C113OOH	4.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{22}O_4$	3.0×10^{5}		Wang et al. (2017)	Q	80, 239
PBWNXGFXFCLKSE-UHFFFAOYSA-N	8.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C114OH	1.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{20}O_3$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
UGVQLPIEIICAJP-UHFFFAOYSA-N	3.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DETLOBPROH	8.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{16}O_4$	9.1×10^{1}		Wang et al. (2017)	Q	80, 239
QNKVJNYVFVQVHN-UHFFFAOYSA-N	1.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HO6CO9C11	4.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{22}O_2$	6.5×10^{2}		Wang et al. (2017)	Q	80, 239
HEIFQPPUFKWMSE-UHFFFAOYSA-N	5.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C122OOH	3.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{24}O_4$	2.3×10^{5}		Wang et al. (2017)	Q	80, 239
PWTYXUGOJRDLPW-UHFFFAOYSA-N	9.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C123CO	1.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{22}O_3$	4.1×10^{3}		Wang et al. (2017)	Q	80, 239
IVLDSNPYDYHHKW-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C123OH	4.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{24}O_3$	9.6×10^{4}		Wang et al. (2017)	Q	80, 239
FTSJAGYKUWYWCN-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C123OOH	4.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{24}O_4$	2.8×10^{5}		Wang et al. (2017)	Q	80, 239
YANZHJXFRFYAEY-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C124OH	1.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{22}O_3$	1.3×10^{4}		Wang et al. (2017)	Q	80, 239
ABVYFIKKAQHKSN-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HO7CO10C12	3.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{24}O_2$	5.1×10^{2}		Wang et al. (2017)	Q	80, 239
AJDNADCNQXGLCC-UHFFFAOYSA-N	4.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C131OH	5.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_3$	2.3×10^{5}		Wang et al. (2017)	Q	80, 239
AONUZHGLRYBQFR-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C132OH	5.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_4$	4.1×10^{8}		Wang et al. (2017)	Q	80, 239
FIXMRMMYQTVSPU-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C132OOH	2.9×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_5$	1.7×10^{8}		Wang et al. (2017)	Q	80, 239
VUANIPKMYHABIK-UHFFFAOYSA-N	1.1×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C133CO	7.1×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{20}O_5$	4.6×10^{9}		Wang et al. (2017)	Q	80, 239
NSPNCPQPMIIWRH-UHFFFAOYSA-N	4.7×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C133OH	3.2×10^{10}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_5$	6.0×10^{10}		Wang et al. (2017)	Q	80, 239
PJPMMZIOBGUFRQ-UHFFFAOYSA-N	8.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C133OOH	8.5×10^{11}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_6$	3.7×10^{10}		Wang et al. (2017)	Q	80, 239
TWNMHUJEMNHLMV-UHFFFAOYSA-N	5.1×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C134CO	4.7×10^{12}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{18}O_6$	2.3×10^{11}		Wang et al. (2017)	Q	80, 239
XVPKZNMZKWIEGC-UHFFFAOYSA-N	2.1×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C134OH	1.0×10^{12}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{20}O_6$	1.1×10^{13}		Wang et al. (2017)	Q	80, 239
CKMYGJKMMJWXII-UHFFFAOYSA-N	8.7×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C134OOH	6.8×10^{14}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{20}O_7$	1.7×10^{12}		Wang et al. (2017)	Q	80, 239
RYVAPXIZXOQMSU-UHFFFAOYSA-N	2.3×10^{8}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:C135OOH	5.0×10^{17}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{18}O_8$	6.6×10^{13}		Wang et al. (2017)	Q	80, 239
VAECXYXKQRKKGE-UHFFFAOYSA-N	9.6×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:BCKAOH	2.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{24}O_3$	8.3×10^{6}		Wang et al. (2017)	Q	80, 239
ARSAOHGCYSGONM-UHFFFAOYSA-N	7.6×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:BCKAOOH	1.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{24}O_4$	4.0×10^{6}		Wang et al. (2017)	Q	80, 239
OXLVMLPVWDEZIL-UHFFFAOYSA-N	7.8×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:BCKBCO	5.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_3$	7.6×10^{5}		Wang et al. (2017)	Q	80, 239
IWYBCVOMQFEOMA-UHFFFAOYSA-N	2.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:BCKBOOH	1.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{24}O_4$	2.6×10^{6}		Wang et al. (2017)	Q	80, 239
SISQWITWYDFXLW-UHFFFAOYSA-N	3.7×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C141OH	1.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{24}O_2$	2.3×10^{3}		Wang et al. (2017)	Q	80, 239
OMNNANPOKVZFEY-UHFFFAOYSA-N	7.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C142OH	2.7×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{24}O_3$	8.5×10^{6}		Wang et al. (2017)	Q	80, 239
TZIWCZUVZZOIAP-UHFFFAOYSA-N	2.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C142OOH	7.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{24}O_4$	1.8×10^{7}		Wang et al. (2017)	Q	80, 239
OJVOLXXWTGQGEJ-UHFFFAOYSA-N	1.9×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C143CO	2.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_4$	5.1×10^{8}		Wang et al. (2017)	Q	80, 239
IPHIBGAHOYIGTO-UHFFFAOYSA-N	5.4×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C143OH	9.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{24}O_4$	5.0×10^{9}		Wang et al. (2017)	Q	80, 239
PUMKKTACSBJGTI-UHFFFAOYSA-N	2.3×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C143OOH	2.5×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{24}O_5$	3.4×10^{9}		Wang et al. (2017)	Q	80, 239
FMXAUTXFPHKMFA-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C145OH	1.0×10^{12}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{24}O_6$	3.1×10^{13}		Wang et al. (2017)	Q	80, 239
CADDZNHIARUDOF-UHFFFAOYSA-N	1.5×10^{9}		Wang et al. (2017)	Q	80, 240
MCM:C145OOH	1.5×10^{15}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{24}O_7$	4.9×10^{13}		Wang et al. (2017)	Q	80, 239
CEBXMSFHIDLJKH-UHFFFAOYSA-N	1.8×10^{10}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:BCBCO	1.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{24}O_2$	6.5×10^{2}		Wang et al. (2017)	Q	80, 239
VLNGGDKMXDHPMK-UHFFFAOYSA-N	8.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PHCOMEOH	3.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_8O_2$	1.2×10^{3}		Wang et al. (2017)	Q	80, 239
ZWVHTXAYIKBMEE-UHFFFAOYSA-N	6.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MPHCOMEOH	1.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_2$	1.3×10^{3}		Wang et al. (2017)	Q	80, 239
CEJINNSYZFLSCS-UHFFFAOYSA-N	4.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PHCOETOH	2.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_2$	7.4×10^{2}		Wang et al. (2017)	Q	80, 239
WLVPRARCUSRDNI-UHFFFAOYSA-N	6.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DMPHCOMOH	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{12}O_2$	7.8×10^{2}		Wang et al. (2017)	Q	80, 239
DBYMZNOFJHQFFD-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:EMPHCOMOH	8.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{14}O_2$	4.5×10^{2}		Wang et al. (2017)	Q	80, 239
MHJXTDDYZBYNEF-UHFFFAOYSA-N	8.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ALCOCH2OOH	4.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_3H_4O_4$	7.6×10^{3}		Wang et al. (2017)	Q	80, 239
RQBGWFCHIWSUOK-UHFFFAOYSA-N	3.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C33CO	4.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_3H_2O_3$	2.8×10^{3}		Wang et al. (2017)	Q	80, 239
ICQNCHSXWNQIHC-UHFFFAOYSA-N	4.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C312COCO3H	4.7×10^{7}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_5$	3.2×10^{5}		Wang et al. (2017)	Q	80, 239
GUGBJTDAGNLAJO-UHFFFAOYSA-N	8.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C413COOOH	3.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_4$	3.5×10^{4}		Wang et al. (2017)	Q	80, 239
XUKQQLOKOLCMAI-UHFFFAOYSA-N	4.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C4CO2OOH	3.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_4$	2.6×10^{4}		Wang et al. (2017)	Q	80, 239
NOBUEMWCPQFCCN-UHFFFAOYSA-N	2.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C4CODIAL	4.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_3$	5.0×10^{3}		Wang et al. (2017)	Q	80, 239
OWIMZZMOFXSCLT-UHFFFAOYSA-N	2.5		Wang et al. (2017)	Q	80, 240
MCM:CO23C3CHO	3.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_3$	3.3×10^{3}		Wang et al. (2017)	Q	80, 239
LVZOZHOAAHWEOQ-UHFFFAOYSA-N	1.7×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CO2C3CHO	4.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_2$	6.0×10^{1}		Wang et al. (2017)	Q	80, 239
PKQIDSVLSKFZQC-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO2C4DIAL	2.8×10^{7}		Wang et al. (2017)	Q	80, 238
$C_4H_2O_4$	5.0×10^{5}		Wang et al. (2017)	Q	80, 239
OURVMEXCDVXLPR-UHFFFAOYSA-N	1.0×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:EGLYOX	4.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_2$	8.0		Wang et al. (2017)	Q	80, 239
RWHQMRRVZJSKGX-UHFFFAOYSA-N	2.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:VGLYOX	1.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_2$	2.6×10^{1}		Wang et al. (2017)	Q	80, 239
SDQVYUNYDAWYIK-UHFFFAOYSA-N	3.5×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C4CO2DCO3H	1.7×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_4O_5$	5.1×10^{6}		Wang et al. (2017)	Q	80, 239
AXIVSVGHKYPZBE-UHFFFAOYSA-N	8.1		Wang et al. (2017)	Q	80, 240
MCM:C4MCO2OOH	2.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	3.6×10^{3}		Wang et al. (2017)	Q	80, 239
RKGLOUQDKXPRQL-UHFFFAOYSA-N	6.3		Wang et al. (2017)	Q	80, 240
MCM:C511OOH	3.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	7.8×10^{4}		Wang et al. (2017)	Q	80, 239
NBNOBTZXOPWFTP-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C5124COOOH	2.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_5$	3.0×10^{6}		Wang et al. (2017)	Q	80, 239
BXDCDQOWFJMSCY-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C512OOH	2.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	9.3×10^{5}		Wang et al. (2017)	Q	80, 239
UGOJGQBYBBLKDX-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C515CO	2.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_4O_4$	1.0×10^{6}		Wang et al. (2017)	Q	80, 239
OONLUXUUWPUJOU-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C515OOH	2.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_5$	3.5×10^{6}		Wang et al. (2017)	Q	80, 239
KCJJHAINVUWKSI-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C54CO	2.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_4O_4$	5.8×10^{5}		Wang et al. (2017)	Q	80, 239
KDLDWLXQVYMIBX-UHFFFAOYSA-N	5.8×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C5CO23CHO	2.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_3$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
IPHREVVCPNNUEQ-UHFFFAOYSA-N	1.1×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C5COCHOOOH	2.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	2.3×10^{5}		Wang et al. (2017)	Q	80, 239
QJMOTDLHJFXUFN-UHFFFAOYSA-N	5.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C5DIALCO	1.4×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_4O_3$	4.9×10^{4}		Wang et al. (2017)	Q	80, 239
SFSCHQJUYKUKJM-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	80, 240
MCM:C5DICARB	1.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_2$	1.1×10^{3}		Wang et al. (2017)	Q	80, 239
GBLMMVFQENXAFZ-UHFFFAOYSA-N	2.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CHOC3COOOH	3.8×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_5$	7.4×10^{5}		Wang et al. (2017)	Q	80, 239
KFSMXRNQWYDJRM-UHFFFAOYSA-N	3.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CO12C4CHO	3.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_3$	9.3×10^{3}		Wang et al. (2017)	Q	80, 239
VUSMENNBCBGZQI-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO13C4CHO	3.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_3$	6.5×10^{3}		Wang et al. (2017)	Q	80, 239
SSMCSEDSANTCBB-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CO23C4CHO	2.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_3$	3.8×10^{3}		Wang et al. (2017)	Q	80, 239
QGGCMCHYJIPQCE-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	80, 240
MCM:CO24C4CHO	2.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_3$	4.3×10^{3}		Wang et al. (2017)	Q	80, 239
XHTYNUBGBUBFOA-UHFFFAOYSA-N	9.3		Wang et al. (2017)	Q	80, 240
MCM:CO2C43CHO	4.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_2$	1.7×10^{1}		Wang et al. (2017)	Q	80, 239
KNTLTMLEQPLVDA-UHFFFAOYSA-N	4.9		Wang et al. (2017)	Q	80, 240
MCM:CO2C4CHO	5.5×10^{2}	8400	Wieser et al. (2023)	Q	437
$C_5H_8O_2$	3.9×10^{1}		Wang et al. (2017)	Q	80, 238
KEHNRUNQZGRQHU-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	80, 239
	7.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO3C4CHO	3.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_2$	2.6×10^{1}		Wang et al. (2017)	Q	80, 239
ZNNXJRURXWWGLN-UHFFFAOYSA-N	6.5		Wang et al. (2017)	Q	80, 240
MCM:IPRGLYOX	4.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_2$	4.9		Wang et al. (2017)	Q	80, 239
FTDZDHIBENIBKZ-UHFFFAOYSA-N	1.9×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:PGLYOX	3.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_2$	5.8		Wang et al. (2017)	Q	80, 239
GDTHVMAIBQVUMV-UHFFFAOYSA-N	1.9×10^{-2}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:C23C54CHO	2.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	7.4×10^{2}		Wang et al. (2017)	Q	80, 239
CBIOWOAHGWGTSI-UHFFFAOYSA-N	2.8		Wang et al. (2017)	Q	80, 240
MCM:C3COCCHO	3.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_2$	2.2×10^{1}		Wang et al. (2017)	Q	80, 239
PVLKSJIUOKAUMV-UHFFFAOYSA-N	7.6		Wang et al. (2017)	Q	80, 240
MCM:C45IC5CHO	2.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	8.0×10^{2}		Wang et al. (2017)	Q	80, 239
WETHXHAOPNKQLZ-UHFFFAOYSA-N	4.5×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C4ECO2OOH	1.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	1.8×10^{3}		Wang et al. (2017)	Q	80, 239
CMRDMVGIWXQQFX-UHFFFAOYSA-N	3.6		Wang et al. (2017)	Q	80, 240
MCM:C511CHO	3.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
SLKPDJWOVVFRFW-UHFFFAOYSA-N	1.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C511CO3H	3.5×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	1.6×10^{6}		Wang et al. (2017)	Q	80, 239
PKVJBWZRBQBAMT-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C512CO3H	3.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	1.6×10^{6}		Wang et al. (2017)	Q	80, 239
OPLKNVAQLNTMAR-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C515CHO	2.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_4$	8.7×10^{5}		Wang et al. (2017)	Q	80, 239
JHVNJBQABGTRPH-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C515CO3H	2.2×10^{10}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_6$	1.1×10^{8}		Wang et al. (2017)	Q	80, 239
XPLLKUAMAYNXAT-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C5CO2DCO3H	1.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_5$	4.5×10^{6}		Wang et al. (2017)	Q	80, 239
DHHXAZIZMIZDQV-UHFFFAOYSA-N	3.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C5DCO2CO3H	1.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_5$	4.2×10^{6}		Wang et al. (2017)	Q	80, 239
GJOWGOOSLUXRQO-UHFFFAOYSA-N	6.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C5MDICARB	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_2$	1.0×10^{3}		Wang et al. (2017)	Q	80, 239
PFLPZDBOPDYOJU-UHFFFAOYSA-N	5.6		Wang et al. (2017)	Q	80, 240
MCM:C5TRONCO3H	2.2×10^{10}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_6$	4.6×10^{7}		Wang et al. (2017)	Q	80, 239
GGHLQXKHXYQGCE-UHFFFAOYSA-N	1.9×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:C6125CO	9.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_3$	6.2×10^{4}		Wang et al. (2017)	Q	80, 239
RFTMILUWMDIPHH-UHFFFAOYSA-N	5.4		Wang et al. (2017)	Q	80, 240
MCM:C6135COOOH	1.7×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	4.8×10^{6}		Wang et al. (2017)	Q	80, 239
HGYTXVUJMUREIP-UHFFFAOYSA-N	2.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C6145COOOH	1.7×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	7.8×10^{6}		Wang et al. (2017)	Q	80, 239
DSJLQKNTJKMXRQ-UHFFFAOYSA-N	2.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C615CO2OOH	1.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	1.2×10^{5}		Wang et al. (2017)	Q	80, 239
MOFLPBJDWVVKPL-UHFFFAOYSA-N	2.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C615CO	2.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	2.8×10^{2}		Wang et al. (2017)	Q	80, 239
BRRWJVYIMRBLKB-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	80, 240
MCM:C616OOH	2.4×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	1.7×10^{7}		Wang et al. (2017)	Q	80, 239
RZNSBZRPHHAABM-UHFFFAOYSA-N	3.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C617OOH	1.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	6.2×10^{3}		Wang et al. (2017)	Q	80, 239
VPKXUGZDYIOAPR-UHFFFAOYSA-N	4.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C618OOH	1.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	2.8×10^{3}		Wang et al. (2017)	Q	80, 239
AMQFKFSLRYYJMS-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C620OOH	2.4×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	1.0×10^{7}		Wang et al. (2017)	Q	80, 239
UWWRYJPKFSIPFS-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C626OOH	2.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	2.3×10^{6}		Wang et al. (2017)	Q	80, 239
DHTMLHKAZOWLFT-UHFFFAOYSA-N	4.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C65OOH	1.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	1.6×10^{4}		Wang et al. (2017)	Q	80, 239
LHKMAYQHAYSMQO-UHFFFAOYSA-N	5.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C6CO134	2.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	1.3×10^{3}		Wang et al. (2017)	Q	80, 239
VIOZHXSHLWOADQ-UHFFFAOYSA-N	6.2		Wang et al. (2017)	Q	80, 240
MCM:C6CO4DB	8.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_4O_4$	2.3×10^{6}		Wang et al. (2017)	Q	80, 239
OGFBTMOHTIWBJU-UHFFFAOYSA-N	1.6×10^{-1}		Wang et al. (2017)	Q	80, 240

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MCM:C6COALCO3H	3.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	4.3×10^{6}		Wang et al. (2017)	Q	80, 239
WRLXIVUJPLXKIG-UHFFFAOYSA-N	6.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C6COCHOOOH	2.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	1.5×10^{6}		Wang et al. (2017)	Q	80, 239
DQAWORJSQGOPLV-UHFFFAOYSA-N	5.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C6CODIAL	2.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	3.2×10^{4}		Wang et al. (2017)	Q	80, 239
PAXFMQWEAJBIJB-UHFFFAOYSA-N	2.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C6DICARB	1.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_2$	6.5×10^{2}		Wang et al. (2017)	Q	80, 239
GVKYFODEMNCLGS-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	80, 240
MCM:CO123C5CHO	2.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_4$	1.7×10^{6}		Wang et al. (2017)	Q	80, 239
GLSSGXNNMIEKBR-UHFFFAOYSA-N	1.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CO235C5CHO	1.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_4$	2.1×10^{5}		Wang et al. (2017)	Q	80, 239
GPIFCHFPYCMSRY-UHFFFAOYSA-N	4.7		Wang et al. (2017)	Q	80, 240
MCM:CO24M3CHO	2.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	8.0×10^{2}		Wang et al. (2017)	Q	80, 239
OQYGUGGUHGKPLC-UHFFFAOYSA-N	2.7		Wang et al. (2017)	Q	80, 240
MCM:CO2C4GLYOX	2.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	7.4×10^{3}		Wang et al. (2017)	Q	80, 239
YEJDUVJLIVLCFZ-UHFFFAOYSA-N	8.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO2C54CHO	3.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_2$	1.8×10^{2}		Wang et al. (2017)	Q	80, 239
IDAHIBMEKOEBRG-UHFFFAOYSA-N	5.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO2M33CHO	2.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_2$	1.1×10^{1}		Wang et al. (2017)	Q	80, 239
HOOWKSPRVCRTJK-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	80, 240
MCM:CO2M3C4CHO	3.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_2$	1.8×10^{2}		Wang et al. (2017)	Q	80, 239
GQHWESFTVGVFIA-UHFFFAOYSA-N	4.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO35C5CHO	2.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
KXLMWINKDVAJKB-UHFFFAOYSA-N	2.6		Wang et al. (2017)	Q	80, 240
MCM:CO3C54CHO	3.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_2$	1.6×10^{1}		Wang et al. (2017)	Q	80, 239
HFHZCESKBNQESK-UHFFFAOYSA-N	1.8		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CO3C5CHO	3.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_2$	2.3×10^{2}		Wang et al. (2017)	Q	80, 239
KKOFYQBBUSZDKJ-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO45C5CHO	2.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	9.1×10^{2}		Wang et al. (2017)	Q	80, 239
WXTRRXXKCNKUIA-UHFFFAOYSA-N	8.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:ECO4	1.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_4$	2.5×10^{5}		Wang et al. (2017)	Q	80, 239
RGMUISDTMIPFQK-UHFFFAOYSA-N	4.2×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:MC5DICARB	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_2$	8.9×10^{2}		Wang et al. (2017)	Q	80, 239
PEBMIJGMJUFNQE-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C4DBM2CO3H	7.8×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_5$	5.1×10^{6}		Wang et al. (2017)	Q	80, 239
OAFSDIWBIPMWQP-UHFFFAOYSA-N	8.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C617CHO	1.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	4.6×10^{2}		Wang et al. (2017)	Q	80, 239
NFXFJRVNKKYMOX-UHFFFAOYSA-N	7.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C617CO3H	2.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	1.2×10^{5}		Wang et al. (2017)	Q	80, 239
GEJLCFNTSCJUHB-UHFFFAOYSA-N	5.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C618CO3H	2.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	1.0×10^{5}		Wang et al. (2017)	Q	80, 239
BCVYZYXNMFZMHQ-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C626CHO	2.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	5.4×10^{4}		Wang et al. (2017)	Q	80, 239
HBIBDTOPQGUCOQ-UHFFFAOYSA-N	2.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C626CO3H	3.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	2.9×10^{6}		Wang et al. (2017)	Q	80, 239
XXGYBOYKTQFTKB-UHFFFAOYSA-N	8.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C6M5CO2OOH	6.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
BPEPZMFTCHTDHQ-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C715CO2OOH	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	5.8×10^{4}		Wang et al. (2017)	Q	80, 239
MXRQCKDWMJYUGS-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C716OOH	1.6×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	8.3×10^{6}		Wang et al. (2017)	Q	80, 239
PDOSKCUHLZEIAA-UHFFFAOYSA-N	2.5×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:C717OOH	1.6×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	4.9×10^{7}		Wang et al. (2017)	Q	80, 239
PIJZITIWWOWVNF-UHFFFAOYSA-N	6.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C718OOH	1.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	2.0×10^{5}		Wang et al. (2017)	Q	80, 239
IUOFUPZPJIEECL-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C731OOH	2.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	4.3×10^{6}		Wang et al. (2017)	Q	80, 239
GGMJSZWHPXYNJN-UHFFFAOYSA-N	4.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C735OOH	1.4×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	8.0×10^{6}		Wang et al. (2017)	Q	80, 239
FKXMDVIITUJJPH-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C736CO	5.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_3$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
XIQVOMVDKSOEBZ-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C736OOH	4.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	1.4×10^{5}		Wang et al. (2017)	Q	80, 239
FLZNSMFAMOSJOT-UHFFFAOYSA-N	4.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C7ADICARB	6.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_2$	1.3×10^{3}		Wang et al. (2017)	Q	80, 239
JOIPXRIQHWMPFU-UHFFFAOYSA-N	8.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C7CO2DBAL	7.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_3$	5.5×10^{4}		Wang et al. (2017)	Q	80, 239
YGMUVGSOGISXBZ-UHFFFAOYSA-N	3.1		Wang et al. (2017)	Q	80, 240
MCM:C7CO2DCO3H	9.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_5$	1.8×10^{6}		Wang et al. (2017)	Q	80, 239
GSEZJGCNNFTSDI-UHFFFAOYSA-N	2.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C7CO4DB	5.8×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_6O_4$	1.5×10^{6}		Wang et al. (2017)	Q	80, 239
RYPSCZRULGRFHH-UHFFFAOYSA-N	4.9×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C7DDICARB	9.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_2$	6.2×10^{2}		Wang et al. (2017)	Q	80, 239
SRVPSCZJUZZLCY-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:C7DICARB	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_2$	3.7×10^{2}		Wang et al. (2017)	Q	80, 239
GLRVVKVYRCSDLF-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO235C6CHO	1.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_4$	2.6×10^{5}		Wang et al. (2017)	Q	80, 239
DKBJFPXQZAZJBK-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:CO25C6CHO	1.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	2.6×10^{4}		Wang et al. (2017)	Q	80, 239
ZTMYUKBUAYLBJN-UHFFFAOYSA-N	4.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:IC7DICARB	1.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_2$	3.1×10^{2}		Wang et al. (2017)	Q	80, 239
XQQMMKHYZYQABV-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MC6CO2OOH	6.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	6.2×10^{3}		Wang et al. (2017)	Q	80, 239
HBFXSTFRJMUUSF-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C4DBMECO3H	6.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_5$	2.2×10^{6}		Wang et al. (2017)	Q	80, 239
MRKOFGXLZVJMLJ-UHFFFAOYSA-N	6.5×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C6CO4M2DB	3.9×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_8O_4$	1.7×10^{6}		Wang et al. (2017)	Q	80, 239
XSTUBABFSAZOJC-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	80, 240
MCM:C6ETCO4DB	4.5×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_8O_4$	8.1×10^{5}		Wang et al. (2017)	Q	80, 239
OAQBTICOMUFUNE-UHFFFAOYSA-N	2.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C718CO3H	1.7×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	2.4×10^{5}		Wang et al. (2017)	Q	80, 239
TVOCFMMHLDKVAZ-UHFFFAOYSA-N	8.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C731CO3H	2.5×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	2.1×10^{6}		Wang et al. (2017)	Q	80, 239
NTZMYPVPFVPPPF-UHFFFAOYSA-N	8.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C7M6CO2OOH	5.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	6.6×10^{3}		Wang et al. (2017)	Q	80, 239
SYXNCLOQMRSNCQ-UHFFFAOYSA-N	5.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C7MCO2DBAL	7.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_3$	3.2×10^{4}		Wang et al. (2017)	Q	80, 239
PDQBXAJOXSGWHJ-UHFFFAOYSA-N	1.8		Wang et al. (2017)	Q	80, 240
MCM:C7MCO2OOH	8.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	3.6×10^{4}		Wang et al. (2017)	Q	80, 239
IVJZKSXAPVTQOQ-UHFFFAOYSA-N	7.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C815CO2OOH	7.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	3.2×10^{4}		Wang et al. (2017)	Q	80, 239
BDUHFTDKOJODDX-UHFFFAOYSA-N	6.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C817CO	3.1×10^{5}	12000	Wieser et al. (2023)	Q	437
$C_8H_{12}O_3$	1.7×10^{4}		Wang et al. (2017)	Q	80, 238
WSCYQCAMZDXSLH-UHFFFAOYSA-N	5.8×10^{3}		Wang et al. (2017)	Q	80, 239
	3.1×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:C830CO	5.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_2$	3.8×10^{2}		Wang et al. (2017)	Q	80, 239
MHDCXCKIQVLVLU-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C831CO	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_3$	5.4×10^{3}		Wang et al. (2017)	Q	80, 239
ZUSGUVUFJOBUST-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C86OOH	1.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_4$	3.0×10^{5}		Wang et al. (2017)	Q	80, 239
DHFNMJQLYJIWHS-UHFFFAOYSA-N	3.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C87CO	1.5×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_4$	7.1×10^{4}		Wang et al. (2017)	Q	80, 239
ZGSYEZWRFTZRGE-UHFFFAOYSA-N	2.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C87OOH	1.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	2.8×10^{6}		Wang et al. (2017)	Q	80, 239
ZOZQVMIZJFBYCH-UHFFFAOYSA-N	9.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C8CO2DBAL	6.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_3$	3.9×10^{4}		Wang et al. (2017)	Q	80, 239
WFUAEUZWLUGFPU-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	80, 240
MCM:C8CO2DCO3H	7.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_5$	1.0×10^{6}		Wang et al. (2017)	Q	80, 239
AFZRTBPBEHNFPV-UHFFFAOYSA-N	1.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C8CO4DB	3.9×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_8O_4$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
XMBXSFIUGNBAMW-UHFFFAOYSA-N	2.4		Wang et al. (2017)	Q	80, 240
MCM:C8DCO2CO3H	8.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_5$	1.2×10^{6}		Wang et al. (2017)	Q	80, 239
LSJULIYFTAQYGE-UHFFFAOYSA-N	1.9×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:CO4DBC8	3.9×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_8O_4$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
UUVQUVHMBIAKFN-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	80, 240
MCM:MC7CO2OOH	5.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	3.0×10^{3}		Wang et al. (2017)	Q	80, 239
XEFYLFAPQOHXQI-UHFFFAOYSA-N	9.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C6CO4MEDB	3.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_4$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
KWNUZJFJQSMOTR-UHFFFAOYSA-N	6.9×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C6IPRCO4DB	4.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_4$	8.7×10^{5}		Wang et al. (2017)	Q	80, 239
PHOIWTKCTUWXFI-UHFFFAOYSA-N	1.9×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:C6PRCO4DB	3.7×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_4$	9.6×10^{5}		Wang et al. (2017)	Q	80, 239
ZAOQHXFQWRKJIE-UHFFFAOYSA-N	1.9×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C7CO4EDB	3.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_4$	1.3×10^{6}		Wang et al. (2017)	Q	80, 239
ZLFZFHOVUMHREF-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	80, 240
MCM:C7ECO4DB	3.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_4$	1.3×10^{6}		Wang et al. (2017)	Q	80, 239
AWHQTSPUFRSDOO-UHFFFAOYSA-N	7.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C827CHO	9.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_3$	8.5×10^{3}		Wang et al. (2017)	Q	80, 239
WRGXNTJIWBXAOX-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C828CHO	7.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	5.8×10^{4}		Wang et al. (2017)	Q	80, 239
YZUHPZZEPOWVFM-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C87CO3H	1.5×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_6$	5.3×10^{7}		Wang et al. (2017)	Q	80, 239
AJHPLULEOIFIGV-UHFFFAOYSA-N	2.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C88CHO	3.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	8.9×10^{4}		Wang et al. (2017)	Q	80, 239
NXCXUGLKKPDWEC-UHFFFAOYSA-N	8.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C914CO	2.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_4$	1.5×10^{7}		Wang et al. (2017)	Q	80, 239
RDBINALOBQAVHT-UHFFFAOYSA-N	5.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C914OOH	2.6×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	1.6×10^{8}		Wang et al. (2017)	Q	80, 239
ZERYOMDBUHTQAV-UHFFFAOYSA-N	3.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C915OOH	4.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	4.2×10^{6}		Wang et al. (2017)	Q	80, 239
IHUGTHJLMVJZBZ-UHFFFAOYSA-N	2.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C916OOH	1.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	4.8×10^{7}		Wang et al. (2017)	Q	80, 239
FURCCROLNKVFJP-UHFFFAOYSA-N	4.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C918OOH	4.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	7.8×10^{5}		Wang et al. (2017)	Q	80, 239
RVRGXPTVZZTPQO-UHFFFAOYSA-N	1.1×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C919OOH	1.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	4.5×10^{7}		Wang et al. (2017)	Q	80, 239
HGDKSMVLGYFVMB-UHFFFAOYSA-N	2.6×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C926OOH	7.3×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	5.5×10^{6}		Wang et al. (2017)	Q	80, 239
YGLJXDYJGXWZRQ-UHFFFAOYSA-N	2.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C930OOH	7.3×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	2.6×10^{7}		Wang et al. (2017)	Q	80, 239
UQPOFUKCKANZIY-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:CO4DBC9	2.5×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_4$	1.2×10^{6}		Wang et al. (2017)	Q	80, 239
KCIAXTRCVKQJBW-UHFFFAOYSA-N	7.1		Wang et al. (2017)	Q	80, 240
MCM:LMLKACO	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	8.1×10^{5}		Wang et al. (2017)	Q	80, 239
JZUAMOXWRDMCCH-UHFFFAOYSA-N	8.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:LMLKAOOH	1.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	1.7×10^{7}		Wang et al. (2017)	Q	80, 239
VTXNRXDJNZTEJV-UHFFFAOYSA-N	9.1×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:LMLKBCO	1.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	5.5×10^{5}		Wang et al. (2017)	Q	80, 239
UMGHNOQMPCKCSD-UHFFFAOYSA-N	6.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:LMLKBOOH	1.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	3.6×10^{7}		Wang et al. (2017)	Q	80, 239
YVDVZIZUYUAKKJ-UHFFFAOYSA-N	3.0×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:LMLKET	1.1×10^{6}	13000	Wieser et al. (2023)	Q	437
$C_9H_{14}O_3$	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
CWEQHJLFCKMWEE-UHFFFAOYSA-N	5.4×10^{4}		Wang et al. (2017)	Q	80, 239
	3.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NORLIMAL	6.1×10^{2}	11000	Wieser et al. (2023)	Q	437
$C_9H_{14}O_2$	4.9×10^{1}		Wang et al. (2017)	Q	80, 238
WPNOYHDEEVPEJH-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	80, 239
	9.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NORPINAL	5.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_2$	2.2×10^{2}		Wang et al. (2017)	Q	80, 239
CRBGTXDFEDFKSU-UHFFFAOYSA-N	4.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C1010OOH	2.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_4$	3.8×10^{5}		Wang et al. (2017)	Q	80, 239
PQCOZMUQYGSZBV-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C1012CO	7.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_3$	6.5×10^{4}		Wang et al. (2017)	Q	80, 239
ZTXNVHZVZBDWRG-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C1012OOH	9.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_4$	3.5×10^{5}		Wang et al. (2017)	Q	80, 239
NQAGNHJKHGEOIP-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C106OOH	6.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_5$	3.2×10^{7}		Wang et al. (2017)	Q	80, 239
QENSMPURVPBEBQ-UHFFFAOYSA-N	1.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C107OOH	2.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_4$	1.6×10^{4}		Wang et al. (2017)	Q	80, 239
JYIMELQJWXRSLA-UHFFFAOYSA-N	3.2×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C108OOH	6.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_5$	1.7×10^{7}		Wang et al. (2017)	Q	80, 239
AIXQDYAMZUITKH-UHFFFAOYSA-N	2.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C109CO	3.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{14}O_3$	5.6×10^{3}		Wang et al. (2017)	Q	80, 239
GPWOGFGLGKGEOT-UHFFFAOYSA-N	8.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C109OOH	3.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_4$	5.8×10^{4}		Wang et al. (2017)	Q	80, 239
ODTCGEGBAGAWAJ-UHFFFAOYSA-N	5.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:LIMALACO	4.3×10^{4}	13000	Wieser et al. (2023)	Q	437
$C_{10}H_{14}O_3$	2.6×10^{4}		Wang et al. (2017)	Q	80, 238
OXUPJDFJWCMZMO-UHFFFAOYSA-N	2.9×10^{3}		Wang et al. (2017)	Q	80, 239
	3.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:LIMALAOOH	2.5×10^{5}	15000	Wieser et al. (2023)	Q	437
$C_{10}H_{16}O_4$	3.5×10^{6}		Wang et al. (2017)	Q	80, 238
DVORBFWFCUOYLW-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
	4.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:LIMALBCO	3.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{14}O_3$	2.0×10^{3}		Wang et al. (2017)	Q	80, 239
OFCYPGCYWHDSNB-UHFFFAOYSA-N	8.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:LIMALBOOH	2.4×10^{5}	15000	Wieser et al. (2023)	Q	437
$C_{10}H_{16}O_4$	2.9×10^{6}		Wang et al. (2017)	Q	80, 238
DCWLKDSHBWMMQU-UHFFFAOYSA-N	2.0×10^{4}		Wang et al. (2017)	Q	80, 239
	1.4×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:LIMAL	4.0×10^{2}	11000	Wieser et al. (2023)	Q	437
$C_{10}H_{16}O_2$	3.8×10^{1}		Wang et al. (2017)	Q	80, 238
OGCGCISRMFSLTC-UHFFFAOYSA-N	7.4×10^{1}		Wang et al. (2017)	Q	80, 239
	2.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PINAL	4.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_2$	2.0×10^{2}		Wang et al. (2017)	Q	80, 239
GCHDWVBHKDJOKU-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:PINALOOH	2.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_4$	1.0×10^{6}		Wang et al. (2017)	Q	80, 239
IKYOAMQPSDRUHL-UHFFFAOYSA-N	5.5×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C116CO	3.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{16}O_3$	2.0×10^{4}		Wang et al. (2017)	Q	80, 239
XGVKCXDPIYHMTH-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C116OOH	2.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_4$	2.0×10^{6}		Wang et al. (2017)	Q	80, 239
GLQKGYMROFUHSE-UHFFFAOYSA-N	2.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C116CHO	2.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{18}O_3$	1.4×10^{5}		Wang et al. (2017)	Q	80, 239
LCDZSXGLJAAQMI-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C116CO3H	3.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{18}O_5$	2.4×10^{6}		Wang et al. (2017)	Q	80, 239
DYOBAPPYFCSOAS-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C1210OOH	2.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_4$	4.7×10^{6}		Wang et al. (2017)	Q	80, 239
KZRFFJDVJJJBDC-UHFFFAOYSA-N	4.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C129CO	1.9×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{16}O_4$	8.7×10^{5}		Wang et al. (2017)	Q	80, 239
RGVZWLUABXGGBI-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C129OOH	2.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{18}O_5$	1.5×10^{7}		Wang et al. (2017)	Q	80, 239
OVAMHHASBHCMIZ-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C1210CO3H	2.8×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{20}O_5$	1.9×10^{6}		Wang et al. (2017)	Q	80, 239
BXGKTBFSJURUHS-UHFFFAOYSA-N	6.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C131CO	1.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{20}O_3$	2.1×10^{4}		Wang et al. (2017)	Q	80, 239
FDPPFMUIMWYEIX-UHFFFAOYSA-N	3.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:BCLKACO	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{20}O_4$	3.2×10^{6}		Wang et al. (2017)	Q	80, 239
ARRZIWJBJSIOKE-UHFFFAOYSA-N	4.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:BCLKAOOH	1.1×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_5$	1.7×10^{7}		Wang et al. (2017)	Q	80, 239
CKBNEDHFWOQWQD-UHFFFAOYSA-N	2.6×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:BCLKBCO	1.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{20}O_4$	2.9×10^{6}		Wang et al. (2017)	Q	80, 239
NZHCLRCYZNBCMK-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:BCLKBOOH	1.1×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_5$	4.6×10^{7}		Wang et al. (2017)	Q	80, 239
CNYMBWKCKYTSRZ-UHFFFAOYSA-N	1.5×10^{6}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:BCLKCCO	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{20}O_4$	1.2×10^{6}		Wang et al. (2017)	Q	80, 239
RVZWWCAHYGTHHX-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:BCLKCOOH	1.1×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_5$	1.5×10^{7}		Wang et al. (2017)	Q	80, 239
OVPKMRRDRUAGIL-UHFFFAOYSA-N	6.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:BCLKET	1.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_3$	1.4×10^{5}		Wang et al. (2017)	Q	80, 239
UGDRYISIDBCIAI-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C141CO	4.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_2$	1.6×10^{2}		Wang et al. (2017)	Q	80, 239
LUPUYUXNGLIEMW-UHFFFAOYSA-N	7.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C146CO	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{20}O_4$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
ODTZTSYYOIXMEF-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C146OOH	1.1×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_5$	1.3×10^{7}		Wang et al. (2017)	Q	80, 239
SPXXDEIFDYFSMG-UHFFFAOYSA-N	1.6×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:BCALACO	2.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{22}O_3$	3.6×10^{3}		Wang et al. (2017)	Q	80, 239
ULXUQSOGQJAAAV-UHFFFAOYSA-N	4.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:BCALAOOH	3.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{24}O_4$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
CATQWYAHYHBBFL-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:BCALBCO	3.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{22}O_3$	2.9×10^{3}		Wang et al. (2017)	Q	80, 239
DVBAGSYXLVWTHM-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:BCALBOOH	2.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{24}O_4$	3.6×10^{4}		Wang et al. (2017)	Q	80, 239
BXDTVEFUTYSWEH-UHFFFAOYSA-N	1.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:BCAL	3.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{24}O_2$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
PJJCDGMFEIUQRZ-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:BCALCCO	2.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{22}O_3$	4.7×10^{3}		Wang et al. (2017)	Q	80, 239
RMGPJKLPPRXORI-UHFFFAOYSA-N	2.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:BCALCOOH	3.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{24}O_4$	1.7×10^{4}		Wang et al. (2017)	Q	80, 239
WQOUANLPJNTVBV-UHFFFAOYSA-N	2.5×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PHGLYOX	1.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_6O_2$	8.9×10^{1}		Wang et al. (2017)	Q	80, 239
OJUGVDODNPJEEC-UHFFFAOYSA-N	8.1×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:MPHGLYOX	1.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_8O_2$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
ILRFLXHICGHRIN-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	80, 240
MCM:DMPHGLYOX	6.5×10^{2}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{10}O_2$	6.6×10^{1}		Wang et al. (2017)	Q	80, 239
COKLAMNWIKZGIN-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	80, 240
MCM:EMPHGLYOX	5.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{12}O_2$	5.3×10^{1}		Wang et al. (2017)	Q	80, 239
LRURTQBJFCJOFP-UHFFFAOYSA-N	8.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:HOCH2COCHO	7.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_4O_3$	4.4×10^{3}		Wang et al. (2017)	Q	80, 239
JLPAWRLRMTZCSF-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	80, 240
MCM:CCOCOCOH	7.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_3$	3.2×10^{3}		Wang et al. (2017)	Q	80, 239
AWMGPEHDHJUMEN-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	80, 240
MCM:CO13C4OH	6.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_3$	2.3×10^{4}		Wang et al. (2017)	Q	80, 239
KATSYVMPKZTIRW-UHFFFAOYSA-N	4.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CO2H3CHO	1.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_3$	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
GTYVZUSWKGYETP-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:H13CO2CHO	1.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_4$	4.6×10^{5}		Wang et al. (2017)	Q	80, 239
RAPYKXPBVBNJGC-UHFFFAOYSA-N	3.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:H1CO23CHO	4.7×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_4$	1.2×10^{6}		Wang et al. (2017)	Q	80, 239
XSEYITBSKRUSNL-UHFFFAOYSA-N	3.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HO1CO3CHO	1.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_3$	4.0×10^{4}		Wang et al. (2017)	Q	80, 239
CUSSNCHZLYDUPJ-UHFFFAOYSA-N	6.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HOCOC4DIAL	1.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_4$	5.3×10^{5}		Wang et al. (2017)	Q	80, 239
JWBVDBDNUQOADG-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C4MCO2OH	8.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	3.2×10^{3}		Wang et al. (2017)	Q	80, 239
YKNUMNAVGAMCFT-UHFFFAOYSA-N	2.6		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C512OH	1.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	1.5×10^{5}		Wang et al. (2017)	Q	80, 239
ZSJOVUGBPPFONP-UHFFFAOYSA-N	5.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C5134CO2OH	9.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_4$	4.2×10^{5}		Wang et al. (2017)	Q	80, 239
UFXCMYYHMGNRSQ-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C513CO	7.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_4$	5.9×10^{6}		Wang et al. (2017)	Q	80, 239
GBFAZHBQOBSKET-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C513OH	3.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	8.9×10^{7}		Wang et al. (2017)	Q	80, 239
VLANIYKAIBIISW-UHFFFAOYSA-N	4.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C513OOH	8.9×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	2.5×10^{8}		Wang et al. (2017)	Q	80, 239
FJRVRXOZJCMNIT-UHFFFAOYSA-N	5.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C514CO23OH	4.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	4.5×10^{6}		Wang et al. (2017)	Q	80, 239
JLVNMCMGUWUGCO-UHFFFAOYSA-N	4.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C520OH	1.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
BXHDMMHJHUOSNS-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C520OOH	7.1×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	3.0×10^{6}		Wang et al. (2017)	Q	80, 239
BCWSZSNCYSGOQJ-UHFFFAOYSA-N	2.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C5CO3OH	9.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_4$	6.2×10^{5}		Wang et al. (2017)	Q	80, 239
UUUQEQKLOQQXBA-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C5DICAROOH	6.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	1.3×10^{7}		Wang et al. (2017)	Q	80, 239
SXCXUVJXNGWYKY-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:CO3H4CHO	1.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	7.1×10^{3}		Wang et al. (2017)	Q	80, 239
GHHQRUFNLVFZPQ-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	80, 240
MCM:H1C23C4CHO	3.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_4$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
VBLXHDGHHJBCMK-UHFFFAOYSA-N	3.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HMVKBCHO	3.6×10^{5}	11000	Wieser et al. (2023)	Q	437
$C_5H_8O_3$	1.1×10^{5}		Wang et al. (2017)	Q	80, 238
XYGGNMZYIGPNCC-UHFFFAOYSA-N	1.3×10^{5}		Wang et al. (2017)	Q	80, 239
	2.5×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HO2CO4CHO	1.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	2.5×10^{4}		Wang et al. (2017)	Q	80, 239
NSUJYXKDWVMPFQ-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HOIPRGLYOX	1.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	3.2×10^{4}		Wang et al. (2017)	Q	80, 239
ROKGRLJNHSUEOC-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:IEC2OOH	3.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	2.0×10^{6}		Wang et al. (2017)	Q	80, 239
KGZJHQJCDPZOFG-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MBOCOCO	3.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	6.8×10^{2}		Wang et al. (2017)	Q	80, 239
OCAJTNNCRSVJNU-UHFFFAOYSA-N	8.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C43OHCOCHO	1.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	2.8×10^{4}		Wang et al. (2017)	Q	80, 239
NMZPCKZSNUOBSC-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	80, 240
MCM:C517CHO	9.5×10^{2}	13000	Wieser et al. (2023)	Q	437
$C_6H_{10}O_3$	1.0×10^{5}		Wang et al. (2017)	Q	80, 238
JGHPNZFTVGSLKF-UHFFFAOYSA-N	7.8×10^{5}		Wang et al. (2017)	Q	80, 239
	2.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C519CHO	2.8×10^{6}	11000	Wieser et al. (2023)	Q	437
$C_6H_{10}O_3$	1.0×10^{5}		Wang et al. (2017)	Q	80, 238
PVAHQKAVPKMXGV-UHFFFAOYSA-N	2.6×10^{5}		Wang et al. (2017)	Q	80, 239
	6.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C5COOHCO3H	4.7×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_6$	3.2×10^{9}		Wang et al. (2017)	Q	80, 239
DETDOHNNOYOALO-UHFFFAOYSA-N	8.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C5MO132OH	1.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	3.0×10^{3}		Wang et al. (2017)	Q	80, 239
YVTXQDAOLHXGGS-UHFFFAOYSA-N	2.7		Wang et al. (2017)	Q	80, 240
MCM:C6134CO2OH	7.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	1.8×10^{5}		Wang et al. (2017)	Q	80, 239
ZUSWTYLGBZLTMD-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C614CO23OH	3.4×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	3.6×10^{6}		Wang et al. (2017)	Q	80, 239
FTHGMBBEYTXWQT-UHFFFAOYSA-N	1.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C615CO2OH	2.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	1.1×10^{5}		Wang et al. (2017)	Q	80, 239
AEWAJJBQFQHEAB-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C616OH	9.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	7.4×10^{6}		Wang et al. (2017)	Q	80, 239
VJOSQGBCXQMKDE-UHFFFAOYSA-N	8.9×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:C617OH	3.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	4.8×10^{3}		Wang et al. (2017)	Q	80, 239
GSQCYSIEWGMUPC-UHFFFAOYSA-N	7.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C620OH	4.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	9.6×10^{6}		Wang et al. (2017)	Q	80, 239
SMLWDBHBBFROKP-UHFFFAOYSA-N	4.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C628OH	4.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	3.6×10^{7}		Wang et al. (2017)	Q	80, 239
XRZKKMNIWXFNJQ-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C628OOH	6.3×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	5.4×10^{7}		Wang et al. (2017)	Q	80, 239
BGLCDSUTRBZUMD-UHFFFAOYSA-N	3.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C629OH	2.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	1.1×10^{7}		Wang et al. (2017)	Q	80, 239
MIXLBBAGKJLCSO-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C629OOH	4.9×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	2.0×10^{7}		Wang et al. (2017)	Q	80, 239
PARGUUHBZPMBOS-UHFFFAOYSA-N	2.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C630CO	2.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	3.4×10^{5}		Wang et al. (2017)	Q	80, 239
AUMGTZPDEFNUMP-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C65OH	3.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	3.4×10^{4}		Wang et al. (2017)	Q	80, 239
ZWRMEYSYDMGCIE-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C67CHO	3.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	6.2×10^{3}		Wang et al. (2017)	Q	80, 239
BZFZPOBVGBFEBG-UHFFFAOYSA-N	8.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C6CO2M2OH	2.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	4.4×10^{6}		Wang et al. (2017)	Q	80, 239
ZFPKEBYORKZJID-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C6CO2OHOOH	3.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	3.3×10^{6}		Wang et al. (2017)	Q	80, 239
LMEOLDNWXYVMAA-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C6CO3MOH	5.4×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	8.3×10^{4}		Wang et al. (2017)	Q	80, 239
WBLLHOUAAGAGCV-UHFFFAOYSA-N	4.0		Wang et al. (2017)	Q	80, 240
MCM:C6COHOCHO	8.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	4.0×10^{5}		Wang et al. (2017)	Q	80, 239
HJNIDOQIVMJXHS-UHFFFAOYSA-N	2.5×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C6DICAROOH	5.5×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	9.6×10^{6}		Wang et al. (2017)	Q	80, 239
HIILQMKIFXFEHC-UHFFFAOYSA-N	2.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C6O132OH	1.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	3.6×10^{3}		Wang et al. (2017)	Q	80, 239
GIDOBZXUXDNRDY-UHFFFAOYSA-N	3.0		Wang et al. (2017)	Q	80, 240
MCM:C6TONOHOOH	2.6×10^{11}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_6$	1.1×10^{10}		Wang et al. (2017)	Q	80, 239
CIXJOARRJVNUNZ-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:H2M3CO4CHO	1.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	2.6×10^{4}		Wang et al. (2017)	Q	80, 239
MIIVJRGFVJVTGE-UHFFFAOYSA-N	9.8		Wang et al. (2017)	Q	80, 240
MCM:H3C25C5CHO	3.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	2.0×10^{6}		Wang et al. (2017)	Q	80, 239
CLPDOVMSDUESLY-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HM22COCHO	6.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	1.8×10^{4}		Wang et al. (2017)	Q	80, 239
UTYMQWKKMYQTHJ-UHFFFAOYSA-N	6.0		Wang et al. (2017)	Q	80, 240
MCM:MC52CO2OH	2.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	4.6×10^{6}		Wang et al. (2017)	Q	80, 239
LGFUKTGFFSPNKZ-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MC5COOHOOH	3.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	6.0×10^{6}		Wang et al. (2017)	Q	80, 239
XFHCIPDXRRXAPB-UHFFFAOYSA-N	8.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MIBKHO4CHO	6.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	1.3×10^{4}		Wang et al. (2017)	Q	80, 239
OYDFBAKICJVUQJ-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C61CHO	6.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	1.4×10^{5}		Wang et al. (2017)	Q	80, 239
BDFRSVKDVGXKLG-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C62CHO	7.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	1.3×10^{5}		Wang et al. (2017)	Q	80, 239
QCTBGQUOJXZEIH-UHFFFAOYSA-N	4.3		Wang et al. (2017)	Q	80, 240
MCM:C6COOHCO3H	3.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_6$	2.4×10^{9}		Wang et al. (2017)	Q	80, 239
BNWBZUAKPODUMK-UHFFFAOYSA-N	3.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C6M5CO2OH	1.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	2.2×10^{4}		Wang et al. (2017)	Q	80, 239
YAAUSHWRBSRFSJ-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:C715CO2OH	1.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	7.6×10^{4}		Wang et al. (2017)	Q	80, 239
KBBGTWJMXYAKIO-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C716OH	2.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	6.8×10^{6}		Wang et al. (2017)	Q	80, 239
QFGSQPDLKNLDDS-UHFFFAOYSA-N	9.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C717OH	5.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	1.6×10^{7}		Wang et al. (2017)	Q	80, 239
SEENFYUXRUQNHQ-UHFFFAOYSA-N	2.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C718OH	5.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_3$	2.7×10^{4}		Wang et al. (2017)	Q	80, 239
ALYGFZDZOCWXMF-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C731OH	8.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_3$	1.7×10^{6}		Wang et al. (2017)	Q	80, 239
KHEBQEUBDOAJRG-UHFFFAOYSA-N	8.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C733CO	5.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	1.9×10^{7}		Wang et al. (2017)	Q	80, 239
IRSIMXCKMCQRGW-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C733OH	1.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	3.3×10^{8}		Wang et al. (2017)	Q	80, 239
WRHSSXYTISGZIA-UHFFFAOYSA-N	3.7×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C733OOH	7.4×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	7.3×10^{8}		Wang et al. (2017)	Q	80, 239
OWEUBRYSVXGVIC-UHFFFAOYSA-N	2.7×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C735OH	2.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	1.7×10^{7}		Wang et al. (2017)	Q	80, 239
PHOAHMZZKPNPAM-UHFFFAOYSA-N	4.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C736OH	8.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	1.3×10^{5}		Wang et al. (2017)	Q	80, 239
QWXLVLIZAXRZBR-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C7ADCOH	1.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	2.8×10^{6}		Wang et al. (2017)	Q	80, 239
SVQINHOHTZDOCH-UHFFFAOYSA-N	7.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C7ADCOOH	1.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	5.1×10^{6}		Wang et al. (2017)	Q	80, 239
COQUITHNSRNVBJ-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C7CO3OHOOH	3.0×10^{11}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_6$	3.2×10^{8}		Wang et al. (2017)	Q	80, 239
YAEIVOJGWQGWPS-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C7DCOH	2.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	1.9×10^{6}		Wang et al. (2017)	Q	80, 239
VIPBNCDHLKDPDM-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C7DCOOH	4.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	5.1×10^{6}		Wang et al. (2017)	Q	80, 239
AVRZSWZUKXCJRK-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C7DDCOH	1.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	2.6×10^{6}		Wang et al. (2017)	Q	80, 239
HYCGRSOMYJQICU-UHFFFAOYSA-N	6.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C7DDCOOH	3.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	1.4×10^{6}		Wang et al. (2017)	Q	80, 239
VSEOFSAKNXJKSZ-UHFFFAOYSA-N	8.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:IC7DCOH	3.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	1.5×10^{6}		Wang et al. (2017)	Q	80, 239
DEDFQTYPJDABTI-UHFFFAOYSA-N	7.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:IC7DCOOH	5.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	5.8×10^{6}		Wang et al. (2017)	Q	80, 239
ZVFWDEWSMKAAIM-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:MC6CO2OH	1.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	1.0×10^{4}		Wang et al. (2017)	Q	80, 239
BNJUZVCUVNAPOM-UHFFFAOYSA-N	3.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C5M2OHCO3H	2.1×10^{9}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_6$	3.2×10^{9}		Wang et al. (2017)	Q	80, 239
BRIBGOXGRALVGI-UHFFFAOYSA-N	9.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C7M15CO2OH	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_3$	3.0×10^{4}		Wang et al. (2017)	Q	80, 239
OEJDBFGEAKTZGI-UHFFFAOYSA-N	6.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C7M6CO2OH	9.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_3$	1.3×10^{4}		Wang et al. (2017)	Q	80, 239
WXVOVBAGQNBDEE-UHFFFAOYSA-N	4.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C7MO3OHOOH	3.0×10^{11}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_6$	2.2×10^{8}		Wang et al. (2017)	Q	80, 239
UOUKTGYLQYQUAO-UHFFFAOYSA-N	4.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C7OHO2CO3H	2.8×10^{9}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_6$	1.7×10^{9}		Wang et al. (2017)	Q	80, 239
AOHPTSIBUCEZIY-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C815CO2OH	1.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_3$	3.8×10^{4}		Wang et al. (2017)	Q	80, 239
IPCSMQASRIZASM-UHFFFAOYSA-N	6.2×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C824CO	1.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_3$	4.6×10^{4}		Wang et al. (2017)	Q	80, 239
BQDQKENHFIFOJZ-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C83COOHOOH	2.7×10^{11}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_6$	2.0×10^{8}		Wang et al. (2017)	Q	80, 239
LBBMWNQOJHPRLQ-UHFFFAOYSA-N	6.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C87OH	2.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	2.1×10^{6}		Wang et al. (2017)	Q	80, 239
DFOLUFIWIMPWQH-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:MC7CO2OH	9.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_3$	6.6×10^{3}		Wang et al. (2017)	Q	80, 239
BSMWBPAKWVVEKL-UHFFFAOYSA-N	1.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C5MEJCO3H	1.7×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_6$	2.2×10^{9}		Wang et al. (2017)	Q	80, 239
IZKMPGKTEBWFPK-UHFFFAOYSA-N	5.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C8O2OHCO3H	2.6×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_6$	1.3×10^{9}		Wang et al. (2017)	Q	80, 239
MBOWYQZNYXRQRC-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C8OHO2CO3H	2.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_6$	1.1×10^{9}		Wang et al. (2017)	Q	80, 239
CJLPRBWVJFSMFP-UHFFFAOYSA-N	8.7		Wang et al. (2017)	Q	80, 240
MCM:C914OH	5.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	8.3×10^{7}		Wang et al. (2017)	Q	80, 239
LFDXAZOJHXEEGS-UHFFFAOYSA-N	2.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C915OH	1.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_3$	2.8×10^{6}		Wang et al. (2017)	Q	80, 239
FAAQZCMVHKUUSB-UHFFFAOYSA-N	8.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C916OH	3.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	1.4×10^{7}		Wang et al. (2017)	Q	80, 239
MXDMOPCDPNEDIT-UHFFFAOYSA-N	6.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C918OH	1.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_3$	4.4×10^{5}		Wang et al. (2017)	Q	80, 239
NFJZVEFTUBPOLY-UHFFFAOYSA-N	1.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C919OH	3.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	1.5×10^{7}		Wang et al. (2017)	Q	80, 239
ULXJXURNPDAXQL-UHFFFAOYSA-N	3.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C926OH	1.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	7.3×10^{6}		Wang et al. (2017)	Q	80, 239
DBPGQZSZWKEZHT-UHFFFAOYSA-N	1.2×10^{5}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C930OH	2.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	5.3×10^{6}		Wang et al. (2017)	Q	80, 239
LNIVXHBNNGOOPM-UHFFFAOYSA-N	3.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:LMLKAOH	2.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	2.6×10^{7}		Wang et al. (2017)	Q	80, 239
XDMVMFNHBSPJDJ-UHFFFAOYSA-N	1.6×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:LMLKBOH	2.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	3.0×10^{7}		Wang et al. (2017)	Q	80, 239
JSAHIYWZESQWRA-UHFFFAOYSA-N	1.1×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:NORLIMOOH	3.8×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{16}O_5$	3.8×10^{8}		Wang et al. (2017)	Q	80, 239
CUMGKBRSRBORIJ-UHFFFAOYSA-N	6.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C1010OH	6.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_3$	5.3×10^{5}		Wang et al. (2017)	Q	80, 239
NQWGZMQLCPYJCB-UHFFFAOYSA-N	8.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C1012OH	3.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_3$	5.6×10^{5}		Wang et al. (2017)	Q	80, 239
ZSBQFHQMMVQAKS-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C106OH	2.5×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_4$	8.1×10^{6}		Wang et al. (2017)	Q	80, 239
LWIDJJPVYZTGLI-UHFFFAOYSA-N	9.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C107OH	3.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_3$	5.9×10^{4}		Wang et al. (2017)	Q	80, 239
DUMRJPIWTJFZCT-UHFFFAOYSA-N	6.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C108OH	2.5×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_4$	3.2×10^{6}		Wang et al. (2017)	Q	80, 239
ZDBVABFEYYIFLR-UHFFFAOYSA-N	5.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C109OH	6.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_3$	4.3×10^{4}		Wang et al. (2017)	Q	80, 239
PUENXTSKKXKPMK-UHFFFAOYSA-N	2.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:LIMALAOH	3.1×10^{4}	15000	Wieser et al. (2023)	Q	437
$C_{10}H_{16}O_3$	5.8×10^{3}		Wang et al. (2017)	Q	80, 238
VNYSFQVUCPNMDZ-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	80, 239
	1.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:LIMALBOH	5.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_3$	1.8×10^{4}		Wang et al. (2017)	Q	80, 239
SMXSHIIAZMJGAE-UHFFFAOYSA-N	5.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:LIMALOH	2.2×10^{10}	18000	Wieser et al. (2023)	Q	437
$C_{10}H_{18}O_4$	4.2×10^{7}		Wang et al. (2017)	Q	80, 238
ISUQULRVPDSRIP-UHFFFAOYSA-N	2.8×10^{8}		Wang et al. (2017)	Q	80, 239
	9.3×10^{5}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:LIMALOOH	4.3×10^{10}	18000	Wieser et al. (2023)	Q	437
$C_{10}H_{18}O_5$	3.5×10^{9}		Wang et al. (2017)	Q	80, 238
OQLBLHLZVAPRGN-UHFFFAOYSA-N	4.0×10^{8}		Wang et al. (2017)	Q	80, 239
	9.6×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PINALOH	8.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_3$	6.0×10^{5}		Wang et al. (2017)	Q	80, 239
NGFXWFWSYUSJMH-UHFFFAOYSA-N	7.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C116OH	9.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_3$	2.6×10^{5}		Wang et al. (2017)	Q	80, 239
JMGXHRKVWURTTA-UHFFFAOYSA-N	5.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C117OH	8.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_4$	4.9×10^{8}		Wang et al. (2017)	Q	80, 239
XYBUENVNXDXQKB-UHFFFAOYSA-N	4.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C117OOH	5.4×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_5$	2.0×10^{8}		Wang et al. (2017)	Q	80, 239
NUIUIELMTMWFAB-UHFFFAOYSA-N	5.9×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C118CO	1.3×10^{10}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{16}O_5$	5.6×10^{8}		Wang et al. (2017)	Q	80, 239
QFBAMJSHDLKQRE-UHFFFAOYSA-N	6.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C118OH	6.2×10^{10}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_5$	3.6×10^{10}		Wang et al. (2017)	Q	80, 239
GQNPBTACCNTXDZ-UHFFFAOYSA-N	2.9×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C118OOH	1.6×10^{12}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_6$	3.0×10^{10}		Wang et al. (2017)	Q	80, 239
DZELKNYJHUANPY-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C1210OH	7.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_3$	2.6×10^{6}		Wang et al. (2017)	Q	80, 239
RDCPBXUNBHOYIW-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C1214OH	7.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_4$	4.7×10^{8}		Wang et al. (2017)	Q	80, 239
LBONAAUBRWCFLP-UHFFFAOYSA-N	2.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C1214OOH	4.4×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_5$	1.8×10^{8}		Wang et al. (2017)	Q	80, 239
RDWLNWMMPUJYPV-UHFFFAOYSA-N	8.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C1215CO	1.0×10^{10}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{18}O_5$	3.2×10^{9}		Wang et al. (2017)	Q	80, 239
MFAMPSJMWGSBSP-UHFFFAOYSA-N	2.8×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C1215OH	4.8×10^{10}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_5$	1.1×10^{11}		Wang et al. (2017)	Q	80, 239
ICTVPTJMPURCGE-UHFFFAOYSA-N	3.2×10^{6}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

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MCM:C1215OOH	1.3×10^{12}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_6$	4.6×10^{10}		Wang et al. (2017)	Q	80, 239
PWIVJRAMQXZVCR-UHFFFAOYSA-N	5.1×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C128CO	3.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{18}O_4$	8.3×10^{7}		Wang et al. (2017)	Q	80, 239
UGSIBTFJEGNWKQ-UHFFFAOYSA-N	6.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C128OH	1.5×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_4$	2.8×10^{9}		Wang et al. (2017)	Q	80, 239
CFXREDIWINSYMD-UHFFFAOYSA-N	1.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C128OOH	4.7×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_5$	2.6×10^{9}		Wang et al. (2017)	Q	80, 239
UJLXMZVGYRRHNB-UHFFFAOYSA-N	3.3×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C129OH	4.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{18}O_4$	3.8×10^{7}		Wang et al. (2017)	Q	80, 239
LZLVFWPHHNPPPO-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C1312CO	2.9×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{20}O_4$	5.9×10^{7}		Wang et al. (2017)	Q	80, 239
OXGUTNXNCKSGQJ-UHFFFAOYSA-N	6.6×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C1312OH	1.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_4$	1.7×10^{9}		Wang et al. (2017)	Q	80, 239
IOOAKPNHTHIGJB-UHFFFAOYSA-N	2.8×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C1312OOH	3.6×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_5$	6.5×10^{8}		Wang et al. (2017)	Q	80, 239
IMCVJRKOQRMDFG-UHFFFAOYSA-N	3.9×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:BCLKAOH	2.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_4$	4.2×10^{7}		Wang et al. (2017)	Q	80, 239
OIHLYIMTKSRRQE-UHFFFAOYSA-N	5.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:BCLKBOH	1.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_4$	3.0×10^{7}		Wang et al. (2017)	Q	80, 239
LFMWXXSOGPOZAN-UHFFFAOYSA-N	7.4×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:BCLKCOH	2.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_4$	3.6×10^{7}		Wang et al. (2017)	Q	80, 239
WUCWLUFQNHHRAC-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C144OOH	4.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{24}O_5$	6.2×10^{8}		Wang et al. (2017)	Q	80, 239
GLUIAMUUMIPXJY-UHFFFAOYSA-N	5.8×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C146OH	2.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_4$	3.2×10^{7}		Wang et al. (2017)	Q	80, 239
MRXVSIMJFRVVPA-UHFFFAOYSA-N	2.0×10^{5}		Wang et al. (2017)	Q	80, 240

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Table A3.6: Ketones (RCOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:BCALAOH	6.3×10^3		Wang et al. (2017)	Q	80, 238
$C_{15}H_{24}O_3$	3.3×10^4		Wang et al. (2017)	Q	80, 239
SOIICZPFVOBBSJ-UHFFFAOYSA-N	6.3×10^3		Wang et al. (2017)	Q	80, 240
MCM:BCALBOH	5.3×10^3		Wang et al. (2017)	Q	80, 238
$C_{15}H_{24}O_3$	2.1×10^4		Wang et al. (2017)	Q	80, 239
WYNIZHBHTSXQQC-UHFFFAOYSA-N	5.9×10^4		Wang et al. (2017)	Q	80, 240
MCM:BCALCOH	6.3×10^3		Wang et al. (2017)	Q	80, 238
$C_{15}H_{24}O_3$	3.4×10^4		Wang et al. (2017)	Q	80, 239
NQPQIVDLCLYNNZ-UHFFFAOYSA-N	1.1×10^4		Wang et al. (2017)	Q	80, 240
MCM:BCALOH	4.4×10^7		Wang et al. (2017)	Q	80, 238
$C_{15}H_{26}O_4$	4.2×10^8		Wang et al. (2017)	Q	80, 239
MPEWUZJEETZOEB-UHFFFAOYSA-N	5.4×10^5		Wang et al. (2017)	Q	80, 240
MCM:BCALOOH	3.2×10^9		Wang et al. (2017)	Q	80, 238
$C_{15}H_{26}O_5$	8.7×10^8		Wang et al. (2017)	Q	80, 239
HSCKVTFOUFPNNB-UHFFFAOYSA-N	3.6×10^7		Wang et al. (2017)	Q	80, 240

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A3.7 Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH)

Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methanoic acid	8.8×10^{1}	6100	Burkholder et al. (2019)	L	
HCOOH	8.8×10^{1}	6100	Burkholder et al. (2015)	L	
(formic acid)	8.8×10^{1}	6100	Sander et al. (2011)	L	
[64-18-6]	8.8×10^{1}	6100	Sander et al. (2006)	L	
BDAGIHXWWSANSR-UHFFFAOYSA-N	6.7×10^{1}	5900	Staudinger and Roberts (2001)	L	
	8.8×10^{1}	6100	Johnson et al. (1996)	M	
	5.4×10^{1}		Khan et al. (1995)	M	
	5.4×10^{1}	5600	Khan and Brimblecombe (1992)	M	
	1.3×10^{2}		Servant et al. (1991)	M	487
	1.5×10^{1}		Hwang et al. (1992)	V	
		5700	Abraham (1984)	V	
		5600	Abraham (1984)	R	488
		5700	Winiwarter et al. (1988)	T	489
	3.7×10^{1}	5700	Jacob (1986)	T	490
	5.5×10^{1}		Keene and Galloway (1986)	T	
	7.5×10^{1}		Johnson (1990)	X	63
	5.9×10^{1}		Gaffney and Senum (1984)	X	389, 491
	5.1×10^{1}		Johnson et al. (1996)	C	
	5.1×10^{1}		Keene et al. (1995)	C	
	5.3×10^{1}		Keene et al. (1995)	C	
	3.7×10^{1}	5700	Lelieveld and Crutzen (1991)	C	
	3.5×10^{1}	5700	Pandis and Seinfeld (1989)	C	
	2.1×10^{2}		Keshavarz et al. (2022)	Q	
	4.0×10^{1}		Duchowicz et al. (2020)	Q	184
	2.2×10^{1}		Wang et al. (2017)	Q	80, 238
	2.5×10^{2}		Wang et al. (2017)	Q	80, 239
	1.0×10^{2}		Wang et al. (2017)	Q	80, 240
	2.3×10^{2}		Hilal et al. (2008)	Q	
	1.2×10^{1}		Modarresi et al. (2007)	Q	67
		5800	Kühne et al. (2005)	Q	
	5.8×10^{1}		Yaffe et al. (2003)	Q	248, 249
	8.6×10^{1}		Abraham (2003)	Q	
	7.7		Katritzky et al. (1998)	Q	
	5.9×10^{1}		Duchowicz et al. (2020)	?	185, 21
		6500	Kühne et al. (2005)	?	
	1.3×10^{1}		Yaws (1999)	?	21
	8.9		Yaws and Yang (1992)	?	21
ethanoic acid	4.0×10^{1}	6200	Burkholder et al. (2019)	L	
CH_3COOH	4.0×10^{1}	6200	Burkholder et al. (2015)	L	
(acetic acid)	4.0×10^{1}	6200	Sander et al. (2011)	L	
[64-19-7]	4.0×10^{1}	6200	Sander et al. (2006)	L	
QTBSBXVTEAMEQO-UHFFFAOYSA-N	4.6×10^{1}	6300	Staudinger and Roberts (2001)	L	
	1.4×10^{1}		von Hartungen et al. (2004)	M	
	4.0×10^{1}	6300	Johnson et al. (1996)	M	

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.4×10^{1}		Khan et al. (1995)	M	
	5.4×10^{1}	8300	Khan and Brimblecombe (1992)	M	
	9.2×10^{1}		Servant et al. (1991)	M	487
			Fredenhagen and Liebster (1932)	M	328
	9.1		Hwang et al. (1992)	V	
		6300	Abraham (1984)	V	
		6200	Abraham (1984)	R	488
	4.8×10^{1}	6400	Plyasunov et al. (2001)	T	
	8.7×10^{1}	6400	Jacob et al. (1989)	T	
		6400	Winiwarter et al. (1988)	T	489
	8.7×10^{1}		Keene and Galloway (1986)	T	
	9.7	4900	Goldstein (1982)	X	298
	9.9×10^{1}		Gaffney and Senum (1984)	X	389, 491
	5.1×10^{1}		Johnson et al. (1996)	C	
	5.2×10^{1}		Keene et al. (1995)	C	
	8.5×10^{1}		Keene et al. (1995)	C	
	1.0×10^{2}		Keshavarz et al. (2022)	Q	
	3.1×10^{1}		Duchowicz et al. (2020)	Q	
	1.4×10^{1}		Wang et al. (2017)	Q	80, 238
	2.9×10^{2}		Wang et al. (2017)	Q	80, 239
	6.5×10^{1}		Wang et al. (2017)	Q	80, 240
	3.3×10^{1}		Li et al. (2014)	Q	241
	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	245
	1.3×10^{2}		Hilal et al. (2008)	Q	
	3.2×10^{1}		Modarresi et al. (2007)	Q	67
		6100	Kühne et al. (2005)	Q	
	9.9×10^{1}		Yaffe et al. (2003)	Q	248, 249
	3.1×10^{1}		Abraham (2003)	Q	
	3.1×10^{1}		English and Carroll (2001)	Q	230, 231
	1.1×10^{1}		Katritzky et al. (1998)	Q	
	2.3×10^{1}		Russell et al. (1992)	Q	279
	3.1×10^{1}		Suzuki et al. (1992)	Q	232
	3.9×10^{1}		Nirmalakhandan and Speece (1988)	Q	
	9.9×10^{1}		Duchowicz et al. (2020)	?	185, 21
	1.1×10^{1}		Maniere et al. (2011)	?	241, 165
		6200	Kühne et al. (2005)	?	
	8.4		Yaws (1999)	?	21
	8.2		Yaws and Yang (1992)	?	21
	3.3×10^{1}		Abraham et al. (1990)	?	
	3.3×10^{1}		Hine and Mookerjee (1975)	?	

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
acetic anhydride	1.7		Duchowicz et al. (2020)	V	186
$C_4H_6O_3$	3.6		Yaws (2003)	X	237
[108-24-7]	6.3×10^{-1}		Duchowicz et al. (2020)	Q	
WFDIJRYMOXRFFG-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	80, 238
	5.3×10^{1}		Wang et al. (2017)	Q	80, 239
	1.7		Wang et al. (2017)	Q	80, 240
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.9		Gharagheizi et al. (2010)	Q	246
	7.1×10^{-1}		Modarresi et al. (2007)	Q	67
	2.3		Yaws (1999)	?	21
propanoic acid	7.1×10^{1}		Kim and Kim (2016)	M	
C_2H_5COOH	1.5×10^{1}		von Hartungen et al. (2004)	M	
(propionic acid)	5.6×10^{1}		Khan et al. (1995)	M	
[79-09-4]	5.5×10^{1}		Khan and Brimblecombe (1992)	M	
XBDQKXXYIPTUBI-UHFFFAOYSA-N	6.1×10^{1}		Servant et al. (1991)	M	487
	2.2×10^{1}		Butler and Ramchandani (1935)	M	
		6800	Abraham (1984)	V	
		6800	Abraham (1984)	R	488
	3.7×10^{1}	6800	Plyasunov et al. (2001)	T	
	2.6×10^{1}		Keshavarz et al. (2022)	Q	
	4.2×10^{1}		Duchowicz et al. (2020)	Q	299
	1.2×10^{1}		Wang et al. (2017)	Q	80, 238
	2.6×10^{2}		Wang et al. (2017)	Q	80, 239
	1.6×10^{1}		Wang et al. (2017)	Q	80, 240
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	245
	7.0×10^{1}		Hilal et al. (2008)	Q	
	2.8×10^{1}		Modarresi et al. (2007)	Q	67
	2.4×10^{1}		Yaffe et al. (2003)	Q	248, 249
	2.2×10^{1}		Abraham (2003)	Q	
	2.3×10^{1}		English and Carroll (2001)	Q	230, 231
	2.4		Katritzky et al. (1998)	Q	
	5.6		Russell et al. (1992)	Q	358
	2.4×10^{1}		Suzuki et al. (1992)	Q	232
	3.4×10^{1}		Nirmalakhandan and Speece (1988)	Q	
	2.2×10^{1}		Duchowicz et al. (2020)	?	185, 21
	1.1×10^{1}		Yaws (1999)	?	21
	2.2×10^{1}		Abraham et al. (1990)	?	
	2.2×10^{1}		Hine and Mookerjee (1975)	?	

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methoxyacetic acid	1.5×10^{3}		Duchowicz et al. (2020)	V	186
$C_3H_6O_3$	3.0×10^{2}		Duchowicz et al. (2020)	Q	
[625-45-6]	3.0×10^{2}		Wang et al. (2017)	Q	80, 238
RMIODHQZRUFFFF-UHFFFAOYSA-N	6.6×10^{2}		Wang et al. (2017)	Q	80, 239
	1.0×10^{3}		Wang et al. (2017)	Q	80, 240
butanoic acid	4.3×10^{1}		Kim and Kim (2016)	M	
C_3H_7COOH	9.7		von Hartungen et al. (2004)	M	
(butyric acid)	4.7×10^{1}		Khan et al. (1995)	M	
[107-92-6]	4.5×10^{1}		Khan and Brimblecombe (1992)	M	
FERIUCNNQQJTOY-UHFFFAOYSA-N	1.8×10^{1}		Butler and Ramchandani (1935)	M	
	9.4		Hwang et al. (1992)	V	
		7100	Abraham (1984)	V	
		7300	Abraham (1984)	R	488
	2.5×10^{1}		Keshavarz et al. (2022)	Q	
	5.0×10^{1}		Duchowicz et al. (2020)	Q	
	9.1		Wang et al. (2017)	Q	80, 238
	1.3×10^{2}		Wang et al. (2017)	Q	80, 239
	1.4×10^{1}		Wang et al. (2017)	Q	80, 240
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	271, 243
	6.2×10^{1}		Raventos-Duran et al. (2010)	Q	244
	9.9		Raventos-Duran et al. (2010)	Q	245
	4.4×10^{1}		Hilal et al. (2008)	Q	
	2.5×10^{1}		Modarresi et al. (2007)	Q	67
	1.7×10^{1}		Abraham (2003)	Q	
	1.8×10^{1}		English and Carroll (2001)	Q	230, 274
	2.8		Russell et al. (1992)	Q	279
	1.8×10^{1}		Suzuki et al. (1992)	Q	232
	2.7×10^{1}		Nirmalakhandan and Speece (1988)	Q	
	1.8×10^{1}		Duchowicz et al. (2020)	?	185, 21
	1.8×10^{1}		Abraham et al. (1990)	?	
	1.8×10^{1}		Hine and Mookerjee (1975)	?	
2-methylpropanoic acid	4.6×10^{1}		Kim and Kim (2016)	M	
$(CH_3)_2CHCOOH$	9.6		von Hartungen et al. (2004)	M	
(isobutyric acid)	1.1×10^{1}		Khan et al. (1995)	M	
[79-31-2]	1.1×10^{1}		Khan and Brimblecombe (1992)	M	
KQNPFQTWMSNSAP-UHFFFAOYSA-N	5.6×10^{1}		Servant et al. (1991)	M	487
	1.4		Mackay et al. (2006c)	V	
	2.5×10^{1}		Keshavarz et al. (2022)	Q	
	1.9×10^{1}		Duchowicz et al. (2020)	Q	
	1.1×10^{1}		Wang et al. (2017)	Q	80, 238
	6.3×10^{1}		Wang et al. (2017)	Q	80, 239
	1.7×10^{1}		Wang et al. (2017)	Q	80, 240
	2.0×10^{1}		Gharagheizi et al. (2012)	Q	
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	244
	9.9		Raventos-Duran et al. (2010)	Q	245

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.5×10^1		Hilal et al. (2008)	Q	
	4.7×10^1		Modarresi et al. (2007)	Q	67
	1.1×10^1		Duchowicz et al. (2020)	?	185, 21
	1.1×10^1		Yaws (1999)	?	21, 12
pentanoic acid	2.3×10^1	6900	Staudinger and Roberts (2001)	L	
C_4H_9COOH	2.4×10^1		Kim and Kim (2016)	M	
(valeric acid)	1.2×10^1		von Hartungen et al. (2004)	M	
[109-52-4]	2.3×10^1	6600	Khan et al. (1995)	M	
NQPDZGIKBAWPEJ-UHFFFAOYSA-N	2.1×10^1	6900	Khan and Brimblecombe (1992)	M	
	1.2×10^1		Mackay et al. (2006c)	V	
	1.2×10^1		Mackay et al. (1995)	V	
	1.6×10^1		Brimblecombe et al. (1992)	V	
		7500	Abraham (1984)	V	
	1.3×10^1		Amoore and Buttery (1978)	V	
		7700	Abraham (1984)	R	488
	7.7		Yaws (2003)	X	237
	1.2×10^1		Keshavarz et al. (2022)	Q	
	5.5×10^1		Duchowicz et al. (2020)	Q	184
	8.5		Wang et al. (2017)	Q	80, 238
	6.6×10^1		Wang et al. (2017)	Q	80, 239
	1.4×10^1		Wang et al. (2017)	Q	80, 240
	9.9		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^1		Raventos-Duran et al. (2010)	Q	244
	7.8		Raventos-Duran et al. (2010)	Q	245
	1.6×10^1		Ghargheizi et al. (2010)	Q	246
	3.3×10^1		Hilal et al. (2008)	Q	
	1.8×10^1		Modarresi et al. (2007)	Q	67
		7200	Kühne et al. (2005)	Q	
	1.4×10^1		Yaffe et al. (2003)	Q	248, 272
	1.1×10^1		Abraham (2003)	Q	
	1.4×10^1		English and Carroll (2001)	Q	230, 231
	2.9		Katritzky et al. (1998)	Q	
	2.2×10^1		Nirmalakhandan et al. (1997)	Q	
	2.1×10^1		Duchowicz et al. (2020)	?	185, 21
		6900	Kühne et al. (2005)	?	
	7.4		Yaws (1999)	?	21
	1.3×10^1		Abraham et al. (1990)	?	
2-methylbutanoic acid	6.7		Duchowicz et al. (2020)	V	186
$C_5H_{10}O_2$	4.9		Yaws (2003)	X	237
[116-53-0]	2.1×10^1		Duchowicz et al. (2020)	Q	
WLAMNBDJUVNPJU-UHFFFAOYSA-N	8.5		Wang et al. (2017)	Q	80, 238
	3.3×10^1		Wang et al. (2017)	Q	80, 239
	1.6×10^1		Wang et al. (2017)	Q	80, 240
	8.3		Ghargheizi et al. (2010)	Q	246
	1.6×10^1		Hilal et al. (2008)	Q	
	4.4×10^1		Modarresi et al. (2007)	Q	67

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methylbutanoic acid	2.7×10^{1}		Kim and Kim (2016)	M	
$(CH_3)_2CHCH_2COOH$	1.1×10^{1}		von Hartungen et al. (2004)	M	
(isovaleric acid)	1.2×10^{1}		Khan et al. (1995)	M	
[503-74-2]	1.2×10^{1}		Khan and Brimblecombe (1992)	M	
GWYFCOCPABKNJV-UHFFFAOYSA-N	1.2×10^{1}		Amoore and Buttery (1978)	M	
	1.6		Mackay et al. (2006c)	V	
	1.6		Mackay et al. (1995)	V	
	7.3		Amoore and Buttery (1978)	V	
	1.1×10^{1}		Yaws (2003)	X	237, 12
	1.2×10^{1}		Keshavarz et al. (2022)	Q	
	2.1×10^{1}		Duchowicz et al. (2020)	Q	299
	8.5		Wang et al. (2017)	Q	80, 238
	6.8×10^{1}		Wang et al. (2017)	Q	80, 239
	1.7×10^{1}		Wang et al. (2017)	Q	80, 240
	2.2×10^{1}		Gharagheizi et al. (2012)	Q	
	9.9		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	244
	7.8		Raventos-Duran et al. (2010)	Q	245
	8.4		Gharagheizi et al. (2010)	Q	246
	2.8×10^{1}		Hilal et al. (2008)	Q	
	2.0×10^{1}		Modarresi et al. (2007)	Q	67
	4.8×10^{1}		Yao et al. (2002)	Q	229
	1.4×10^{1}		English and Carroll (2001)	Q	230, 231
	1.2×10^{1}		Duchowicz et al. (2020)	?	185, 21
	7.0		Yaws (1999)	?	21, 12
	1.2×10^{1}		Abraham et al. (1990)	?	
2,2-dimethylpropanoic acid	3.5		Khan et al. (1995)	M	
$(CH_3)_3CCOOH$	3.5		Khan and Brimblecombe (1992)	M	
(pivalic acid)	8.4		Yaws (2003)	X	237
[75-98-9]	1.2×10^{1}		Keshavarz et al. (2022)	Q	
IUGYQRQAERSCNH-UHFFFAOYSA-N	9.4		Duchowicz et al. (2020)	Q	
	9.9		Raventos-Duran et al. (2010)	Q	242, 243
	9.9		Raventos-Duran et al. (2010)	Q	244
	7.8		Raventos-Duran et al. (2010)	Q	245
	6.9		Gharagheizi et al. (2010)	Q	246
	1.2×10^{1}		Hilal et al. (2008)	Q	
	1.6×10^{1}		Modarresi et al. (2007)	Q	67
	3.8		Yaffe et al. (2003)	Q	248, 249
	9.0×10^{-1}		Katritzky et al. (1998)	Q	
	3.6		Duchowicz et al. (2020)	?	185, 21

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexanoic acid	1.3×10^1	6100	Staudinger and Roberts (2001)	L	
$C_5H_{11}COOH$	9.9		Kim and Kim (2016)	M	
(caproic acid)	7.5		von Hartungen et al. (2004)	M	
[142-62-1]	1.3×10^1	6300	Khan et al. (1995)	M	
FUZZWVXGSFPDMH-UHFFFAOYSA-N	1.3×10^1	5900	Khan and Brimblecombe (1992)	M	
	1.7×10^1		Mackay et al. (2006c)	V	
	1.7		Mackay et al. (1995)	V	
	1.1×10^1		Brimblecombe et al. (1992)	V	
	2.0×10^1		Hwang et al. (1992)	V	
		8700	Abraham (1984)	V	
		8100	Abraham (1984)	R	488
	2.4×10^1		Yaws (2003)	X	237, 12
	6.1		Keshavarz et al. (2022)	Q	
	5.9×10^1		Duchowicz et al. (2020)	Q	184
	1.7×10^1		Gharagheizi et al. (2012)	Q	
	6.2		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^1		Raventos-Duran et al. (2010)	Q	244
	6.2		Raventos-Duran et al. (2010)	Q	245
	1.4×10^1		Gharagheizi et al. (2010)	Q	246
	2.4×10^1		Hilal et al. (2008)	Q	
	1.7×10^1		Modarresi et al. (2007)	Q	67
		7500	Kühne et al. (2005)	Q	
	1.4×10^1		Yaffe et al. (2003)	Q	248, 249
	8.3		Abraham (2003)	Q	
	3.9×10^1		Yao et al. (2002)	Q	229, 267
	1.1×10^1		English and Carroll (2001)	Q	230, 231
	7.9		Katritzky et al. (1998)	Q	
	1.7×10^1		Nirmalakhandan et al. (1997)	Q	
	1.3×10^1		Duchowicz et al. (2020)	?	185, 21
		7200	Kühne et al. (2005)	?	
	1.5×10^1		Yaws (1999)	?	21, 12
	1.5×10^1		Abraham et al. (1990)	?	
2-methylpentanoic acid	1.1×10^1		Hilal et al. (2008)	Q	
$C_6H_{12}O_2$	3.6×10^1		Modarresi et al. (2007)	Q	67
[97-61-0]					
OVBFMEVBMNZIBR-UHFFFAOYSA-N					
2-ethylbutanoic acid	6.2		Duchowicz et al. (2020)	V	186
$C_6H_{12}O_2$	4.3		Yaws (2003)	X	237
[88-09-5]	2.3×10^1		Duchowicz et al. (2020)	Q	
OXQGTIUCKGYOAA-UHFFFAOYSA-N	8.9		Gharagheizi et al. (2012)	Q	
	6.2		Raventos-Duran et al. (2010)	Q	242, 243
	9.9		Raventos-Duran et al. (2010)	Q	244
	6.2		Raventos-Duran et al. (2010)	Q	245
	7.6		Gharagheizi et al. (2010)	Q	246
	9.0		Hilal et al. (2008)	Q	
	3.2×10^1		Modarresi et al. (2007)	Q	67

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.1		Yaffe et al. (2003)	Q	248, 249
	7.9×10^{-1}		Katritzky et al. (1998)	Q	
heptanoic acid	1.5×10^{1}		Kim and Kim (2016)	M	
$C_7H_{14}O_2$	1.5×10^{1}		Duchowicz et al. (2020)	V	186
[111-14-8]	9.6		Brimblecombe et al. (1992)	V	
MNWFXJYAOYHMED-UHFFFAOYSA-N		8500	Abraham (1984)	V	
		8500	Abraham (1984)	R	488
	6.1×10^{1}		Duchowicz et al. (2020)	Q	
	5.5		Wang et al. (2017)	Q	80, 238
	2.9×10^{1}		Wang et al. (2017)	Q	80, 239
	2.0×10^{1}		Wang et al. (2017)	Q	80, 240
	1.0×10^{1}		Gharagheizi et al. (2012)	Q	
	1.7×10^{1}		Hilal et al. (2008)	Q	
	1.6×10^{1}		Modarresi et al. (2007)	Q	67
		7800	Kühne et al. (2005)	Q	
	3.0×10^{1}		Yaffe et al. (2003)	Q	248, 249
	6.4		Abraham (2003)	Q	
	2.9×10^{1}		Yao et al. (2002)	Q	229
	4.3		Katritzky et al. (1998)	Q	
		7900	Kühne et al. (2005)	?	
	2.5×10^{1}		Yaws (1999)	?	21, 12
	1.3×10^{1}		Abraham et al. (1990)	?	
4,4-dimethylpentanoic acid	4.3		Zhang et al. (2010)	Q	287, 288
$C_7H_{14}O_2$	1.4×10^{1}		Zhang et al. (2010)	Q	287, 289
[95823-36-2]	1.6×10^{3}		Zhang et al. (2010)	Q	287, 290
HMMSZUQCCUWXRA-UHFFFAOYSA-N	1.6		Zhang et al. (2010)	Q	287, 291
2-ethyl-2-methylbutanoic acid	4.3		Zhang et al. (2010)	Q	287, 288
$C_7H_{14}O_2$	5.4		Zhang et al. (2010)	Q	287, 289
[19889-37-3]	2.3×10^{2}		Zhang et al. (2010)	Q	287, 290
LHJPKLWGGMAUAN-UHFFFAOYSA-N	1.6		Zhang et al. (2010)	Q	287, 291
octanoic acid	1.1×10^{1}		Duchowicz et al. (2020)	V	186
$C_8H_{16}O_2$	1.5×10^{-1}		Mackay et al. (2006c)	V	
(caprylic acid)	1.5×10^{-1}		Mackay et al. (1995)	V	
[124-07-2]	7.6		Brimblecombe et al. (1992)	V	
WWZKQHOCKIZLMA-UHFFFAOYSA-N		9600	Abraham (1984)	V	
		8900	Abraham (1984)	R	488
	1.9×10^{1}		Yaws (2003)	X	237, 12
	6.4×10^{1}		Duchowicz et al. (2020)	Q	
	6.5		Gharagheizi et al. (2012)	Q	
	1.2×10^{1}		Gharagheizi et al. (2010)	Q	246
	1.3×10^{1}		Hilal et al. (2008)	Q	
	1.2×10^{1}		Modarresi et al. (2007)	Q	67
		8200	Kühne et al. (2005)	Q	
	1.2×10^{1}		Yaffe et al. (2003)	Q	248, 249
	5.7		Abraham (2003)	Q	

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.7×10^{1}		Yao et al. (2002)	Q	229
	5.8		Katritzky et al. (1998)	Q	
		8400	Kühne et al. (2005)	?	
	1.0×10^{1}		Yaws (1999)	?	21, 12
	1.1×10^{1}		Abraham et al. (1990)	?	
2-ethylhexanoic acid	3.5		HSDB (2015)	V	
$C_8H_{16}O_2$	3.4		Hilal et al. (2008)	Q	
[149-57-5]	2.4×10^{1}		Modarresi et al. (2007)	Q	67
OBETXYAYXDNJHR-UHFFFAOYSA-N					
endothal	2.6×10^{10}		Duchowicz et al. (2020)	V	186
$C_8H_{10}O_5$	1.4×10^{6}		Duchowicz et al. (2020)	Q	
[145-73-3]					
GXEKYRXVRROBEV-UHFFFAOYSA-N					
nonanoic acid	6.1		Duchowicz et al. (2020)	V	186
$C_9H_{18}O_2$	3.8		Brimblecombe et al. (1992)	V	
(pelargic acid)	2.0×10^{1}		Yaws (2003)	X	237, 12
[112-05-0]	6.9		Hilal et al. (2008)	C	
FBUKVWPVBMHYJY-UHFFFAOYSA-N	6.5×10^{1}		Duchowicz et al. (2020)	Q	
	4.0		Gharagheizi et al. (2012)	Q	
	1.3×10^{1}		Gharagheizi et al. (2010)	Q	246
	9.9		Hilal et al. (2008)	Q	
	1.2×10^{1}		Modarresi et al. (2007)	Q	67
	1.2×10^{1}		Yaffe et al. (2003)	Q	248, 272
	4.2		Abraham (2003)	Q	
	2.3×10^{1}		Yao et al. (2002)	Q	229
	5.6		Katritzky et al. (1998)	Q	
	3.0		Maniere et al. (2011)	?	12, 165
	1.1×10^{1}		Yaws (1999)	?	21, 12
decanoic acid	7.4		Duchowicz et al. (2020)	V	186
$C_{10}H_{20}O_2$	6.5		Hilal et al. (2008)	C	
[334-48-5]	6.7×10^{1}		Duchowicz et al. (2020)	Q	
GHVNFZFCNZKVNT-UHFFFAOYSA-N	7.7		Hilal et al. (2008)	Q	
	1.0×10^{1}		Modarresi et al. (2007)	Q	67
	3.0		Abraham (2003)	Q	
	1.9×10^{2}		Yaws (1999)	?	21, 12
3,3,5,5-tetramethylhexanoic acid	1.9		Zhang et al. (2010)	Q	287, 288
$C_{10}H_{20}O_2$	3.5		Zhang et al. (2010)	Q	287, 289
[1135681-77-4]	1.0×10^{3}		Zhang et al. (2010)	Q	287, 290
WRPPDRMFGQJMAR-UHFFFAOYSA-N	6.1×10^{-1}		Zhang et al. (2010)	Q	287, 291
pinonic acid	6.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_3$	3.0×10^{5}		Wang et al. (2017)	Q	80, 239
[473-72-3]	6.2×10^{5}		Wang et al. (2017)	Q	80, 240
SIZDUQQDBXJXLQ-UHFFFAOYSA-N	5.9×10^{4}		Isaacman-VanWertz et al. (2016)	Q	441

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
undecanoic acid	7.7		Yaws (2003)	X	237
$C_{11}H_{22}O_2$	1.8×10^{1}		Gharagheizi et al. (2010)	Q	246
[112-37-8]	5.8		Hilal et al. (2008)	Q	
ZDPHROOEEOARMN-UHFFFAOYSA-N	2.2		Abraham (2003)	Q	
dodecanoic acid	4.5		Hilal et al. (2008)	Q	
$C_{12}H_{24}O_2$	1.7		Abraham (2003)	Q	
[143-07-7]	1.7×10^{1}		Yao et al. (2002)	Q	229
POULHZVOKOAJMA-UHFFFAOYSA-N	8.4×10^{1}		Yaws (1999)	?	21, 12
tridecanoic acid	8.0		Yaws (2003)	X	237
$C_{13}H_{26}O_2$	3.8×10^{1}		Gharagheizi et al. (2010)	Q	246
[638-53-9]	1.2		Abraham (2003)	Q	
SZHOJFHSIKHZHA-UHFFFAOYSA-N					
tetradecanoic acid	2.0×10^{1}		Duchowicz et al. (2020)	V	186
$C_{14}H_{28}O_2$	7.1×10^{1}		Duchowicz et al. (2020)	Q	
[544-63-8]	9.4×10^{-1}		Abraham (2003)	Q	
TUNFSRHWOTWDNC-UHFFFAOYSA-N					
pentadecanoic acid	7.1×10^{-1}		Abraham (2003)	Q	
$C_{15}H_{30}O_2$					
[1002-84-2]					
WQEPLUUGTLDZJY-UHFFFAOYSA-N					
hexadecanoic acid	4.9×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{16}H_{32}O_2$	7.2×10^{1}		Duchowicz et al. (2020)	Q	
(palmitic acid)	3.0		Gharagheizi et al. (2012)	Q	
[57-10-3]	5.2×10^{-1}		Abraham (2003)	Q	
IPCSVZSSVZVIGE-UHFFFAOYSA-N					
heptadecanoic acid	3.8×10^{-1}		Abraham (2003)	Q	
$C_{17}H_{34}O_2$					
(margaric acid)					
[506-12-7]					
KEMQGTRYUADPNZ-UHFFFAOYSA-N					
octadecanoic acid	2.1×10^{1}		Duchowicz et al. (2020)	V	186
$C_{18}H_{36}O_2$	2.5×10^{5}		Mackay et al. (1995)	V	
(stearic acid)	7.3×10^{1}		Duchowicz et al. (2020)	Q	
[57-11-4]	8.4×10^{-1}		Hilal et al. (2008)	Q	
QIQXTHQIDYTFRH-UHFFFAOYSA-N	3.5		Modarresi et al. (2007)	Q	67
	3.0×10^{-1}		Abraham (2003)	Q	
nonadecanoic acid	2.3×10^{-1}		Abraham (2003)	Q	
$C_{19}H_{38}O_2$					
[646-30-0]					
ISYWECDDZWTKFF-UHFFFAOYSA-N					

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
eicosanoic acid $C_{20}H_{40}O_2$ (arachidic acid) [506-30-9] VKOBVWXKNCXXDE-UHFFFAOYSA-N	1.7×10^{-1}		Abraham (2003)	Q	
heneicosanoic acid $C_{21}H_{42}O_2$ [2363-71-5] CKDDRHZIAZRDBW-UHFFFAOYSA-N	1.3×10^{-1}		Abraham (2003)	Q	
docosanoic acid $C_{22}H_{44}O_2$ (behenic acid) [112-85-6] UKMSUNONTOPOIO-UHFFFAOYSA-N	9.5×10^{-2}		Abraham (2003)	Q	
tricosanoic acid $C_{23}H_{46}O_2$ [2433-96-7] XEZVDURJDFGERA-UHFFFAOYSA-N	7.2×10^{-2}		Abraham (2003)	Q	
tetracosanoic acid $C_{24}H_{48}O_2$ (lignoceric acid) [557-59-5] QZZGJDVWLFXDLK-UHFFFAOYSA-N	5.4×10^{-2}		Abraham (2003)	Q	
propenoic acid $C_3H_4O_2$ (acrylic acid) [79-10-7] NIXOWILDQLNWCW-UHFFFAOYSA-N	2.7×10^{1}		Duchowicz et al. (2020)	V	186
	3.1×10^{1}		Lide and Frederikse (1995)	V	
	1.2×10^{2}		Duchowicz et al. (2020)	Q	
	3.3×10^{1}		Wang et al. (2017)	Q	80, 238
	2.2×10^{1}		Wang et al. (2017)	Q	80, 239
	4.6×10^{1}		Wang et al. (2017)	Q	80, 240
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	245
	2.2×10^{1}		Hilal et al. (2008)	Q	
	9.4×10^{2}		Modarresi et al. (2007)	Q	67
	2.4×10^{1}		Yaws (1999)	?	21
	2.4×10^{1}		Yaws and Yang (1992)	?	21
2-butenoic acid $C_4H_6O_2$ (crotonic acid) [3724-65-0] LDHQCZJRKDOVOX-UHFFFAOYSA-N	2.3×10^{1}		Duchowicz et al. (2020)	V	186
	5.1×10^{1}		Duchowicz et al. (2020)	Q	
	4.2×10^{1}		Wang et al. (2017)	Q	80, 238
	2.2×10^{1}		Wang et al. (2017)	Q	80, 239
	5.0×10^{1}		Wang et al. (2017)	Q	80, 240
	2.3×10^{1}		Hilal et al. (2008)	Q	
	1.1×10^{2}		Modarresi et al. (2007)	Q	67

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(E)-2-butenoic acid $C_4H_6O_2$ (*trans*-crotonic acid) [107-93-7] LDHQCZJRKDOVOX-NSCUHMNNSA-N	4.1×10^{1}		HSDB (2015)	V	
(Z)-2-butenoic acid	1.5×10^{2}		Duchowicz et al. (2020)	V	186
$C_4H_6O_2$	5.1×10^{1}		Duchowicz et al. (2020)	Q	
(isocrotonic acid)	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
[503-64-0]	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	244
LDHQCZJRKDOVOX-IHWYPQMZSA-N	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	245
	2.3×10^{1}		Hilal et al. (2008)	Q	
	1.1×10^{2}		Modarresi et al. (2007)	Q	67
2-methyl-2-propenoic acid	2.5×10^{1}		Khan et al. (1992)	M	
$C_4H_6O_2$	1.0		Mackay et al. (2006c)	V	
(methacrylic acid)	9.2		Keshavarz et al. (2022)	Q	
[79-41-4]	5.0×10^{1}		Duchowicz et al. (2020)	Q	299
CERQOIWHTDAKMF-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	80, 238
	1.7×10^{1}		Wang et al. (2017)	Q	80, 239
	8.3		Wang et al. (2017)	Q	80, 240
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	245
	1.9×10^{1}		Hilal et al. (2008)	Q	
	1.4×10^{2}		Modarresi et al. (2007)	Q	67
	2.5×10^{1}		Duchowicz et al. (2020)	?	185, 21
methacrylic acid epoxide $C_4H_6O_3$ CSEUSVYSDPXJAP-UHFFFAOYSA-N	1.2×10^{3}		Pye et al. (2013)	Q	492
benzenecarboxylic acid	2.9×10^{2}		Li et al. (2007)	M	
C_6H_5COOH	2.6×10^{2}		Duchowicz et al. (2020)	V	186
(benzoic acid)	2.5×10^{2}		Mackay et al. (2006c)	V	
[65-85-0]	1.4×10^{2}		Lide and Frederikse (1995)	V	
WPYMKLBDIGXBTP-UHFFFAOYSA-N	2.1		Mackay et al. (1995)	V	
	1.7×10^{2}		Meylan and Howard (1991)	V	
	1.4×10^{2}	6500	Goldstein (1982)	X	298
	1.4×10^{2}		Howard (1989)	X	412
	3.1×10^{2}		Duchowicz et al. (2020)	Q	
	4.6×10^{2}		Wang et al. (2017)	Q	80, 238
	5.1×10^{2}		Wang et al. (2017)	Q	80, 239
	3.5×10^{2}		Wang et al. (2017)	Q	80, 240
	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	2.4×10^{2}		Hilal et al. (2008)	Q	
		6700	Kühne et al. (2005)	Q	

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.1×10^{1}		Meylan and Howard (1991)	Q	
	1.5×10^{3}		Maniere et al. (2011)	?	12, 165
		6200	Kühne et al. (2005)	?	
	2.4×10^{2}		Yaws and Yang (1992)	?	21
sorbic acid $C_6H_8O_2$ [110-44-1] WSWCOQWTEOXDQX-MQQKCMAXSA-N	3.3×10^{1}		Abraham et al. (2019)	Q	
	2.0×10^{2}		HSDB (2015)	Q	99
D(-)-isoascorbic acid $C_6H_8O_6$ (erythorbic acid) [89-65-6] CIWBSHSKHKDKBQ-DUZGATOHSA-N	2.4×10^{2}		HSDB (2015)	Q	99
shikimic acid $C_7H_{10}O_5$ [138-59-0] JXOHGGNKMLTUBP-UHFFFAOYSA-N	3.7×10^{8}		HSDB (2015)	Q	99
4-hydroxybenzoic acid $C_7H_6O_3$ [99-96-7] FJKROLUGYXJWQN-UHFFFAOYSA-N	1.4×10^{6}		Duchowicz et al. (2020)	V	186
	1.4×10^{6}		HSDB (2015)	V	
	2.7×10^{6}		Duchowicz et al. (2020)	Q	
3,4,5-trihydroxybenzoic acid $C_7H_6O_5$ (gallic acid) [149-91-7] LNTHITQWFMADLM-UHFFFAOYSA-N	1.2×10^{14}		HSDB (2015)	Q	99
2-methylbenzoic acid $C_8H_8O_2$ (*o*-toluic acid) [118-90-1] ZWLPBLYKEWSWPD-UHFFFAOYSA-N	9.7		Abraham et al. (2019)	Q	
	2.7×10^{2}		Wang et al. (2017)	Q	80, 238
	8.0×10^{1}		Wang et al. (2017)	Q	80, 239
	9.3×10^{1}		Wang et al. (2017)	Q	80, 240
	8.2×10^{1}		Zhang et al. (2010)	Q	287, 288
	3.2×10^{1}		Zhang et al. (2010)	Q	287, 289
	9.9×10^{1}		Zhang et al. (2010)	Q	287, 290
	1.1×10^{2}		Zhang et al. (2010)	Q	287, 291
3-methylbenzoic acid $C_8H_8O_2$ (*m*-toluic acid) [99-04-7] GPSDUZXPYCFOSQ-UHFFFAOYSA-N	6.6		Mackay et al. (2006c)	V	
	1.4×10^{-1}		Mackay et al. (1995)	V	
	3.9×10^{1}		Abraham et al. (2019)	Q	
	2.7×10^{2}		Wang et al. (2017)	Q	80, 238
	3.7×10^{2}		Wang et al. (2017)	Q	80, 239
	3.6×10^{2}		Wang et al. (2017)	Q	80, 240
	8.2×10^{1}		Zhang et al. (2010)	Q	287, 288
	1.2×10^{2}		Zhang et al. (2010)	Q	287, 289
	5.1×10^{2}		Zhang et al. (2010)	Q	287, 290
	1.1×10^{2}		Zhang et al. (2010)	Q	287, 291

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methylbenzoic acid	2.7×10^2		Wang et al. (2017)	Q	80, 238
$C_8H_8O_2$	4.2×10^2		Wang et al. (2017)	Q	80, 239
(p-toluic acid)	4.7×10^2		Wang et al. (2017)	Q	80, 240
[99-94-5]	8.2×10^1		Zhang et al. (2010)	Q	287, 288
LPNBBFKOUUSUDB-UHFFFAOYSA-N	1.4×10^2		Zhang et al. (2010)	Q	287, 289
	8.8×10^2		Zhang et al. (2010)	Q	287, 290
	1.1×10^2		Zhang et al. (2010)	Q	287, 291
		7000	Kühne et al. (2005)	Q	
		7500	Kühne et al. (2005)	?	
2-hydroxy-benzoic acid	1.3×10^3		Duchowicz et al. (2020)	V	186
$C_7H_6O_3$	8.0×10^2		Mackay et al. (2006c)	V	
(salicylic acid)	6.9×10^2		Mackay et al. (1995)	V	
[69-72-7]	1.8		Mackay et al. (1995)	V	
YGSDEFSMJLZEOE-UHFFFAOYSA-N	9.0×10^1		Yaws (2003)	X	237
	1.5×10^3		Duchowicz et al. (2020)	Q	
	1.6×10^3		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^2		Raventos-Duran et al. (2010)	Q	244
	6.2×10^2		Raventos-Duran et al. (2010)	Q	245
	8.9×10^1		Gharagheizi et al. (2010)	Q	246
benzeneethanoic acid	2.4×10^2		Duchowicz et al. (2020)	V	186
$C_8H_8O_2$	1.5×10^2		Mackay et al. (2006c)	V	
(phenylacetic acid)	1.8×10^2		Mackay et al. (1995)	V	
[103-82-2]	1.4×10^1		Mackay et al. (1995)	V	
WLJVXDMOQOGPHL-UHFFFAOYSA-N	3.4×10^2		Duchowicz et al. (2020)	Q	
	4.1×10^2		Wang et al. (2017)	Q	80, 238
	2.1×10^3		Wang et al. (2017)	Q	80, 239
	3.6×10^3		Wang et al. (2017)	Q	80, 240
	1.2×10^3		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^3		Raventos-Duran et al. (2010)	Q	244
	2.0×10^2		Raventos-Duran et al. (2010)	Q	245
	9.9×10^2		Hilal et al. (2008)	Q	
	3.2×10^2		Modarresi et al. (2007)	Q	67
	2.4×10^2		Yaffe et al. (2003)	Q	248, 249
	5.1×10^1		Katritzky et al. (1998)	Q	
phthalic anhydride	6.1×10^2		Duchowicz et al. (2020)	V	186
$C_8H_4O_3$	1.6×10^3		Lide and Frederikse (1995)	V	
[85-44-9]	1.2×10^1		Yaws (2003)	X	237
LGRFSURHDFAFJT-UHFFFAOYSA-N	4.4×10^1		Duchowicz et al. (2020)	Q	
	1.2×10^1		Gharagheizi et al. (2010)	Q	246
1,2-benzenedicarboxylic acid	4.9×10^5		Duchowicz et al. (2020)	V	186
$C_8H_6O_4$	4.9×10^5		HSDB (2015)	V	
(phthalic acid)	8.2×10^6		Duchowicz et al. (2020)	Q	
[88-99-3]					
XNGIFLGASWRNHJ-UHFFFAOYSA-N					

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
terephthalic acid $C_8H_6O_4$ [100-21-0] KKEYFWRCBNTPAC-UHFFFAOYSA-N	2.5×10^{7} 4.8×10^{9}		HSDB (2015) Gharagheizi et al. (2012)	Q Q	447
isophthalic acid $C_8H_6O_4$ [121-91-5] QQVIHTHCMHWDBS-UHFFFAOYSA-N	4.0×10^{9} 7.3×10^{4} 4.5×10^{6} 7.1×10^{8} 3.7×10^{9}		Yaws (2003) Abraham et al. (2019) HSDB (2015) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q Q Q	237 99 246
dehydroacetic acid $C_8H_8O_4$ [520-45-6] PGRHXDWITVMQBC-UHFFFAOYSA-N	2.9×10^{1}		HSDB (2015)	V	
2-methoxybenzoic acid $C_8H_8O_3$ [579-75-9] ILUJQPXNXACGAN-UHFFFAOYSA-N	2.5×10^{3}		Abraham et al. (2019)	Q	
4-methoxybenzoic acid $C_8H_8O_3$ [100-09-4] ZEYHEAKUIGZSGI-UHFFFAOYSA-N	1.8×10^{3}		Abraham et al. (2019)	Q	
caffeic acid $C_9H_8O_4$ [331-39-5] QAIPRVGONGVQAS-DUXPYHPUSA-N	7.0×10^{10}		HSDB (2015)	Q	99
4-methylphthalic anhydride $C_9H_6O_3$ [19438-61-0] ZOXBWJMCXHTKNU-UHFFFAOYSA-N	1.4 6.4×10^{4} 3.5×10^{1} 3.6×10^{1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
3-phenyl-2-propenoic acid $C_9H_8O_2$ (cinnamic acid) [621-82-9] WBYWAXJHAXSJNI-UHFFFAOYSA-N	5.8×10^{2} 4.1×10^{2} 9.9×10^{2} 1.6×10^{2} 7.8×10^{2}		Duchowicz et al. (2020) Duchowicz et al. (2020) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010)	V Q Q Q Q	186 242, 243 244 245
trans-cinnamic acid $C_9H_8O_2$ [140-10-3] WBYWAXJHAXSJNI-VOTSOKGWSA-N	2.8×10^{11}		Abraham et al. (2019)	Q	
p-coumaric acid $C_9H_8O_3$ [501-98-4] NGSWKAQJJWESNS-ZZXKWVIFSA-N	7.2×10^{5}		Abraham et al. (2019)	Q	

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4-dimethoxybenzoic acid $C_9H_{10}O_4$ (veratric acid) [93-07-2] DAUAQNGYDSHRET-UHFFFAOYSA-N	1.1×10^5		Abraham et al. (2019)	Q	
3,4,5-trimethoxybenzoic acid $C_{10}H_{12}O_5$ (eudesmic acid) [118-41-2] SJSOFNCYXJUNBT-UHFFFAOYSA-N	7.3×10^5		Abraham et al. (2019)	Q	
1-naphthaleneacetic acid	3.3×10^2		Maniere et al. (2011)	?	12, 493, 165
$C_{12}H_{10}O_2$	7.9×10^3		Maniere et al. (2011)	?	12, 494, 165
[86-87-3] PRPINYUDVPFIRX-UHFFFAOYSA-N					
2-naphthoxyacetic acid $C_{12}H_{10}O_3$ [120-23-0] RZCJYMOBWVJQGV-UHFFFAOYSA-N	3.5×10^5		Ebert et al. (2023)	?	318
p-tert-butylbenzoic acid	3.5×10^1		Zhang et al. (2010)	Q	287, 288
$C_{11}H_{14}O_2$	4.5×10^1		Zhang et al. (2010)	Q	287, 289
[98-73-7]	3.6×10^2		Zhang et al. (2010)	Q	287, 290
KDVYCTOWXSLNNI-UHFFFAOYSA-N	4.2×10^1		Zhang et al. (2010)	Q	287, 291
trinexapac	3.9×10^6		Duchowicz et al. (2020)	V	186
$C_{11}H_{12}O_5$	4.3×10^8		Duchowicz et al. (2020)	Q	
[104273-73-6] DFFWZNDCNBOKDI-UHFFFAOYSA-N					
benzoic acid, anhydride	7.0		Zhang et al. (2010)	Q	287, 288
$C_{14}H_{10}O_3$	3.7×10^2		Zhang et al. (2010)	Q	287, 289
[93-97-0]	6.5×10^3		Zhang et al. (2010)	Q	287, 290
CHIHQLCVLOXUJW-UHFFFAOYSA-N	6.4×10^2		Zhang et al. (2010)	Q	287, 291
pyromellitic acid	1.6×10^{13}		Yaws (2003)	X	237, 495
$C_{10}H_6O_8$	3.0×10^{13}		Gharagheizi et al. (2012)	Q	
[89-05-4]	1.6×10^{13}		Gharagheizi et al. (2010)	Q	246
CYIDZMCFTVVTJO-UHFFFAOYSA-N					
pyromellitic dianhydride	1.3×10^3		HSDB (2015)	Q	99
$C_{10}H_2O_6$	1.3×10^3		Zhang et al. (2010)	Q	287, 288
[89-32-7]	1.4×10^{11}		Zhang et al. (2010)	Q	287, 289
ANSXAPJVJOKRDJ-UHFFFAOYSA-N	4.8×10^4		Zhang et al. (2010)	Q	287, 290
	9.7×10^5		Zhang et al. (2010)	Q	287, 291

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
naproxen $C_{14}H_{14}O_3$ [22204-53-1] CMWTZPSULFXXJA-VIFPVBQESA-N	2.5×10^{5}		Abraham et al. (2019)	Q	
(Z,Z)-9,12-octadecadienoic acid $C_{18}H_{32}O_2$ (linoleic acid) [60-33-3] OYHQOLUKZRVURQ-HZJYTTRNSA-N	4.9×10^{1}		HSDB (2015)	V	
rosmarinic acid $C_{18}H_{16}O_8$ [537-15-5] DOUMFZQKYFQNTF-WUTVXBCWSA-N	3.7×10^{21}		HSDB (2015)	Q	447
abietic acid $C_{20}H_{30}O_2$ [514-10-3] RSWGJHLUYNHPMX-ONCXSQPRSA-N	1.5×10^{5} 1.7×10^{5}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237, 12 246
ethanedioic acid HOOCCOOH (oxalic acid) [144-62-7] MUBZPKHOEPUJKR-UHFFFAOYSA-N	6.1×10^{6} 6.1×10^{6} 6.1×10^{6} 7.1×10^{6} 3.1×10^{4} 4.2×10^{5} 6.9×10^{4} 1.6×10^{4} 1.6×10^{3} 3.7×10^{7} 4.9×10^{4} 2.0×10^{4} 3.9×10^{5} 4.2×10^{5} 2.4×10^{3} 2.3×10^{5} 4.1×10^{5} 4.9×10^{6} 6.9×10^{4}	 9800 7300 	Burkholder et al. (2019) Burkholder et al. (2015) Compernolle and Müller (2014a) Clegg et al. (1996) Brimblecombe et al. (1992) Yaws (2003) Gaffney and Senum (1984) Keshavarz et al. (2022) Duchowicz et al. (2020) Gharagheizi et al. (2012) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Gharagheizi et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Meylan and Howard (1991) Saxena and Hildemann (1996) Duchowicz et al. (2020)	L L V V V X X Q Q Q Q Q Q Q Q Q Q E ?	 237, 12 389, 491 242, 243 244 245 246 67 401 185, 21
propanedioic acid $HOOCCH_2COOH$ (malonic acid) [141-82-2] OFOBLEOULBTSOW-UHFFFAOYSA-N	2.4×10^{8} 2.4×10^{8} 3.7×10^{4} 3.8×10^{8} 9.3×10^{7} 2.1×10^{1} 2.5×10^{5} 6.2×10^{6} 2.5×10^{6}	 11000 14000 	Burkholder et al. (2019) Burkholder et al. (2015) Duchowicz et al. (2020) Compernolle and Müller (2014a) Compernolle and Müller (2014a) Duchowicz et al. (2020) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010)	L L V V V Q Q Q Q	 186 242, 243 244 245

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{5}		Modarresi et al. (2007)	Q	67
	3.9×10^{6}		Saxena and Hildemann (1996)	E	401
butanedioic acid	3.1×10^{7}		Burkholder et al. (2019)	L	
$HOOC(CH_2)_2COOH$	3.1×10^{7}		Burkholder et al. (2015)	L	
(succinic acid)	2.8×10^{7}		Duchowicz et al. (2020)	V	186
[110-15-6]	2.7×10^{7}		HSDB (2015)	V	
KDYFGRWQOYBRFD-UHFFFAOYSA-N	4.1×10^{7}	11000	Compernolle and Müller (2014a)	V	
	2.0×10^{7}	12000	Compernolle and Müller (2014a)	V	
	7.2×10^{5}		Yaws (2003)	X	237
	6.5×10^{4}		Duchowicz et al. (2020)	Q	
	1.4×10^{7}		Gharagheizi et al. (2012)	Q	
	4.9×10^{6}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{6}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{6}		Raventos-Duran et al. (2010)	Q	245
	3.2×10^{5}		Gharagheizi et al. (2010)	Q	246
	3.0×10^{6}		Saxena and Hildemann (1996)	E	401
pentanedioic acid	3.8×10^{7}		Burkholder et al. (2019)	L	
$HOOC(CH_2)_3COOH$	3.8×10^{7}		Burkholder et al. (2015)	L	
(glutaric acid)	1.9×10^{7}		Mentel et al. (2004)	M	
[110-94-1]	5.1×10^{7}	12000	Compernolle and Müller (2014a)	V	
JFCQEDHGNNZCLN-UHFFFAOYSA-N	2.4×10^{7}	13000	Compernolle and Müller (2014a)	V	
	1.0×10^{5}		Yaws (2003)	X	237, 496
	5.0×10^{6}		Gharagheizi et al. (2012)	Q	
	4.9×10^{6}		Raventos-Duran et al. (2010)	Q	271, 243
	3.9×10^{7}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{6}		Raventos-Duran et al. (2010)	Q	245
	3.5×10^{5}		Gharagheizi et al. (2010)	Q	246
	2.2×10^{7}		Hilal et al. (2008)	Q	
	2.3×10^{5}		Modarresi et al. (2007)	Q	67
	2.0×10^{6}		Saxena and Hildemann (1996)	E	401
3-hydroxy glutaric acid	6.7×10^{8}		Isaacman-VanWertz et al. (2016)	Q	441
$C_5H_8O_5$					
[638-18-6]					
ZQHYXNSQOIDNTL-UHFFFAOYSA-N					
hexanedioic acid	6.6×10^{7}		Burkholder et al. (2019)	L	
$HOOC(CH_2)_4COOH$	6.6×10^{7}		Burkholder et al. (2015)	L	
(adipic acid)	2.1×10^{6}		Duchowicz et al. (2020)	V	186
[124-04-9]	2.1×10^{6}		HSDB (2015)	V	
WNLRTRBMVRJNCN-UHFFFAOYSA-N	6.6×10^{7}	13000	Compernolle and Müller (2014a)	V	
	1.1×10^{1}		Lide and Frederikse (1995)	V	
	1.8×10^{5}	11000	Goldstein (1982)	X	298
	3.3×10^{6}		Duchowicz et al. (2020)	Q	
	2.2×10^{6}		Gharagheizi et al. (2012)	Q	
	3.9×10^{6}		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^{7}		Raventos-Duran et al. (2010)	Q	244

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.9×10^5		Raventos-Duran et al. (2010)	Q	245
	2.5×10^7		Hilal et al. (2008)	Q	
	2.5×10^5		Modarresi et al. (2007)	Q	67
	2.0×10^6		Saxena and Hildemann (1996)	E	401
tricarballylic acid $C_6H_8O_6$ [99-14-9] KQTIIICEAUMSDG-UHFFFAOYSA-N	1.9×10^9		Isaacman-VanWertz et al. (2016)	Q	441
heptanedioic acid	2.6×10^7		Duchowicz et al. (2020)	V	186
$C_7H_{12}O_4$	8.1×10^7	15000	Compernolle and Müller (2014a)	V	
(pimelic acid)	4.1×10^6		Duchowicz et al. (2020)	Q	
[111-16-0] WLJVNTCWHIRURA-UHFFFAOYSA-N					
3-acetyl pentanedioic acid $C_7H_{10}O_5$ [149474-71-5] TZPGYCKKEMNHRS-UHFFFAOYSA-N	4.5×10^9		Isaacman-VanWertz et al. (2016)	Q	441
octanedioic acid	1.8×10^6		Duchowicz et al. (2020)	V	186
$C_8H_{14}O_4$	7.7×10^7	14000	Compernolle and Müller (2014a)	V	
(suberic acid)	4.8×10^6		Duchowicz et al. (2020)	Q	
[505-48-6] TYFQFVWCELRYAO-UHFFFAOYSA-N					
3-methyl-1,2,3-butanetricarboxylic acid $C_8H_{12}O_6$ [77370-41-3] VMWJGTKDJFMTFZ-UHFFFAOYSA-N	1.9×10^8		Isaacman-VanWertz et al. (2016)	Q	441
nonanedioic acid	8.9×10^7	17000	Compernolle and Müller (2014a)	V	
$C_9H_{16}O_4$	3.6×10^6		Yaws (2003)	X	237, 12
(azelaic acid)	1.9×10^5		Gharagheizi et al. (2012)	Q	
[123-99-9]	9.3×10^5		Gharagheizi et al. (2010)	Q	246
BDJRBEYXGGNYIS-UHFFFAOYSA-N					
decanedioic acid	7.6×10^7		Compernolle and Müller (2014a)	V	
$C_{10}H_{18}O_4$	1.7×10^6		Yaws (2003)	X	237, 12
(sebacic acid)	1.6×10^5		Gharagheizi et al. (2012)	Q	
[111-20-6]	1.4×10^6		Gharagheizi et al. (2010)	Q	246
CXMXRPHRNRROMY-UHFFFAOYSA-N					
dodecanedioic acid $C_{12}H_{22}O_4$ [693-23-2] TVIDDXQYHWJXFK-UHFFFAOYSA-N	9.9×10^5		Ebert et al. (2023)	?	316

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cis-butenedioic acid	1.4×10^{8}		Lide and Frederikse (1995)	V	
$HOOC(CH)_2COOH$	1.3×10^{6}		Yaws (2003)	X	237
(maleic acid)	6.8×10^{6}		Gharagheizi et al. (2012)	Q	
[110-16-7]	1.3×10^{6}		Gharagheizi et al. (2010)	Q	246
VZCYOOQTPOCHFL-UPHRSURJSA-N	9.9×10^{6}		Saxena and Hildemann (1996)	E	401
citraconic acid	3.6×10^{7}		Yaws (2003)	X	237
$C_5H_6O_4$	4.0×10^{6}		Gharagheizi et al. (2012)	Q	
[498-23-7]	3.7×10^{7}		Gharagheizi et al. (2010)	Q	246
HNEGQIOMVPPMNR-IHWYPQMZSA-N					
itaconic acid	1.3×10^{6}		Yaws (2003)	X	237, 12
$C_5H_6O_4$	1.3×10^{7}		Gharagheizi et al. (2012)	Q	
[97-65-4]	1.3×10^{6}		Gharagheizi et al. (2010)	Q	246
LVHBHZANLOWSRM-UHFFFAOYSA-N					
1,4-cyclohexanedicarboxylic acid	1.1×10^{6}		Yaws (2003)	X	237, 154
$C_8H_{12}O_4$	2.3×10^{6}		Gharagheizi et al. (2012)	Q	
[619-82-9]	1.1×10^{6}		Gharagheizi et al. (2010)	Q	246
PXGZQGDTEZPERC-UHFFFAOYSA-N					
pinic acid	1.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	7.1×10^{7}		Wang et al. (2017)	Q	80, 239
[473-73-4]	3.2×10^{7}		Wang et al. (2017)	Q	80, 240
LEVONNIFUFSRKZ-UHFFFAOYSA-N	1.0×10^{7}		Isaacman-VanWertz et al. (2016)	Q	441
methanoic peroxyacid	2.9×10^{1}		Sauer (1997)	M	449
$HCOOOH$	5.2		HSDB (2015)	Q	99
(peroxyformic acid)					
[107-32-4]					
SCKXCAADGDQQCS-UHFFFAOYSA-N					
ethanoic peroxyacid	8.3	5300	Burkholder et al. (2019)	L	
CH_3COOOH	8.3	5300	Burkholder et al. (2015)	L	
(peroxyacetic acid)	8.3	5300	Sander et al. (2011)	L	
[79-21-0]	7.3	5600	Staudinger and Roberts (2001)	L	
KFSLWBXXFJQRDL-UHFFFAOYSA-N	2.4×10^{1}		Sauer (1997)	M	449
	8.3	5300	O'Sullivan et al. (1996)	M	
	6.5	5900	Lind and Kok (1994)	M	52
	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
	9.6		Wang et al. (2017)	Q	80, 239
	1.3×10^{-1}		Wang et al. (2017)	Q	80, 240
	7.8		Raventos-Duran et al. (2010)	Q	242, 243
	2.5		Raventos-Duran et al. (2010)	Q	244
	7.8		Raventos-Duran et al. (2010)	Q	245
	1.8×10^{1}		Hilal et al. (2008)	Q	
	9.3×10^{1}		Modarresi et al. (2007)	Q	67
		6100	Kühne et al. (2005)	Q	
		5300	Kühne et al. (2005)	?	

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:M2C43CO2H	8.0		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	1.7×10^{1}		Wang et al. (2017)	Q	80, 239
XFOASZQZPWEJAA-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:M33C3CO2H	4.9		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	1.7×10^{1}		Wang et al. (2017)	Q	80, 239
VUAXHMVRKOTJKP-UHFFFAOYSA-N	9.6		Wang et al. (2017)	Q	80, 240
MCM:C721OOH	1.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	2.8×10^{6}		Wang et al. (2017)	Q	80, 239
ZLURETBBUKLNQX-UHFFFAOYSA-N	6.2×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C721CO3H	1.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	5.5×10^{6}		Wang et al. (2017)	Q	80, 239
HYEGRGIGVZWWFM-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C811OOH	9.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_4$	3.3×10^{6}		Wang et al. (2017)	Q	80, 239
RYDSGVCXHLRTGT-UHFFFAOYSA-N	2.5×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C823OOH	8.7×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_4$	3.0×10^{6}		Wang et al. (2017)	Q	80, 239
KIIRSRLFRXTUMU-UHFFFAOYSA-N	2.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NORPINIC	1.7×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	2.0×10^{7}		Wang et al. (2017)	Q	80, 239
KLGKVMMWRDYKJM-UHFFFAOYSA-N	6.3×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C811CO3H	1.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	3.7×10^{6}		Wang et al. (2017)	Q	80, 239
ZVOGBTSHONFRIW-UHFFFAOYSA-N	2.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C823CO3H	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	1.6×10^{6}		Wang et al. (2017)	Q	80, 239
IESQFENJEQJSTC-UHFFFAOYSA-N	3.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:LIMONIC	1.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	6.6×10^{7}		Wang et al. (2017)	Q	80, 239
JUCWCJYNDRRZKR-UHFFFAOYSA-N	1.8×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C137OOH	8.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_4$	3.7×10^{6}		Wang et al. (2017)	Q	80, 239
RDYPCLKIKFUKHY-UHFFFAOYSA-N	4.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C137CO2H	1.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_4$	1.7×10^{8}		Wang et al. (2017)	Q	80, 239
IYTMEDMFNUDFPT-UHFFFAOYSA-N	1.7×10^{8}		Wang et al. (2017)	Q	80, 240
MCM:C137CO3H	9.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_5$	2.4×10^{6}		Wang et al. (2017)	Q	80, 239
WIBVBPZGNYNCKK-UHFFFAOYSA-N	1.8×10^{5}		Wang et al. (2017)	Q	80, 240

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:TM123BCO2H	1.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_2$	9.1×10^{1}		Wang et al. (2017)	Q	80, 239
RIZUCYSQUWMQLX-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:TM124BCO2H	1.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_2$	4.1×10^{2}		Wang et al. (2017)	Q	80, 239
OPVAJFQBSDUNQA-UHFFFAOYSA-N	5.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:TMBCO2H	1.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}O_2$	2.6×10^{2}		Wang et al. (2017)	Q	80, 239
UMVOQQDNEYOJOK-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C2OHOCO2H	2.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_4$	2.0×10^{7}		Wang et al. (2017)	Q	80, 239
RBNPOMFGQQGHHO-UHFFFAOYSA-N	2.1×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:HOC2H4CO2H	3.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_3$	1.1×10^{5}		Wang et al. (2017)	Q	80, 239
ALRHLSYJTWAHJZ-UHFFFAOYSA-N	7.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HC3CO2H	1.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_3$	3.6×10^{5}		Wang et al. (2017)	Q	80, 239
RMQJECWPWQIIPW-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:HMACO2H	6.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_3$	8.3×10^{2}		Wang et al. (2017)	Q	80, 239
AAMTXHVZOHPPQR-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HO2C3CO2H	3.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	6.9×10^{4}		Wang et al. (2017)	Q	80, 239
WHBMMWSBFZVSSR-UHFFFAOYSA-N	6.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HOC3H6CO2H	2.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	1.4×10^{5}		Wang et al. (2017)	Q	80, 239
SJZRECIVHVDYJC-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:HOIPRCO2H	3.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	4.5×10^{4}		Wang et al. (2017)	Q	80, 239
DBXBTMSZEOQQDU-UHFFFAOYSA-N	6.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:IPRHOCO2H	9.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	2.3×10^{4}		Wang et al. (2017)	Q	80, 239
BWLBGMIXKSTLSX-UHFFFAOYSA-N	5.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C46CO2H	4.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	1.5×10^{5}		Wang et al. (2017)	Q	80, 239
NJMYQRVWBCSLEU-UHFFFAOYSA-N	5.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HC4ACO2H	6.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	2.3×10^{5}		Wang et al. (2017)	Q	80, 239
BERUOTKXCOOJJM-UHFFFAOYSA-N	6.0×10^{5}		Wang et al. (2017)	Q	80, 240

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HC4CCO2H	6.9×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	2.0×10^5		Wang et al. (2017)	Q	80, 239
NCQCQZXQBYAHBZ-UHFFFAOYSA-N	6.5×10^5		Wang et al. (2017)	Q	80, 240
MCM:HM22CO2H	1.7×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	2.1×10^4		Wang et al. (2017)	Q	80, 239
RDFQSFOGKVZWKF-UHFFFAOYSA-N	1.8×10^4		Wang et al. (2017)	Q	80, 240
MCM:HO2C43CO2H	2.8×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	1.6×10^4		Wang et al. (2017)	Q	80, 239
VEXDRERIMPLZLU-UHFFFAOYSA-N	3.2×10^4		Wang et al. (2017)	Q	80, 240
MCM:HO2C4CO2H	2.3×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	8.0×10^4		Wang et al. (2017)	Q	80, 239
FMHKPLXYWVCLME-UHFFFAOYSA-N	8.1×10^5		Wang et al. (2017)	Q	80, 240
MCM:HOBUT2CO2H	2.3×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	3.5×10^4		Wang et al. (2017)	Q	80, 239
JYTYEGKJKIXWOJ-UHFFFAOYSA-N	7.1×10^5		Wang et al. (2017)	Q	80, 240
MCM:C518CO2H	4.6×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	2.8×10^4		Wang et al. (2017)	Q	80, 239
COPVWTGWHHSRKU-UHFFFAOYSA-N	2.0×10^4		Wang et al. (2017)	Q	80, 240
MCM:H2M2C4CO2H	1.4×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	3.0×10^4		Wang et al. (2017)	Q	80, 239
PQJUMPXLDAZULJ-UHFFFAOYSA-N	3.2×10^5		Wang et al. (2017)	Q	80, 240
MCM:H2M3C4CO2H	2.2×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	2.9×10^4		Wang et al. (2017)	Q	80, 239
BNTHHYUWQILHSA-UHFFFAOYSA-N	2.4×10^5		Wang et al. (2017)	Q	80, 240
MCM:HM22C3CO2H	1.4×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	2.3×10^4		Wang et al. (2017)	Q	80, 239
WLKUATLKPJGHKX-UHFFFAOYSA-N	1.6×10^5		Wang et al. (2017)	Q	80, 240
MCM:HM2C43CO2H	2.2×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	2.3×10^4		Wang et al. (2017)	Q	80, 239
QSMSJHRQUBQMKD-UHFFFAOYSA-N	4.7×10^4		Wang et al. (2017)	Q	80, 240
MCM:HM33C3CO2H	1.4×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.7×10^4		Wang et al. (2017)	Q	80, 239
NGRPJOQCQYDOJX-UHFFFAOYSA-N	6.6×10^5		Wang et al. (2017)	Q	80, 240
MCM:HO2C54CO2H	2.2×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.6×10^4		Wang et al. (2017)	Q	80, 239
IOXPMKQXROCYFL-UHFFFAOYSA-N	6.3×10^5		Wang et al. (2017)	Q	80, 240
MCM:HO3C5CO2H	2.0×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	3.7×10^4		Wang et al. (2017)	Q	80, 239
ABIKNKURIGPIRJ-UHFFFAOYSA-N	6.2×10^5		Wang et al. (2017)	Q	80, 240

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C622CO2H	3.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_3$	4.7×10^{4}		Wang et al. (2017)	Q	80, 239
PHVXTLWKDLVJPT-UHFFFAOYSA-N	2.7×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C624CO2H	3.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_3$	3.0×10^{4}		Wang et al. (2017)	Q	80, 239
IOGKLHPXZHQWIC-UHFFFAOYSA-N	4.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:H3M3C5CO2H	1.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_3$	1.7×10^{4}		Wang et al. (2017)	Q	80, 239
BHWOTLCMMUBASI-UHFFFAOYSA-N	2.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C811OH	3.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_3$	1.7×10^{6}		Wang et al. (2017)	Q	80, 239
UVNHICQQCWWSMK-UHFFFAOYSA-N	9.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C812OH	3.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_4$	2.9×10^{8}		Wang et al. (2017)	Q	80, 239
VFUDATRQVLCLSF-UHFFFAOYSA-N	1.2×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C812OOH	1.8×10^{9}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_5$	4.9×10^{8}		Wang et al. (2017)	Q	80, 239
TXANCYYWZQZPGK-UHFFFAOYSA-N	1.5×10^{8}		Wang et al. (2017)	Q	80, 240
MCM:C823OH	3.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_3$	2.0×10^{6}		Wang et al. (2017)	Q	80, 239
HTVBHPNLYICQSI-UHFFFAOYSA-N	9.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C825OH	5.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_4$	3.7×10^{7}		Wang et al. (2017)	Q	80, 239
GZVYHBJSBFFFII-UHFFFAOYSA-N	5.9×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C825OOH	2.8×10^{9}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_5$	7.8×10^{8}		Wang et al. (2017)	Q	80, 239
XYVJCWMMBMHSFM-UHFFFAOYSA-N	1.8×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C137OH	3.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_3$	1.7×10^{6}		Wang et al. (2017)	Q	80, 239
GRQGZSRLPJOOBF-UHFFFAOYSA-N	2.1×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C139OH	6.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_4$	7.6×10^{9}		Wang et al. (2017)	Q	80, 239
RQGWJIBQKQBFEC-UHFFFAOYSA-N	1.4×10^{8}		Wang et al. (2017)	Q	80, 240
MCM:C139OOH	1.8×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_5$	1.7×10^{10}		Wang et al. (2017)	Q	80, 239
MQHLLQIJDGKDCT-UHFFFAOYSA-N	9.8×10^{8}		Wang et al. (2017)	Q	80, 240
MCM:C44OOH	7.3×10^{8}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_5$	4.1×10^{7}		Wang et al. (2017)	Q	80, 239
RIVXGQNQRYOWAN-UHFFFAOYSA-N	1.9×10^{5}		Wang et al. (2017)	Q	80, 240

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MALDALCO2H	3.4×10^4		Wang et al. (2017)	Q	80, 238
$C_4H_4O_3$	6.0×10^3		Wang et al. (2017)	Q	80, 239
ZOIRMVZWDRLJPI-UHFFFAOYSA-N	5.9×10^3		Wang et al. (2017)	Q	80, 240
MCM:PRPAL2CO2H	9.8×10^3		Wang et al. (2017)	Q	80, 238
$C_4H_6O_3$	5.0×10^3		Wang et al. (2017)	Q	80, 239
VOKUMXABRRXHAR-UHFFFAOYSA-N	2.0×10^3		Wang et al. (2017)	Q	80, 240
MCM:C3MCOCO2H	2.3×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_6O_3$	9.6×10^3		Wang et al. (2017)	Q	80, 239
VXAWORVMCLXEKH-UHFFFAOYSA-N	7.8×10^2		Wang et al. (2017)	Q	80, 240
MCM:CO1M22CO2H	5.4×10^3		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	1.3×10^3		Wang et al. (2017)	Q	80, 239
SUMZWDXUXLTFFX-UHFFFAOYSA-N	6.5×10^2		Wang et al. (2017)	Q	80, 240
MCM:MC3ODBCO2H	2.3×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_6O_3$	9.3×10^3		Wang et al. (2017)	Q	80, 239
QPFVAKLVWFPTSX-UHFFFAOYSA-N	3.4×10^3		Wang et al. (2017)	Q	80, 240
MCM:C3EODBCO2H	2.0×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	8.3×10^3		Wang et al. (2017)	Q	80, 239
XIZBOUDCWHEQCF-UHFFFAOYSA-N	4.6×10^2		Wang et al. (2017)	Q	80, 240
MCM:C3M2COCO2H	1.6×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	9.1×10^3		Wang et al. (2017)	Q	80, 239
HLFIROOBCUFLFC-UHFFFAOYSA-N	5.8×10^3		Wang et al. (2017)	Q	80, 240
MCM:C522CO2H	1.3×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	2.3×10^4		Wang et al. (2017)	Q	80, 239
NSMTVDIDRFOALU-UHFFFAOYSA-N	9.3×10^3		Wang et al. (2017)	Q	80, 240
MCM:RGDCO2H	2.0×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	8.5×10^3		Wang et al. (2017)	Q	80, 239
HNXWTHGWCGDLKB-UHFFFAOYSA-N	3.0×10^3		Wang et al. (2017)	Q	80, 240
MCM:C615CO2H	3.6×10^6		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	5.4×10^5		Wang et al. (2017)	Q	80, 239
BRDQYLNZHVUNQF-UHFFFAOYSA-N	2.6×10^4		Wang et al. (2017)	Q	80, 240
MCM:C722OOH	3.0×10^8		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	1.6×10^7		Wang et al. (2017)	Q	80, 239
XJSSOLXEKAZFKL-UHFFFAOYSA-N	8.0×10^5		Wang et al. (2017)	Q	80, 240
MCM:IP3ODBCO2H	1.9×10^4		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	4.5×10^3		Wang et al. (2017)	Q	80, 239
HLXOYOZOZOGAJW-UHFFFAOYSA-N	1.1×10^3		Wang et al. (2017)	Q	80, 240
MCM:PC3ODBCO2H	1.7×10^4		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	5.4×10^3		Wang et al. (2017)	Q	80, 239
SHOOYBDWMZRRKO-UHFFFAOYSA-N	2.2×10^3		Wang et al. (2017)	Q	80, 240

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C721CHO	1.2×10^4		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_3$	2.8×10^5		Wang et al. (2017)	Q	80, 239
MQTHUXQLMJSVGN-UHFFFAOYSA-N	2.9×10^4		Wang et al. (2017)	Q	80, 240
MCM:C729CO2H	1.0×10^4		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_3$	1.1×10^5		Wang et al. (2017)	Q	80, 239
NHNJUKWYLMFOQP-UHFFFAOYSA-N	1.7×10^4		Wang et al. (2017)	Q	80, 240
MCM:C823CO	1.0×10^4		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_3$	2.2×10^5		Wang et al. (2017)	Q	80, 239
KUOQBJGRIDTXEZ-UHFFFAOYSA-N	7.1×10^3		Wang et al. (2017)	Q	80, 240
MCM:C822CO2H	4.4×10^4	15000	Wieser et al. (2023)	Q	437
$C_9H_{14}O_3$	8.5×10^3		Wang et al. (2017)	Q	80, 238
ADULCIYKWVJSFE-UHFFFAOYSA-N	9.3×10^4		Wang et al. (2017)	Q	80, 239
	3.0×10^4		Wang et al. (2017)	Q	80, 240
MCM:C830CO2H	9.1×10^3		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_3$	1.9×10^5		Wang et al. (2017)	Q	80, 239
NWNQYPOMHUZLML-UHFFFAOYSA-N	2.3×10^4		Wang et al. (2017)	Q	80, 240
MCM:C89CO2H	9.1×10^3		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_3$	2.0×10^5		Wang et al. (2017)	Q	80, 239
RFGXRYLTPBBFIG-UHFFFAOYSA-N	7.4×10^4		Wang et al. (2017)	Q	80, 240
MCM:C126CO2H	1.0×10^4		Wang et al. (2017)	Q	80, 238
$C_{13}H_{20}O_3$	2.4×10^5		Wang et al. (2017)	Q	80, 239
FRZAETYQWIEERW-UHFFFAOYSA-N	2.6×10^5		Wang et al. (2017)	Q	80, 240
MCM:C137CO	1.0×10^4		Wang et al. (2017)	Q	80, 238
$C_{13}H_{20}O_3$	2.2×10^5		Wang et al. (2017)	Q	80, 239
FQUQDHNCRLRZNB-UHFFFAOYSA-N	7.8×10^4		Wang et al. (2017)	Q	80, 240
MCM:C136CO2H	8.9×10^3		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_3$	1.5×10^5		Wang et al. (2017)	Q	80, 239
MUFZWTUKICSBHZ-UHFFFAOYSA-N	7.8×10^3		Wang et al. (2017)	Q	80, 240
MCM:COHM2CO2H	2.0×10^5		Wang et al. (2017)	Q	80, 238
$C_4H_6O_4$	7.1×10^5		Wang et al. (2017)	Q	80, 239
DDNPKLYNPFAIEE-UHFFFAOYSA-N	2.0×10^2		Wang et al. (2017)	Q	80, 240
MCM:C1H4C5CO2H	1.8×10^7		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	3.4×10^7		Wang et al. (2017)	Q	80, 239
NIVGPRREFKECGM-UHFFFAOYSA-N	3.2×10^6		Wang et al. (2017)	Q	80, 240
MCM:ECOCO2H	7.3×10^3		Wang et al. (2017)	Q	80, 238
$C_4H_6O_3$	4.1×10^1		Wang et al. (2017)	Q	80, 239
TYEYBOSBBBHJIV-UHFFFAOYSA-N	5.8		Wang et al. (2017)	Q	80, 240
MCM:C41CO2H	6.5×10^3		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	4.6×10^3		Wang et al. (2017)	Q	80, 239
GCXJINGJZAOJHR-UHFFFAOYSA-N	3.0×10^3		Wang et al. (2017)	Q	80, 240

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C5CO14OH	2.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_3$	1.6×10^{4}		Wang et al. (2017)	Q	80, 239
XGTKSWVCNVUVHG-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:CO2C4CO2H	5.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	4.6×10^{5}		Wang et al. (2017)	Q	80, 239
JOOXCMJARBKPKM-UHFFFAOYSA-N	7.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:CO3C4CO2H	5.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	1.5×10^{4}		Wang et al. (2017)	Q	80, 239
FHSUFDYFOHSYHI-UHFFFAOYSA-N	5.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:IPGLYOXOH	6.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	1.7×10^{1}		Wang et al. (2017)	Q	80, 239
QHKABHOOEWYVLI-UHFFFAOYSA-N	5.4		Wang et al. (2017)	Q	80, 240
MCM:PGLYOXOH	5.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	2.0×10^{1}		Wang et al. (2017)	Q	80, 239
KDVFRMMRZOCFLS-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	80, 240
MCM:C51CO2H	5.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	1.6×10^{5}		Wang et al. (2017)	Q	80, 239
NFIWUVRBASXMGK-UHFFFAOYSA-N	1.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C5CODBCO2H	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	1.6×10^{4}		Wang et al. (2017)	Q	80, 239
YUICRCSHEOZHST-UHFFFAOYSA-N	2.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C5DBCOCO2H	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
LRRPKULXSOVRRZ-UHFFFAOYSA-N	2.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C6DCRBBOH	2.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
VUZJJUOKMOGBDH-UHFFFAOYSA-N	4.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:CO2C54CO2H	5.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	8.7×10^{4}		Wang et al. (2017)	Q	80, 239
UZTJTTKEYGHTNM-UHFFFAOYSA-N	3.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:CO2M33CO2H	3.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	8.5×10^{2}		Wang et al. (2017)	Q	80, 239
CBZZWRQRPKSEQI-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:CO3C5CO2H	4.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	2.6×10^{5}		Wang et al. (2017)	Q	80, 239
CLJBDOUIEHLLEN-UHFFFAOYSA-N	3.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C732OOH	3.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	1.8×10^{9}		Wang et al. (2017)	Q	80, 239
ASSSOSHEUJWVOL-UHFFFAOYSA-N	2.0×10^{6}		Wang et al. (2017)	Q	80, 240

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C7ADCCO2H	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	1.3×10^{4}		Wang et al. (2017)	Q	80, 239
GJIWJSZYGQVZNC-UHFFFAOYSA-N	6.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C7CDCCO2H	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	7.8×10^{3}		Wang et al. (2017)	Q	80, 239
OAGXHOMWGVMDLP-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C7DCCO2H	1.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	8.5×10^{3}		Wang et al. (2017)	Q	80, 239
LUXOYEZTEWTGMD-UHFFFAOYSA-N	4.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C7DDCCO2H	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	8.5×10^{3}		Wang et al. (2017)	Q	80, 239
MDDQAVHYGMRQBB-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:CO25C6CO2H	2.7×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	2.2×10^{7}		Wang et al. (2017)	Q	80, 239
WUQQVFQGWWMQLD-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:IC7DCCO2H	1.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	6.9×10^{3}		Wang et al. (2017)	Q	80, 239
TZKNMZPMBZQSMV-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C732CO3H	3.6×10^{9}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_6$	2.2×10^{9}		Wang et al. (2017)	Q	80, 239
IARLEAITRRLVEZ-UHFFFAOYSA-N	2.7×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:KLIMONIC	4.5×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	3.4×10^{10}		Wang et al. (2017)	Q	80, 239
POLIOAJLCGOOTJ-UHFFFAOYSA-N	1.1×10^{9}		Wang et al. (2017)	Q	80, 240
MCM:C827CO2H	1.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	1.3×10^{6}		Wang et al. (2017)	Q	80, 239
UOMMGFNPUVSKTE-UHFFFAOYSA-N	4.9×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C88CO2H	4.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	6.6×10^{7}		Wang et al. (2017)	Q	80, 239
LOFCXTWTTIFNLN-UHFFFAOYSA-N	3.2×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:KLIMONONIC	2.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_4$	5.4×10^{7}		Wang et al. (2017)	Q	80, 239
RRLLKTDJWPIWHS-UHFFFAOYSA-N	8.5×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C928CO2H	1.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_4$	5.6×10^{7}		Wang et al. (2017)	Q	80, 239
SANKOOWGNYBKOU-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:LIMONONIC	5.7×10^{4}	15000	Wieser et al. (2023)	Q	437
$C_{10}H_{16}O_3$	5.8×10^{3}		Wang et al. (2017)	Q	80, 238
NJOIWWRMLFSDTM-UHFFFAOYSA-N	5.9×10^{4}		Wang et al. (2017)	Q	80, 239
	2.4×10^{5}		Wang et al. (2017)	Q	80, 240

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C1011CO2H	4.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_3$	1.5×10^{5}		Wang et al. (2017)	Q	80, 239
IUOPXZCJHJMHNP-UHFFFAOYSA-N	2.4×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C1211OOH	3.5×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_5$	1.7×10^{9}		Wang et al. (2017)	Q	80, 239
PTZJPBFCCQIPAZ-UHFFFAOYSA-N	8.1×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C1211CO2H	4.7×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{20}O_5$	9.3×10^{10}		Wang et al. (2017)	Q	80, 239
QUEDJGCZCJPFDA-UHFFFAOYSA-N	2.8×10^{8}		Wang et al. (2017)	Q	80, 240
MCM:C1211CO3H	3.6×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{20}O_6$	4.5×10^{9}		Wang et al. (2017)	Q	80, 239
DVDQWECWXWLOQZ-UHFFFAOYSA-N	8.1×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C131CO2H	2.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_4$	1.4×10^{8}		Wang et al. (2017)	Q	80, 239
QDUXHZZYSCMHPK-UHFFFAOYSA-N	5.9×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C147CO	1.4×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{20}O_5$	3.2×10^{8}		Wang et al. (2017)	Q	80, 239
MMRJODLWTRWNRH-UHFFFAOYSA-N	2.5×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C147OOH	1.7×10^{11}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_6$	1.0×10^{9}		Wang et al. (2017)	Q	80, 239
MOUQEZQXHGSYER-UHFFFAOYSA-N	3.0×10^{8}		Wang et al. (2017)	Q	80, 240
MCM:C141CO2H	5.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{24}O_3$	2.1×10^{5}		Wang et al. (2017)	Q	80, 239
VGNFSHPHIKPNED-UHFFFAOYSA-N	3.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HOCH2COCO2H	1.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_3H_4O_4$	5.3×10^{2}		Wang et al. (2017)	Q	80, 239
HHDDCCUIIUWNGJ-UHFFFAOYSA-N	4.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:H3C2C4CO2H	8.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	2.0×10^{6}		Wang et al. (2017)	Q	80, 239
IQZHXDCQZNRIRW-UHFFFAOYSA-N	2.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:HMVKBCO2H	1.7×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	2.1×10^{6}		Wang et al. (2017)	Q	80, 239
ISMQTZHDOHOVBT-UHFFFAOYSA-N	6.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C517CO2H	1.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	1.3×10^{7}		Wang et al. (2017)	Q	80, 239
APPVMSIJNZFGHP-UHFFFAOYSA-N	2.0×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C519CO2H	1.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	3.8×10^{6}		Wang et al. (2017)	Q	80, 239
ULHNCRHSCMPZGW-UHFFFAOYSA-N	3.8×10^{6}		Wang et al. (2017)	Q	80, 240

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C732OH	1.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	4.7×10^{8}		Wang et al. (2017)	Q	80, 239
PKQMWBHBXJKPID-UHFFFAOYSA-N	4.2×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C734CO	8.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	6.6×10^{7}		Wang et al. (2017)	Q	80, 239
CPJVKYXUMUTCGW-UHFFFAOYSA-N	3.2×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C734OH	1.9×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	8.7×10^{10}		Wang et al. (2017)	Q	80, 239
RDRUHSRUZHRAFB-UHFFFAOYSA-N	4.4×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C734OOH	1.1×10^{12}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_6$	2.0×10^{11}		Wang et al. (2017)	Q	80, 239
ABEMFUWOTMEDPB-UHFFFAOYSA-N	1.3×10^{8}		Wang et al. (2017)	Q	80, 240
MCM:H3C25CCO2H	4.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	4.1×10^{9}		Wang et al. (2017)	Q	80, 239
FMZPEVNVWACALO-UHFFFAOYSA-N	2.7×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C813OH	2.1×10^{10}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_5$	6.5×10^{8}		Wang et al. (2017)	Q	80, 239
UHMOZKUUXAVADP-UHFFFAOYSA-N	2.0×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C813OOH	6.2×10^{11}		Wang et al. (2017)	Q	80, 238
$C_8H_{14}O_6$	1.7×10^{8}		Wang et al. (2017)	Q	80, 239
FNGYAHKKJFMZCA-UHFFFAOYSA-N	4.3×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C825CO	2.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	2.6×10^{5}		Wang et al. (2017)	Q	80, 239
PGSQVIJDIYGHPF-UHFFFAOYSA-N	4.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HOPINONIC	8.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_4$	6.0×10^{7}		Wang et al. (2017)	Q	80, 239
MZHKOIVHCBFXJV-UHFFFAOYSA-N	1.0×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C1211OH	1.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_4$	2.7×10^{8}		Wang et al. (2017)	Q	80, 239
JNTJQAWMLAKHDW-UHFFFAOYSA-N	2.8×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C1212OH	1.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_5$	4.7×10^{11}		Wang et al. (2017)	Q	80, 239
OINCQTVJDDDYTJ-UHFFFAOYSA-N	8.9×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C1212OOH	6.5×10^{11}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_6$	1.8×10^{11}		Wang et al. (2017)	Q	80, 239
KZNQDAPBLSOIIR-UHFFFAOYSA-N	1.8×10^{10}		Wang et al. (2017)	Q	80, 240
MCM:C1213CO	1.5×10^{12}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{18}O_6$	3.3×10^{12}		Wang et al. (2017)	Q	80, 239
IKFUCIVDZJUENZ-UHFFFAOYSA-N	2.1×10^{9}		Wang et al. (2017)	Q	80, 240

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C1213OH	7.1×10^{12}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_6$	9.8×10^{11}		Wang et al. (2017)	Q	80, 239
DPGLQQDGNMDAAZ-UHFFFAOYSA-N	1.3×10^{8}		Wang et al. (2017)	Q	80, 240
MCM:C1213OOH	1.9×10^{14}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{20}O_7$	1.3×10^{13}		Wang et al. (2017)	Q	80, 239
ZUGVXCQEOPRNFT-UHFFFAOYSA-N	3.9×10^{8}		Wang et al. (2017)	Q	80, 240
MCM:C1310CO	4.3×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{20}O_5$	3.9×10^{11}		Wang et al. (2017)	Q	80, 239
NHYXXXJOGAKHPV-UHFFFAOYSA-N	2.6×10^{9}		Wang et al. (2017)	Q	80, 240
MCM:C1310OH	2.0×10^{10}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_5$	1.0×10^{11}		Wang et al. (2017)	Q	80, 239
PXEJSKZGVMTSCR-UHFFFAOYSA-N	1.7×10^{9}		Wang et al. (2017)	Q	80, 240
MCM:C1310OOH	5.4×10^{11}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{22}O_6$	1.1×10^{12}		Wang et al. (2017)	Q	80, 239
HXUMLFGRLLCICH-UHFFFAOYSA-N	5.9×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C147OH	3.3×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_5$	5.6×10^{8}		Wang et al. (2017)	Q	80, 239
IPYASLZXSQHCRG-UHFFFAOYSA-N	7.8×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C151OH	6.3×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{26}O_5$	2.4×10^{10}		Wang et al. (2017)	Q	80, 239
RRTATIWWWPYIIC-UHFFFAOYSA-N	3.7×10^{9}		Wang et al. (2017)	Q	80, 240
MCM:C151OOH	4.7×10^{11}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{26}O_6$	1.9×10^{11}		Wang et al. (2017)	Q	80, 239
FDHNLWUJMDRLQD-UHFFFAOYSA-N	2.8×10^{10}		Wang et al. (2017)	Q	80, 240
MCM:CO13C3CO2H	6.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_4$	1.5×10^{4}		Wang et al. (2017)	Q	80, 239
YEZSWHPLZBZVLH-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C512CO2H	4.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	6.3×10^{7}		Wang et al. (2017)	Q	80, 239
CGRSCFNOTZUXCX-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C6COALCO2H	4.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	2.3×10^{7}		Wang et al. (2017)	Q	80, 239
TWNJAPRLIZAXHA-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C617CO2H	2.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	9.6×10^{5}		Wang et al. (2017)	Q	80, 239
ZXMACHDUAJJJBQ-UHFFFAOYSA-N	2.4×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C618CO2H	2.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	2.3×10^{5}		Wang et al. (2017)	Q	80, 239
MXMJWVQRGMMLRI-UHFFFAOYSA-N	5.8×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.7: Carboxylic acids (RCOOH) and peroxy carboxylic acids (RCOOOH) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C626CO2H	3.7×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	8.3×10^{7}		Wang et al. (2017)	Q	80, 239
JCTYMUINHXVDEP-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C732CO	3.7×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	5.0×10^{7}		Wang et al. (2017)	Q	80, 239
ATXVRLJHWCSFDB-UHFFFAOYSA-N	2.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C718CO2H	2.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	1.6×10^{7}		Wang et al. (2017)	Q	80, 239
OBYKYHDGLQUNDK-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C731CO2H	3.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_4$	2.0×10^{8}		Wang et al. (2017)	Q	80, 239
URWVDUFOGQNELZ-UHFFFAOYSA-N	3.8×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C87CO2H	1.7×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	3.6×10^{8}		Wang et al. (2017)	Q	80, 239
GZPOIVSRXTZTQZ-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C116CO2H	4.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{18}O_4$	1.8×10^{8}		Wang et al. (2017)	Q	80, 239
HWWVGCXKFWUOCT-UHFFFAOYSA-N	1.3×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C1211CO	4.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{18}O_4$	4.2×10^{7}		Wang et al. (2017)	Q	80, 239
VVPUYBXPESADLR-UHFFFAOYSA-N	8.7×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C1210CO2H	3.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{20}O_4$	2.8×10^{8}		Wang et al. (2017)	Q	80, 239
MERIWEKKXYNSHZ-UHFFFAOYSA-N	8.3×10^{5}		Wang et al. (2017)	Q	80, 240

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A3.8 Esters (RCOOR)

Table A3.8: Esters (RCOOR)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3-dioxolan-2-one $C_3H_4O_3$ (ethylene carbonate) [96-49-1] KMTRUDSVKNLOMY-UHFFFAOYSA-N	3.6×10^{-2}		HSDB (2015)	Q	99
carbonic acid, dimethyl ester	1.6×10^{-1}	4900	Burkholder et al. (2019)	L	
$C_3H_6O_3$	1.6×10^{-1}	4900	Burkholder et al. (2015)	L	
(dimethyl carbonate)	1.5×10^{-1}	5000	Brockbank (2013)	L	1
[616-38-6]	1.6×10^{-1}	4900	Böhme et al. (2008)	M	
IEJIGPNLZYLLBP-UHFFFAOYSA-N	1.6×10^{-1}	5000	Dohnal et al. (2010)	V	1
	2.5×10^{-1}		Wang et al. (2017)	Q	80, 238
	2.1×10^{-1}		Wang et al. (2017)	Q	80, 239
	2.1×10^{-1}		Wang et al. (2017)	Q	80, 240
	1.6×10^{-2}		HSDB (2015)	Q	99
dimethyl dicarbonate $C_4H_6O_5$ [4525-33-1] GZDFHIJNHHMENY-UHFFFAOYSA-N	2.2×10^{-2}		HSDB (2015)	Q	99
carbonic acid, diethyl ester	1.0×10^{-1}	6000	Burkholder et al. (2019)	L	
$C_5H_{10}O_3$	1.0×10^{-1}	6000	Burkholder et al. (2015)	L	
(diethyl carbonate)	1.0×10^{-1}	6400	Brockbank (2013)	L	1
[105-58-8]	1.1×10^{-1}	6100	Böhme et al. (2008)	M	
OIFBSDVPJOWBCH-UHFFFAOYSA-N	1.1×10^{-1}		Duchowicz et al. (2020)	V	186
	1.1×10^{-1}		HSDB (2015)	V	
	1.0×10^{-1}	6100	Dohnal et al. (2010)	V	1
	1.5×10^{-2}		Duchowicz et al. (2020)	Q	
	1.6×10^{-1}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	6.9×10^{-2}		Hilal et al. (2008)	Q	
	2.8×10^{-2}		Modarresi et al. (2007)	Q	67
	1.1×10^{-1}		Yaws (1999)	?	21, 12
methyl methanoate	4.1×10^{-2}	4000	Burkholder et al. (2019)	L	
$HCOOCH_3$	4.1×10^{-2}	4000	Burkholder et al. (2015)	L	
(methyl formate)	4.2×10^{-2}	3800	Brockbank (2013)	L	1
[107-31-3]	4.1×10^{-2}	4000	Sander et al. (2011)	L	
TZIHFWKZFHZASV-UHFFFAOYSA-N	4.2×10^{-2}	3900	Plyasunov et al. (2004)	L	
	4.1×10^{-2}	4000	Kutsuna et al. (2005)	M	
	4.6×10^{-2}		Wittig et al. (2001)	M	
	4.1×10^{-2}		Hoff et al. (1993)	M	
	3.9×10^{-2}	4100	Hartkopf and Karger (1973)	M	
	4.9×10^{-2}		Mackay et al. (2006c)	V	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.9×10^{-2}		Mackay et al. (1995)	V	
	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	3.8×10^{-1}		Duchowicz et al. (2020)	Q	
	5.3×10^{-2}		Wang et al. (2017)	Q	80, 238
	1.0×10^{-1}		Wang et al. (2017)	Q	80, 239
	8.7×10^{-2}		Wang et al. (2017)	Q	80, 240
	4.4×10^{-2}		Li et al. (2014)	Q	241
	5.4×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	5.8×10^{-2}		Hilal et al. (2008)	Q	
	5.8×10^{-2}		Modarresi et al. (2007)	Q	67
		4100	Kühne et al. (2005)	Q	
	4.6×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	3.4×10^{-2}		English and Carroll (2001)	Q	230, 231
	2.9×10^{-2}		Katritzky et al. (1998)	Q	
	8.0×10^{-2}		Suzuki et al. (1992)	Q	232
	6.4×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	4.4×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		4200	Kühne et al. (2005)	?	
	5.2×10^{-3}		Yaws (1999)	?	21, 12
	4.4×10^{-2}		Betterton (1992)	?	497
	4.4×10^{-2}		Abraham et al. (1990)	?	
	4.4×10^{-2}		Hine and Mookerjee (1975)	?	497
ethyl methanoate	3.4×10^{-2}	4600	Burkholder et al. (2019)	L	
$HCOOC_2H_5$	3.4×10^{-2}	4600	Burkholder et al. (2015)	L	
(ethyl formate)	3.3×10^{-2}	4000	Brockbank (2013)	L	1
[109-94-4]	3.4×10^{-2}	4600	Sander et al. (2011)	L	
WBJINCZRORDGAQ-UHFFFAOYSA-N	3.5×10^{-2}	4600	Plyasunov et al. (2004)	L	
	3.4×10^{-2}	4600	Kutsuna et al. (2005)	M	
	4.0×10^{-2}		Wittig et al. (2001)	M	
	2.3×10^{-2}		Richon et al. (1985)	M	38
	1.9×10^{-3}	4600	Hartkopf and Karger (1973)	M	
	4.9×10^{-2}		Mackay et al. (2006c)	V	
	4.9×10^{-2}		Mackay et al. (1995)	V	
	3.1×10^{-2}		Abraham (1984)	V	
	3.5×10^{-2}		Hine and Mookerjee (1975)	V	
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	1.8×10^{-1}		Duchowicz et al. (2020)	Q	184
	4.1×10^{-2}		Wang et al. (2017)	Q	80, 238
	4.8×10^{-2}		Wang et al. (2017)	Q	80, 239
	5.0×10^{-2}		Wang et al. (2017)	Q	80, 240
	4.7×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	245

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.1×10^{-2}		Hilal et al. (2008)	Q	
	5.5×10^{-2}		Modarresi et al. (2007)	Q	67
	2.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.6×10^{-2}		English and Carroll (2001)	Q	230, 231
	3.5×10^{-2}		Katritzky et al. (1998)	Q	
	6.2×10^{-2}		Suzuki et al. (1992)	Q	232
	5.7×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.6×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	4.5×10^{-2}		Yaws (1999)	?	21, 28
	1.7×10^{-2}		Abraham and Weathersby (1994)	?	21
	1.4×10^{-3}		Hoff et al. (1993)	?	21
	3.1×10^{-2}		Abraham et al. (1990)	?	
propyl methanoate $HCOOC_3H_7$ (propyl formate) [110-74-7] KFNNIILCVOLYIR-UHFFFAOYSA-N	2.6×10^{-2}	5100	Burkholder et al. (2019)	L	
	2.6×10^{-2}	5100	Burkholder et al. (2015)	L	
	3.1×10^{-2}	4800	Brockbank (2013)	L	1
	2.6×10^{-2}	5100	Sander et al. (2011)	L	
	2.8×10^{-2}	4900	Plyasunov et al. (2004)	L	
	2.6×10^{-2}	5100	Kutsuna et al. (2005)	M	
	2.3×10^{-2}		Duchowicz et al. (2020)	V	186
	2.1×10^{-2}		Mackay et al. (2006c)	V	
	2.7×10^{-2}		Hine and Mookerjee (1975)	V	
	2.7×10^{-2}		Yaws (2003)	X	237, 87
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	
	2.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.3×10^{-2}		Hilal et al. (2008)	Q	
	4.5×10^{-2}		Modarresi et al. (2007)	Q	67
	1.3×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	1.9×10^{-2}		English and Carroll (2001)	Q	230, 231
	3.5×10^{-2}		Katritzky et al. (1998)	Q	
	4.7×10^{-2}		Suzuki et al. (1992)	Q	232
	4.4×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.3×10^{-2}		Yaws (1999)	?	21, 87
	2.7×10^{-2}		Abraham et al. (1990)	?	
isopropyl methanoate $HCOOC_3H_7$ (isopropyl formate) [625-55-8] RMOUBSOVHSONPZ-UHFFFAOYSA-N	1.9×10^{-2}		Plyasunov et al. (2004)	L	
	1.3×10^{-2}		Duchowicz et al. (2020)	V	186
	1.2×10^{-2}		Hine and Mookerjee (1975)	V	
	8.2×10^{-2}		Duchowicz et al. (2020)	Q	
	4.4×10^{-2}		Wang et al. (2017)	Q	80, 238
	3.1×10^{-2}		Wang et al. (2017)	Q	80, 239
	7.8×10^{-2}		Wang et al. (2017)	Q	80, 240
	4.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.1×10^{-2}		Hilal et al. (2008)	Q	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.3×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.0×10^{-2}		English and Carroll (2001)	Q	230, 274
	3.8×10^{-2}		Katritzky et al. (1998)	Q	
	4.3×10^{-2}		Suzuki et al. (1992)	Q	232
	3.9×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.2×10^{-2}		Abraham et al. (1990)	?	
butyl methanoate $HCOOC_4H_9$ (butyl formate) [592-84-7] NMJJFJNHVMGPGM-UHFFFAOYSA-N	2.6×10^{-2}	3700	Brockbank (2013)	L	1
	1.9×10^{-2}		Plyasunov et al. (2004)	L	
	1.9×10^{-2}		Wittig et al. (2001)	M	
	1.9×10^{-2}		Duchowicz et al. (2020)	V	186
	1.7×10^{-2}		Yaws (2003)	X	237, 402
	2.3×10^{-1}		Duchowicz et al. (2020)	Q	
	3.0×10^{-2}		Wang et al. (2017)	Q	80, 238
	2.1×10^{-2}		Wang et al. (2017)	Q	80, 239
	3.5×10^{-2}		Wang et al. (2017)	Q	80, 240
	1.4×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
	4.1×10^{-2}		Modarresi et al. (2007)	Q	67
	2.0×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	3.5×10^{-2}		Katritzky et al. (1998)	Q	
	1.9×10^{-2}		Yaws (1999)	?	21, 402
(1-methylpropyl)-methanoate $C_5H_{10}O_2$ (*sec*-butyl formate) [589-40-2] OAEQYDZVVPONKW-UHFFFAOYSA-N	1.9×10^{-2}		Gharagheizi et al. (2012)	Q	
(2-methylpropyl)-methanoate $HCOOC_4H_9$ (isobutyl formate) [542-55-2] AVMSWPWPYJVYKY-UHFFFAOYSA-N	1.6×10^{-2}	5200	Brockbank (2013)	L	1
	1.6×10^{-2}	5200	Plyasunov et al. (2004)	L	
	1.9×10^{-2}		Duchowicz et al. (2020)	V	186
	1.8×10^{-2}		Mackay et al. (2006c)	V	
	1.8×10^{-2}		Mackay et al. (1995)	V	
	1.7×10^{-2}		Hine and Mookerjee (1975)	V	
	1.8×10^{-2}		Yaws (2003)	X	237
	9.1×10^{-2}		Duchowicz et al. (2020)	Q	
	9.5×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.0×10^{-2}		Hilal et al. (2008)	Q	
	3.3×10^{-2}		Modarresi et al. (2007)	Q	67
	2.0×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.5×10^{-2}		English and Carroll (2001)	Q	230, 260
	3.9×10^{-2}		Katritzky et al. (1998)	Q	
	3.3×10^{-2}		Suzuki et al. (1992)	Q	232
	3.1×10^{-2}		Nirmalakhandan and Speece (1988)	Q	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.3×10^{-2}		Yaws (1999)	?	21
	1.7×10^{-2}		Abraham et al. (1990)	?	
(1,1-dimethylethyl)-methanoate	1.4×10^{-2}	3600	Brockbank (2013)	L	1
$HCOOC_4H_9$	1.4×10^{-2}	3600	Arp and Schmidt (2004)	M	
(*tert*-butyl formate; TBF)	2.5×10^{-2}		Yaws (2003)	X	258
[762-75-4]	2.5×10^{-2}		Yaws (2003)	X	237
RUPAXCPQAAOIPB-UHFFFAOYSA-N	7.3×10^{-2}		Dupeux et al. (2022)	Q	259
	2.9×10^{-2}		Keshavarz et al. (2022)	Q	
	4.0×10^{-2}		Duchowicz et al. (2020)	Q	299
	2.3×10^{-2}		Wang et al. (2017)	Q	80, 238
	1.1×10^{-2}		Wang et al. (2017)	Q	80, 239
	6.6×10^{-2}		Wang et al. (2017)	Q	80, 240
	4.5×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
	1.4×10^{-2}		Duchowicz et al. (2020)	?	185, 21
pentyl methanoate	1.7×10^{-2}	6000	Brockbank (2013)	L	1
$C_6H_{12}O_2$	1.6×10^{-2}	5800	Plyasunov et al. (2004)	L	
(pentyl formate)	1.5×10^{-2}		Yaws (2003)	X	237
[638-49-3]	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
DIQMPQMYFZXDAX-UHFFFAOYSA-N	1.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
	1.3×10^{-2}		Hilal et al. (2008)	Q	
	7.5×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	2.8×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	2.5×10^{-2}		Yaws (1999)	?	21
3-pentyl methanoate	1.2×10^{-2}		Gharagheizi et al. (2012)	Q	
$C_6H_{12}O_2$					
(3-pentyl formate)					
[58368-67-5]					
YMJOAYHERILFIM-UHFFFAOYSA-N					
1,1-dimethylpropyl methanoate	1.7×10^{-2}		Yaws (2003)	X	237
$C_6H_{12}O_2$	3.0×10^{-2}		Gharagheizi et al. (2012)	Q	
(1,1-dimethylpropyl formate)	1.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
[757-88-0]					
SVZIJXUUTNJSEJ-UHFFFAOYSA-N					
1,2-dimethylpropyl methanoate	1.7×10^{-2}		Yaws (2003)	X	237
$C_6H_{12}O_2$	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
(1,2-dimethylpropyl formate)	1.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66794-46-5]					
XEQSPMCNFJQDHU-UHFFFAOYSA-N					
1-methylbutyl methanoate	1.7×10^{-2}		Yaws (2003)	X	237
$C_6H_{12}O_2$	1.7×10^{-2}		Gharagheizi et al. (2012)	Q	
(1-methylbutyl formate)	1.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
[58368-66-4]					
JNRQSKFTIYCDIP-UHFFFAOYSA-N					

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2-dimethylpropyl methanoate	1.5×10^{-2}		Yaws (2003)	X	237
$C_6H_{12}O_2$	3.1×10^{-3}		Gharagheizi et al. (2012)	Q	
(2,2-dimethylpropyl formate)	1.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
[23361-67-3]					
DGMIPKNXUDSQGI-UHFFFAOYSA-N					
2-methylbutyl methanoate	1.6×10^{-2}		Yaws (2003)	X	237
$C_6H_{12}O_2$	5.2×10^{-3}		Gharagheizi et al. (2012)	Q	
(2-methylbutyl formate)	1.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
[35073-27-9]					
DWORILFBIRYUDC-UHFFFAOYSA-N					
3-methylbutyl methanoate	1.2×10^{-2}	5700	Plyasunov et al. (2004)	L	
$HCOOC_5H_{11}$	1.5×10^{-2}		Hine and Mookerjee (1975)	V	
(isoamyl formate)	1.2×10^{-2}		Yaws (2003)	X	237
[110-45-2]	3.9×10^{-2}		Keshavarz et al. (2022)	Q	
XKYICAQFSCFURC-UHFFFAOYSA-N	9.7×10^{-2}		Duchowicz et al. (2020)	Q	299
	8.5×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
	1.7×10^{-2}		Hilal et al. (2008)	Q	
	3.3×10^{-2}		Modarresi et al. (2007)	Q	67
	1.6×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.1×10^{-2}		English and Carroll (2001)	Q	230, 231
	3.4×10^{-2}		Katritzky et al. (1998)	Q	
	2.5×10^{-2}		Suzuki et al. (1992)	Q	232
	2.4×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.5×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	1.5×10^{-2}		Abraham et al. (1990)	?	
hexyl methanoate	1.0×10^{-2}		Plyasunov et al. (2004)	L	
$C_7H_{14}O_2$	1.0×10^{-2}		Yaws (2003)	X	237
(hexyl formate)	8.0×10^{-3}		Gharagheizi et al. (2012)	Q	
[629-33-4]	8.2×10^{-3}		Gharagheizi et al. (2010)	Q	246
OUGPMNMLWKSBRI-UHFFFAOYSA-N	1.1×10^{-2}		Hilal et al. (2008)	Q	
	1.6×10^{-2}		Nirmalakhandan et al. (1997)	Q	
heptyl methanoate	6.7×10^{-3}		Yaws (2003)	X	237
$C_8H_{16}O_2$	5.9×10^{-3}		Gharagheizi et al. (2012)	Q	
(heptyl formate)	5.2×10^{-3}		Gharagheizi et al. (2010)	Q	246
[112-23-2]					
XEAMDSXSXYAICO-UHFFFAOYSA-N					
octyl methanoate	1.7×10^{-3}		Yaws (2003)	X	237
$C_9H_{18}O_2$	3.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
(octyl formate)	5.1×10^{-3}		Yaws (1999)	?	21
[112-32-3]					
AVBRYQRTMPHARE-UHFFFAOYSA-N					

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
nonyl methanoate $C_{10}H_{20}O_2$ (nonyl formate) [5451-92-3] MOGJOLMSQWGXPA-UHFFFAOYSA-N	2.3×10^{-3} 3.9×10^{-3} 2.1×10^{-3}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
decyl methanoate $C_{11}H_{22}O_2$ (decyl formate) [5451-52-5] BCLJZFLDSCTULJ-UHFFFAOYSA-N	1.5×10^{-3} 4.8×10^{-3} 1.4×10^{-3}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
undecyl methanoate $C_{12}H_{24}O_2$ (undecyl formate) [5454-24-0] OASFNORBKVGDRW-UHFFFAOYSA-N	9.3×10^{-4} 6.0×10^{-3} 9.3×10^{-4}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
dodecyl methanoate $C_{13}H_{26}O_2$ (dodecyl formate) [28303-42-6] WPSGFSPBRBRLIQ-UHFFFAOYSA-N	6.2×10^{-4} 6.6×10^{-4}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
vinyl methanoate $C_3H_4O_2$ (vinyl formate) [692-45-5] GFJVXXWOPWLRNU-UHFFFAOYSA-N	5.2×10^{-2} 5.2×10^{-2} 1.2×10^{-2} 5.3×10^{-2}		Yaws (2003) Yaws (2003) Dupeux et al. (2022) Gharagheizi et al. (2010)	X X Q Q	258 237 259 246
benzyl methanoate $C_8H_8O_2$ (benzyl formate) [104-57-4] UYWQUFXKFGHYNT-UHFFFAOYSA-N	2.0	7100	Brockbank (2013)	L	1
methyl ethanoate CH_3COOCH_3 (methyl acetate) [79-20-9] KXKVLQRXCPHEJC-UHFFFAOYSA-N	8.5×10^{-2} 2.0×10^{-2} 8.5×10^{-2} 8.1×10^{-2} 8.1×10^{-2} 1.2×10^{-1} 6.6×10^{-2} 8.3×10^{-2} 4.2×10^{-2} 7.7×10^{-2} 7.7×10^{-2} 8.6×10^{-2} 1.1×10^{-1} 8.7×10^{-2}	5900 5000 5900 4800 4900 7500 4500 4900 5000 4800	Burkholder et al. (2019) Burkholder et al. (2015) Brockbank (2013) Plyasunov et al. (2004) Fenclová et al. (2014) Hiatt (2013) Arp and Schmidt (2004) Hovorka et al. (2002) Kaneko et al. (1994) Ioffe et al. (1984) Kieckbusch and King (1979b) Buttery et al. (1969) Butler and Ramchandani (1935) McKeown and Stowell (1927)	L L L L M M M M M M M M M M	498, 1 499, 500 1 1 14 501

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^{-1}		Mackay et al. (2006c)	V	
	1.1×10^{-1}		Mackay et al. (1995)	V	
	4.8×10^{-2}	3300	Djerki and Laub (1988)	V	
	1.1×10^{-1}	4800	Bagno et al. (1991)	T	473
	1.8×10^{-1}		Yaws (2003)	X	258
	9.6×10^{-2}		Dupeux et al. (2022)	Q	259
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	1.7×10^{-1}		Duchowicz et al. (2020)	Q	
	3.4×10^{-2}		Wang et al. (2017)	Q	80, 238
	1.2×10^{-1}		Wang et al. (2017)	Q	80, 239
	2.5×10^{-1}		Wang et al. (2017)	Q	80, 240
	7.3×10^{-2}		Li et al. (2014)	Q	241
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.4×10^{-2}		Hilal et al. (2008)	Q	
	6.0×10^{-2}		Modarresi et al. (2007)	Q	67
		4500	Kühne et al. (2005)	Q	
	8.6×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	5.4×10^{-2}		Yao et al. (2002)	Q	229
	7.0×10^{-2}		English and Carroll (2001)	Q	230, 231
	3.8×10^{-2}		Katritzky et al. (1998)	Q	
	5.6×10^{-2}		Suzuki et al. (1992)	Q	232
	3.9×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	8.6×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		4900	Kühne et al. (2005)	?	
	1.4×10^{-1}		Yaws (1999)	?	21, 12
	8.0×10^{-2}		Abraham et al. (1990)	?	
ethyl ethanoate	6.5×10^{-2}	5600	Burkholder et al. (2019)	L	502, 1
$CH_3COOC_2H_5$	5.9×10^{-2}	5900	Burkholder et al. (2015)	L	
(ethyl acetate)	6.5×10^{-2}	5600	Brockbank (2013)	L	1
[141-78-6]	5.9×10^{-2}	5900	Sander et al. (2011)	L	
XEKOWRVHYACXOJ-UHFFFAOYSA-N	6.3×10^{-2}	5500	Plyasunov et al. (2004)	L	
	5.9×10^{-2}	5200	Kutsuna and Kaneyasu (2021)	M	
	5.2×10^{-2}	4800	Ammari and Schroen (2019)	M	11
	6.2×10^{-2}	5500	Fenclová et al. (2014)	M	1
	5.1×10^{-2}		Aprea et al. (2007)	M	
	5.9×10^{-2}	5900	Kutsuna et al. (2005)	M	
	3.9×10^{-2}		van Ruth et al. (2002)	M	14
	4.1×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 361
	3.0×10^{-2}		van Ruth et al. (2001)	M	14
			Dewulf et al. (1999)	M	362
	6.6×10^{-2}		Druaux et al. (1998)	M	
	3.4×10^{-2}		Welke et al. (1998)	M	
	5.7×10^{-2}		Landy et al. (1995)	M	
	2.8×10^{-2}		Kaneko et al. (1994)	M	14
	4.4×10^{-2}	3900	Kolb et al. (1992)	M	277

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^{-1}		Pividal et al. (1992)	M	80
	4.3×10^{-2}		Guitart et al. (1989)	M	14
	6.2×10^{-2}		Jones et al. (1988)	M	
	4.3×10^{-2}		Richon et al. (1985)	M	38
	1.3×10^{-1}		Ioffe et al. (1984)	M	80
	5.8×10^{-2}	5300	Kieckbusch and King (1979b)	M	501
	5.7×10^{-2}		Nelson and Hoff (1968)	M	297
	7.4×10^{-2}		Butler and Ramchandani (1935)	M	
	7.3×10^{-2}		Mackay et al. (2006c)	V	
	3.1×10^{-2}		Philippe et al. (2003)	V	14
	7.3×10^{-2}		Mackay et al. (1995)	V	
	3.6×10^{-1}		Hwang et al. (1992)	V	
	7.1×10^{-2}		Yaws (2003)	X	258
	4.7×10^{-2}	5700	Janini and Quaddora (1986)	X	298
	3.9×10^{-2}		Nahon et al. (2000)	C	14
	7.8×10^{-2}		Dupeux et al. (2022)	Q	259
	2.2×10^{-2}		Keshavarz et al. (2022)	Q	
	6.9×10^{-2}		Duchowicz et al. (2020)	Q	299
	2.8×10^{-2}		Wang et al. (2017)	Q	80, 238
	6.2×10^{-2}		Wang et al. (2017)	Q	80, 239
	2.5×10^{-1}		Wang et al. (2017)	Q	80, 240
	5.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.6×10^{-2}		Hilal et al. (2008)	Q	
	4.9×10^{-2}		Modarresi et al. (2007)	Q	67
		4800	Kühne et al. (2005)	Q	
	7.3×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	5.4×10^{-2}		Yao et al. (2002)	Q	229
	5.3×10^{-2}		English and Carroll (2001)	Q	230, 231
	4.5×10^{-2}		Katritzky et al. (1998)	Q	
	1.6×10^{-1}		Russell et al. (1992)	Q	279
	4.3×10^{-2}		Suzuki et al. (1992)	Q	232
	4.1×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	7.4×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		5200	Kühne et al. (2005)	?	
	7.1×10^{-2}		Yaws (1999)	?	21
	8.8×10^{-2}		Hoff et al. (1993)	?	21
	5.8×10^{-2}		Abraham et al. (1990)	?	
ethyl ethanoate-1-13C $CH_3COOC_2H_5$ (ethyl acetate-1-13C) [3424-59-7] XEKOWRVHYACXOJ-AZXPZELESA-N	7.1×10^{-2}	6500	Hiatt (2013)	M	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
propyl ethanoate	4.4×10^{-2}	6100	Burkholder et al. (2019)	L	503, 1
$CH_3COOC_3H_7$	4.4×10^{-2}	6000	Brockbank (2013)	L	1
(propyl acetate)	4.5×10^{-2}	5900	Plyasunov et al. (2004)	L	
[109-60-4]	4.5×10^{-2}	5900	Fenclová et al. (2014)	M	1
YKYONYBAUNKHLG-UHFFFAOYSA-N	3.9×10^{-2}		van Ruth et al. (2002)	M	14
	3.0×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 361
	1.8×10^{-2}		van Ruth et al. (2001)	M	14
	3.7×10^{-2}		Welke et al. (1998)	M	
	2.1×10^{-2}		Kaneko et al. (1994)	M	14
	3.1×10^{-2}		Richon et al. (1985)	M	38
	4.5×10^{-2}	5500	Kieckbusch and King (1979b)	M	501
	4.6×10^{-2}		Mackay et al. (2006c)	V	
	4.6×10^{-2}		Mackay et al. (1995)	V	
	5.0×10^{-2}		Hine and Mookerjee (1975)	V	
	5.0×10^{-2}		Butler and Ramchandani (1935)	V	
	3.7×10^{-2}		Yaws (2003)	X	258
	3.7×10^{-2}		Yaws (2003)	X	237
	4.4×10^{-2}	6000	Janini and Quaddora (1986)	X	298
	5.0×10^{-2}		Dupeux et al. (2022)	Q	259
	2.9×10^{-2}		Keshavarz et al. (2022)	Q	
	7.7×10^{-2}		Duchowicz et al. (2020)	Q	
	2.5×10^{-2}		Wang et al. (2017)	Q	80, 238
	3.9×10^{-2}		Wang et al. (2017)	Q	80, 239
	2.1×10^{-1}		Wang et al. (2017)	Q	80, 240
	2.4×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.9×10^{-2}		Hilal et al. (2008)	Q	
	4.2×10^{-2}		Modarresi et al. (2007)	Q	67
	4.6×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	2.6×10^{-2}		Yao et al. (2002)	Q	229
	4.0×10^{-2}		English and Carroll (2001)	Q	230, 231
	4.1×10^{-2}		Katritzky et al. (1998)	Q	
	9.9×10^{-2}		Russell et al. (1992)	Q	279
	3.3×10^{-2}		Suzuki et al. (1992)	Q	232
	3.3×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	4.5×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	3.4×10^{-2}		Yaws (1999)	?	21
	4.5×10^{-2}		Abraham et al. (1990)	?	
methyl methoxyacetate $C_4H_8O_3$ [6290-49-9] QRMHDGWGLNLHMN-UHFFFAOYSA-N	2.5		Hovorka et al. (2002)	M	38

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-propenyl ethanoate	7.6×10^{-2}		HSDB (2015)	V	
$C_5H_8O_2$	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
[591-87-7]	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	244
FWZUNOYOVVKUNF-UHFFFAOYSA-N	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	7.0×10^{-2}		Hilal et al. (2008)	Q	
	8.4×10^{-2}		Modarresi et al. (2007)	Q	67
2-propyl ethanoate	3.3×10^{-2}	6100	Brockbank (2013)	L	1
$CH_3COOC_3H_7$	3.3×10^{-2}	5600	Plyasunov et al. (2004)	L	
(isopropyl acetate)	1.3×10^{-2}		Kaneko et al. (1994)	M	14
[108-21-4]	3.5×10^{-2}		Hine and Mookerjee (1975)	V	
JMMWKPVZQRWMSS-UHFFFAOYSA-N	3.7×10^{-2}		Yaws (2003)	X	258
	2.9×10^{-2}	5500	Janini and Quaddora (1986)	X	298
	4.5×10^{-2}		Dupeux et al. (2022)	Q	259
	2.9×10^{-2}		Keshavarz et al. (2022)	Q	
	3.0×10^{-2}		Duchowicz et al. (2020)	Q	184
	2.6×10^{-2}		Wang et al. (2017)	Q	80, 238
	3.9×10^{-2}		Wang et al. (2017)	Q	80, 239
	1.7×10^{-1}		Wang et al. (2017)	Q	80, 240
	6.0×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-2}		Hilal et al. (2008)	Q	
	2.8×10^{-2}		Modarresi et al. (2007)	Q	67
	4.6×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	3.3×10^{-2}		Yao et al. (2002)	Q	229
	3.9×10^{-2}		English and Carroll (2001)	Q	230, 274
	4.2×10^{-2}		Katritzky et al. (1998)	Q	
	2.9×10^{-2}		Suzuki et al. (1992)	Q	232
	2.9×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	3.6×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	3.6×10^{-2}		Yaws (1999)	?	21
	3.5×10^{-2}		Abraham et al. (1990)	?	
2-methoxyethyl ethanoate	3.0		Hovorka et al. (2002)	M	38
$C_5H_{10}O_3$	9.0		HSDB (2015)	V	
(methyl cellosolve acetate)					
[110-49-6]					
XLLIQLLCWZCATF-UHFFFAOYSA-N					
glycerol monoacetate	2.4×10^{4}		HSDB (2015)	Q	99
$C_5H_{10}O_4$					
(acetin)					
[26446-35-5]					
KMZHZAAOEWVPSE-UHFFFAOYSA-N					
1-propen-2-ol, acetate	5.5×10^{-3}		HSDB (2015)	Q	99
$C_5H_8O_2$					
(isopropenyl acetate)					
[108-22-5]					
HETCEOQFVDFGSY-UHFFFAOYSA-N					

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
butyl ethanoate	3.8×10^{-2}	6300	Brockbank (2013)	L	1
$CH_3COOC_4H_9$	3.5×10^{-2}	6300	Plyasunov et al. (2004)	L	
(butyl acetate)	2.4×10^{-2}		Kim and Kim (2014)	M	
[123-86-4]	3.5×10^{-2}	6300	Fenclová et al. (2014)	M	1
DKPFZGUDAPQIHT-UHFFFAOYSA-N	2.1×10^{-2}		Helburn et al. (2008)	M	
	2.8×10^{-2}		van Ruth et al. (2002)	M	14
	2.3×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 361
	1.7×10^{-2}		van Ruth et al. (2001)	M	14
	2.7×10^{-2}		Welke et al. (1998)	M	
	1.3×10^{-2}		Kaneko et al. (1994)	M	14
	2.3×10^{-2}	4300	Kolb et al. (1992)	M	277
	3.5×10^{-2}	7100	Ioffe et al. (1984)	M	
	3.5×10^{-2}	6000	Kieckbusch and King (1979b)	M	501
	3.2×10^{-2}		Mackay et al. (2006c)	V	
	3.2×10^{-2}		Mackay et al. (1995)	V	
	2.7×10^{-2}		Hwang et al. (1992)	V	
	3.0×10^{-2}		Hine and Mookerjee (1975)	V	
	4.2×10^{-2}		Yaws (2003)	X	258
	3.5×10^{-2}	7500	Janini and Quaddora (1986)	X	298
	2.1×10^{-2}	3200	Goldstein (1982)	X	298
	4.3×10^{-2}		Dupeux et al. (2022)	Q	259
	3.9×10^{-2}		Keshavarz et al. (2022)	Q	
	8.2×10^{-2}		Duchowicz et al. (2020)	Q	
	2.0×10^{-2}		Wang et al. (2017)	Q	80, 238
	2.9×10^{-2}		Wang et al. (2017)	Q	80, 239
	1.7×10^{-1}		Wang et al. (2017)	Q	80, 240
	1.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.3×10^{-2}		Hilal et al. (2008)	Q	
	3.0×10^{-2}		Modarresi et al. (2007)	Q	67
		5500	Kühne et al. (2005)	Q	
	3.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.4×10^{-2}		Yao et al. (2002)	Q	229, 267
	3.1×10^{-2}		English and Carroll (2001)	Q	230, 231
	4.1×10^{-2}		Katritzky et al. (1998)	Q	
	5.3×10^{-2}		Russell et al. (1992)	Q	358
	1.6×10^{-2}		Suzuki et al. (1992)	Q	232
	2.6×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	3.5×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		5300	Kühne et al. (2005)	?	
	3.8×10^{-2}		Yaws (1999)	?	21
	3.5×10^{-2}		Abraham et al. (1990)	?	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-butyl ethanoate	2.3×10^{-2}	6000	Brockbank (2013)	L	1
$C_6H_{12}O_2$	2.3×10^{-2}	6200	Plyasunov et al. (2004)	L	
(*sec*-butyl acetate)	2.3×10^{-2}		HSDB (2015)	V	
[105-46-4]	2.4×10^{-2}		Yaws (2003)	X	258
DCKVNWZUADLDEH-UHFFFAOYSA-N	2.4×10^{-2}		Yaws (2003)	X	237, 12
	2.5×10^{-2}		Dupeux et al. (2022)	Q	259
	2.3×10^{-2}		Wang et al. (2017)	Q	80, 238
	2.6×10^{-2}		Wang et al. (2017)	Q	80, 239
	1.2×10^{-1}		Wang et al. (2017)	Q	80, 240
	2.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.9×10^{-2}		Modarresi et al. (2007)	Q	67
	2.4×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.7×10^{-2}		Yao et al. (2002)	Q	229
			Katritzky et al. (1998)	Q	504
	1.8×10^{-2}		Yaws (1999)	?	21, 12
1,1-dimethylethyl ethanoate	1.2×10^{-2}	6100	Brockbank (2013)	L	1
$C_6H_{12}O_2$	1.1×10^{-2}	5600	Plyasunov et al. (2004)	L	
(*tert*-butyl acetate)	1.1×10^{-2}		Duchowicz et al. (2020)	V	186
[540-88-5]	3.2×10^{-2}		Yaws (2003)	X	258
WMOVHXAZOJBABW-UHFFFAOYSA-N	3.2×10^{-2}		Yaws (2003)	X	237
	2.6×10^{-2}		Dupeux et al. (2022)	Q	259
	1.4×10^{-2}		Duchowicz et al. (2020)	Q	
	1.4×10^{-2}		Wang et al. (2017)	Q	80, 238
	1.6×10^{-2}		Wang et al. (2017)	Q	80, 239
	7.4×10^{-2}		Wang et al. (2017)	Q	80, 240
	2.4×10^{-2}		HSDB (2015)	Q	99
	5.8×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.2×10^{-2}		Modarresi et al. (2007)	Q	67
	1.9×10^{-2}		Yao et al. (2002)	Q	229
	2.9×10^{-2}		Yaws (1999)	?	21
2-methylpropyl ethanoate	2.6×10^{-2}	6000	Brockbank (2013)	L	1
$CH_3COOC_4H_9$	2.4×10^{-2}	6200	Plyasunov et al. (2004)	L	
(isobutyl acetate)	1.0×10^{-2}		Kaneko et al. (1994)	M	14
[110-19-0]	1.9×10^{-2}		Mackay et al. (2006c)	V	
GJRQTCIYDGXPES-UHFFFAOYSA-N	1.9×10^{-2}		Mackay et al. (1995)	V	
	2.2×10^{-2}		Hine and Mookerjee (1975)	V	
	3.7×10^{-2}		Yaws (2003)	X	258
	2.3×10^{-2}		Yaws (2003)	X	237
	3.7×10^{-2}		Dupeux et al. (2022)	Q	259
	3.9×10^{-2}		Keshavarz et al. (2022)	Q	
	3.2×10^{-2}		Duchowicz et al. (2020)	Q	184
	1.0×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.7×10^{-2}		Hilal et al. (2008)	Q	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.2×10^{-2}		Modarresi et al. (2007)	Q	67
		5500	Kühne et al. (2005)	Q	
	1.8×10^{-2}		Yao et al. (2002)	Q	229
	3.1×10^{-2}		English and Carroll (2001)	Q	230, 231
	9.5×10^{-2}		Russell et al. (1992)	Q	279
	2.3×10^{-2}		Suzuki et al. (1992)	Q	232
	2.2×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.2×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		4600	Kühne et al. (2005)	?	
	2.3×10^{-2}		Yaws (1999)	?	21
	2.2×10^{-2}		Abraham et al. (1990)	?	
pentyl ethanoate	2.5×10^{-2}	7200	Brockbank (2013)	L	1
$CH_3COOC_5H_{11}$	2.7×10^{-2}	6700	Plyasunov et al. (2004)	L	
(amyl acetate)	1.3×10^{-1}	5000	Meynier et al. (2003)	M	38
[628-63-7]	9.3×10^{-3}		Kaneko et al. (1994)	M	14
PGMYKACGEOXYJE-UHFFFAOYSA-N	3.4×10^{-2}		Hellmann (1987)	M	87
	2.8×10^{-2}	6500	Kieckbusch and King (1979b)	M	501
	2.4×10^{-2}		Mackay et al. (2006c)	V	
	2.4×10^{-2}		Mackay et al. (1995)	V	
	2.5×10^{-2}		Hine and Mookerjee (1975)	V	
	2.8×10^{-2}		Yaws (2003)	X	258
	2.8×10^{-2}		Yaws (2003)	X	237
	2.5×10^{-2}		Meynier et al. (2003)	C	
	3.3×10^{-2}		Dupeux et al. (2022)	Q	259
	5.3×10^{-2}		Keshavarz et al. (2022)	Q	
	8.6×10^{-2}		Duchowicz et al. (2020)	Q	
	1.4×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.0×10^{-2}		Hilal et al. (2008)	Q	
	2.8×10^{-2}		Modarresi et al. (2007)	Q	67
	2.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.1×10^{-2}		Yao et al. (2002)	Q	229, 267
	2.3×10^{-2}		English and Carroll (2001)	Q	230, 260
	3.8×10^{-2}		Katritzky et al. (1998)	Q	
	2.1×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	2.6×10^{-2}		Russell et al. (1992)	Q	279
	1.9×10^{-2}		Suzuki et al. (1992)	Q	232
	2.1×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.3×10^{-2}		Taft et al. (1985)	Q	
	2.5×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	2.9×10^{-2}		Yaws (1999)	?	21
	2.8×10^{-2}		Abraham et al. (1990)	?	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methylbutyl ethanoate	2.8×10^{-2}		Yaws (2003)	X	237
$C_7H_{14}O_2$	7.4×10^{-3}		Gharagheizi et al. (2012)	Q	
(2-methylbutyl acetate)	2.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
[624-41-9]					
XHIUFYZDQBSEMF-UHFFFAOYSA-N					
1,2-dimethylpropyl ethanoate	2.9×10^{-2}		Yaws (2003)	X	237
$C_7H_{14}O_2$	1.2×10^{-2}		Gharagheizi et al. (2012)	Q	
(1,2-dimethylpropyl acetate)	2.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
[5343-96-4]					
ZLSXRPTWWRGMTJ-UHFFFAOYSA-N					
1-ethylpropyl ethanoate	1.3×10^{-2}		Gharagheizi et al. (2012)	Q	
$C_7H_{14}O_2$					
(1-ethylpropyl acetate)					
[620-11-1]					
PBKYSIMDORTIEU-UHFFFAOYSA-N					
1,1-dimethylpropyl ethanoate	2.9×10^{-2}		Yaws (2003)	X	258
$C_7H_{14}O_2$	2.9×10^{-2}		Yaws (2003)	X	237
(*tert*-pentyl acetate)	2.0×10^{-2}		Dupeux et al. (2022)	Q	259
[625-16-1]	3.3×10^{-2}		Gharagheizi et al. (2012)	Q	
JCCIFDCPHCKATH-UHFFFAOYSA-N	2.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
2,2-dimethylpropyl ethanoate	2.6×10^{-2}		Yaws (2003)	X	237
$C_7H_{14}O_2$	2.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
(neopentyl acetate)					
[926-41-0]					
QLNYTCSELYEEPV-UHFFFAOYSA-N					
1,2-propanediol, diacetate	7.0×10^{1}		HSDB (2015)	Q	99
$C_7H_{12}O_4$					
[623-84-7]					
MLHOXUWWKVQEJB-UHFFFAOYSA-N					
2-pentanol, acetate	1.2×10^{-2}		HSDB (2015)	Q	99
$C_7H_{14}O_2$	1.9×10^{-2}		Gharagheizi et al. (2012)	Q	
[626-38-0]					
GQKZRWSUJHVIPE-UHFFFAOYSA-N					
3-methylbutyl ethanoate	2.1×10^{-2}	6700	Brockbank (2013)	L	1
$CH_3COOC_5H_{11}$	2.0×10^{-2}	6500	Plyasunov et al. (2004)	L	
(isoamyl acetate)	2.2×10^{-2}	6600	Ammari and Schroen (2019)	M	11
[123-92-2]	8.8×10^{-2}	4300	Meynier et al. (2003)	M	38
MLFHJEHSLIIPHL-UHFFFAOYSA-N	8.8×10^{-3}		Kaneko et al. (1994)	M	14
	2.6×10^{-2}		Mackay et al. (2006c)	V	
	2.6×10^{-2}		Mackay et al. (1995)	V	
	2.1×10^{-2}		Meylan and Howard (1991)	V	
	1.7×10^{-2}		Hine and Mookerjee (1975)	V	
	2.2×10^{-2}		Yaws (2003)	X	237
	2.4×10^{-2}	5000	Goldstein (1982)	X	298

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.7×10^{-2}		Meynier et al. (2003)	C	
	5.3×10^{-2}		Keshavarz et al. (2022)	Q	
	7.0		Abney (2021)	Q	399
	3.3×10^{-2}		Duchowicz et al. (2020)	Q	299
	1.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.6×10^{-2}		Hilal et al. (2008)	Q	
	3.2×10^{-2}		Modarresi et al. (2007)	Q	67
	1.8×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.6×10^{-2}		Yao et al. (2002)	Q	229
	2.4×10^{-2}		English and Carroll (2001)	Q	230, 231
	3.8×10^{-2}		Katritzky et al. (1998)	Q	
	1.7×10^{-2}		Suzuki et al. (1992)	Q	232
	1.8×10^{-2}		Meylan and Howard (1991)	Q	
	1.8×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.7×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	2.1×10^{-2}		Yaws (1999)	?	21
	1.7×10^{-2}		Abraham et al. (1990)	?	
hexyl ethanoate $CH_3COOC_6H_{13}$ (hexyl acetate) [142-92-7] AOGQPLXWSUTHQB-UHFFFAOYSA-N	2.0×10^{-2}	7100	Brockbank (2013)	L	1, 505
	1.7×10^{-2}	7300	Plyasunov et al. (2004)	L	
	1.4×10^{-2}		Souchon et al. (2004)	M	
	1.5×10^{-2}		Karl et al. (2003)	M	
	5.2×10^{-3}		Mackay et al. (2006c)	V	
	5.2×10^{-3}		Mackay et al. (1995)	V	
	1.8×10^{-2}		Hine and Mookerjee (1975)	V	
	2.0×10^{-2}		Yaws (2003)	X	258
	2.0×10^{-2}		Yaws (2003)	X	237
	3.6×10^{-2}		Dupeux et al. (2022)	Q	259
	7.1×10^{-2}		Keshavarz et al. (2022)	Q	
	8.9×10^{-2}		Duchowicz et al. (2020)	Q	184
	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
	1.4×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	67
	2.0×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.0×10^{-2}		Yao et al. (2002)	Q	229, 267
	1.7×10^{-2}		English and Carroll (2001)	Q	230, 231
	3.6×10^{-2}		Katritzky et al. (1998)	Q	
	9.9×10^{-3}		Russell et al. (1992)	Q	279
	1.5×10^{-2}		Suzuki et al. (1992)	Q	232
	2.2×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	2.0×10^{-2}		Yaws (1999)	?	21
	1.8×10^{-2}		Abraham et al. (1990)	?	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
4-methyl-2-pentyl ethanoate	1.7×10^{-2}		HSDB (2015)	V	
$C_8H_{16}O_2$	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
(4-methyl-2-pentyl acetate)	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
[108-84-9]	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
CPIVYSAVIPTCCX-UHFFFAOYSA-N	1.1×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	67
	1.8×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	3.4×10^{-2}		Katritzky et al. (1998)	Q	
cyclohexyl ethanoate	1.0×10^{-1}	7000	Brockbank (2013)	L	1, 506
$C_8H_{14}O_2$	8.2×10^{-2}		HSDB (2015)	Q	99
(cyclohexyl acetate)					
[622-45-7]					
YYLLIJHXUHJATK-UHFFFAOYSA-N					
ethanol, 2-(2-ethoxyethoxy)-, acetate	4.3×10^{2}		HSDB (2015)	V	
$C_8H_{16}O_4$					
(diethylene glycol monoethyl ether acetate)					
[112-15-2]					
FPZWZCWUIYYYBU-UHFFFAOYSA-N					
phenyl ethanoate	1.3	7200	Brockbank (2013)	L	1
$C_8H_8O_2$	1.5×10^{-1}		HSDB (2015)	Q	99
(phenyl acetate)					
[122-79-2]					
IPBVNPXQWQGGJP-UHFFFAOYSA-N					
heptyl ethanoate	1.2×10^{-2}		Yaws (2003)	X	258
$C_9H_{18}O_2$	1.1×10^{-2}		Yaws (2003)	X	237
(heptyl acetate)	2.4×10^{-2}		Dupeux et al. (2022)	Q	259
[112-06-1]	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
ZCZSIDMEHXZRLG-UHFFFAOYSA-N	1.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
			Brockbank (2013)	W	507
phenylmethyl ethanoate	8.5×10^{-1}	6800	Brockbank (2013)	L	1
$C_9H_{10}O_2$	8.7×10^{-1}		Duchowicz et al. (2020)	V	186
(benzyl acetate)	9.0×10^{-1}		HSDB (2015)	V	
[140-11-4]	7.6×10^{-1}		Dupeux et al. (2022)	Q	259
QUKGYYKBILRGFE-UHFFFAOYSA-N	5.2×10^{-1}		Duchowicz et al. (2020)	Q	
	7.0×10^{-1}		Modarresi et al. (2007)	Q	67
	9.2×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	5.4×10^{-1}		Katritzky et al. (1998)	Q	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
octyl ethanoate	8.6×10^{-3}		Yaws (2003)	X	258
$CH_3COOC_8H_{17}$	8.6×10^{-3}		Yaws (2003)	X	237
(octyl acetate)	1.8×10^{-2}		Dupeux et al. (2022)	Q	259
[112-14-1]	1.2×10^{-2}		Gharagheizi et al. (2012)	Q	
YLYBTZIQSIBWLI-UHFFFAOYSA-N	1.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
			Brockbank (2013)	W	508
2-ethylhexyl ethanoate	1.1×10^{-2}		Mackay et al. (2006c)	V	
$C_{10}H_{20}O_2$	1.1×10^{-2}		Mackay et al. (1995)	V	
(2-ethylhexyl acetate)	1.3×10^{-2}		Yaws (2003)	X	237
[103-09-3]	6.6×10^{-3}		HSDB (2015)	Q	99
WOYWLLHHWAMFCB-UHFFFAOYSA-N	2.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
	9.8×10^{-3}		Yao et al. (2002)	Q	229
	1.3×10^{-2}		Yaws (1999)	?	21
nonyl ethanoate	4.1×10^{-2}		Yaws (2003)	X	258
$C_{11}H_{22}O_2$	2.1×10^{-2}		Dupeux et al. (2022)	Q	259
(nonyl acetate)					
[143-13-5]					
GJQIMXVRFNLMTB-UHFFFAOYSA-N					
decyl ethanoate	2.8×10^{-3}		Yaws (2003)	X	258
$C_{12}H_{24}O_2$	1.2×10^{-2}		Dupeux et al. (2022)	Q	259
(decyl acetate)	8.0×10^{-3}		Gharagheizi et al. (2012)	Q	
[112-17-4]					
NUPSHWCALHZGOV-UHFFFAOYSA-N					
undecyl ethanoate	1.5×10^{-2}		Gharagheizi et al. (2012)	Q	
$C_{13}H_{26}O_2$					
(undecyl acetate)					
[1731-81-3]					
CKQGCFFDQIFZFA-UHFFFAOYSA-N					
ethanol, 2,2'-[1,2-ethanediylbis(oxy)]bis-, diacetate	3.7×10^{7}		HSDB (2015)	Q	99
$C_{10}H_{18}O_6$					
(triethylene glycol, diacetate)					
[111-21-7]					
OVOUKWFJRHALDD-UHFFFAOYSA-N					
1-methoxy-2-propyl ethanoate	2.9		Duchowicz et al. (2020)	V	186
$C_6H_{12}O_3$	8.7×10^{-1}		Duchowicz et al. (2020)	Q	
(1-methoxy-2-propyl acetate)	2.5		Raventos-Duran et al. (2010)	Q	242, 243
[108-65-6]	1.6		Raventos-Duran et al. (2010)	Q	244
LLHKCFNBLRBOGN-UHFFFAOYSA-N	2.5		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-1}		Hilal et al. (2008)	Q	
	6.3×10^{-1}		Modarresi et al. (2007)	Q	67

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-ethoxyethyl ethanoate	3.0		Brockbank (2013)	L	
$C_6H_{12}O_3$	3.0		Hovorka et al. (2002)	M	38
(2-ethoxyethyl acetate)	1.5		Johanson and Dynésius (1988)	M	14
[111-15-9]	3.4		Keshavarz et al. (2022)	Q	
SVONRAPFKPVNKG-UHFFFAOYSA-N	7.5×10^{-1}		Duchowicz et al. (2020)	Q	184
	2.5		Raventos-Duran et al. (2010)	Q	242, 243
	2.5		Raventos-Duran et al. (2010)	Q	244
	2.5		Raventos-Duran et al. (2010)	Q	245
	1.9		Hilal et al. (2008)	Q	
	7.2×10^{-1}		Modarresi et al. (2007)	Q	67
	3.1		Duchowicz et al. (2020)	?	185, 21
	7.0		Yaws (1999)	?	21, 12
2-butoxyethyl ethanoate	1.8		Brockbank (2013)	L	
$C_8H_{16}O_3$	1.8	25000	Kim et al. (2000)	M	
(butyl cellosolve acetate)	6.1		Keshavarz et al. (2022)	Q	
[112-07-2]	9.6×10^{-1}		Duchowicz et al. (2020)	Q	299
NQBXSWAWVZHKBZ-UHFFFAOYSA-N	1.2		Raventos-Duran et al. (2010)	Q	242, 243
	1.6		Raventos-Duran et al. (2010)	Q	244
	1.6		Raventos-Duran et al. (2010)	Q	245
	1.3		Hilal et al. (2008)	Q	
	5.2×10^{-1}		Modarresi et al. (2007)	Q	67
	1.8		Duchowicz et al. (2020)	?	185, 21
2-(2-butoxyethoxy)-ethanol, ethanoate	2.8×10^{1}		Duchowicz et al. (2020)	V	186
$C_{10}H_{20}O_4$	2.8×10^{1}		HSDB (2015)	V	
[124-17-4]	1.1×10^{1}		Duchowicz et al. (2020)	Q	
VXQBJTKSVGFQOL-UHFFFAOYSA-N	6.2×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	4.1×10^{1}		Hilal et al. (2008)	Q	
	7.2		Modarresi et al. (2007)	Q	67
1,2-ethanediol, diethanoate	1.2×10^{2}		Duchowicz et al. (2020)	V	186
$C_6H_{10}O_4$	1.2×10^{2}		HSDB (2015)	V	
[111-55-7]	1.3×10^{2}		Yaws (2003)	X	237, 87
JTXMVXSTHSMVQF-UHFFFAOYSA-N	6.4		Duchowicz et al. (2020)	Q	
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	245
	1.4×10^{2}		Gharagheizi et al. (2010)	Q	246
	1.3×10^{1}		Hilal et al. (2008)	Q	
	9.3×10^{1}		Yaws (1999)	?	21, 87
geranyl acetate	4.1×10^{-3}		HSDB (2015)	Q	99
$C_{12}H_{20}O_2$					
[105-87-3]					
HIGQPQRQIQDZMP-DHZHZOJOSA-N					

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
linalyl acetate	1.8×10^{-2}		Dupeux et al. (2022)	Q	259
$C_{12}H_{20}O_2$	5.8×10^{-3}		HSDB (2015)	Q	99
[115-95-7]					
UWKAYLJWKGQEPM-UHFFFAOYSA-N					
cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate	1.2×10^{-2}		HSDB (2015)	Q	99
$C_{12}H_{22}O_2$					
(menthyl acetate)					
[16409-45-3]					
XHXUANMFYXWVNG-UHFFFAOYSA-N					
methyl propanoate	5.8×10^{-2}	5700	Brockbank (2013)	L	1
$C_2H_5COOCH_3$	5.5×10^{-2}	5400	Plyasunov et al. (2004)	L	
(methyl propionate)	5.2×10^{-2}		Ioffe et al. (1984)	M	
[554-12-1]	5.7×10^{-2}		Buttery et al. (1969)	M	
RJUFJBKOKNCXHH-UHFFFAOYSA-N	6.1×10^{-2}		Mackay et al. (2006c)	V	
	6.1×10^{-2}		Mackay et al. (1995)	V	
	1.3×10^{-1}	3900	Djerki and Laub (1988)	V	
	6.1×10^{-2}		Hine and Mookerjee (1975)	V	
	5.4×10^{-2}	5400	Bagno et al. (1991)	T	473
	2.2×10^{-2}		Keshavarz et al. (2022)	Q	
	2.0×10^{-1}		Duchowicz et al. (2020)	Q	184
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	5.2×10^{-2}		Modarresi et al. (2007)	Q	67
	5.8×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	5.3×10^{-2}		Yao et al. (2002)	Q	229
	5.3×10^{-2}		English and Carroll (2001)	Q	230, 231
	3.9×10^{-2}		Katritzky et al. (1998)	Q	
	4.4×10^{-2}		Suzuki et al. (1992)	Q	232
	4.0×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	5.7×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	5.2×10^{-2}		Yaws (1999)	?	21
	5.8×10^{-2}	5000	Betterton (1992)	?	509
	5.7×10^{-2}		Abraham et al. (1990)	?	
methyl 2-hydroxypropanoate	9.1	5000	Sanz and Gmehling (2005)	M	
$C_4H_8O_3$	4.7		Wang et al. (2017)	Q	80, 238
(methyl lactate)	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
[547-64-8]	1.4×10^{1}		Wang et al. (2017)	Q	80, 240
LPEKGGXMPWTOCB-UHFFFAOYSA-N	1.2×10^{3}		HSDB (2015)	Q	99

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethyl propanoate	3.8×10^{-2}	5900	Brockbank (2013)	L	1
$C_2H_5COOC_2H_5$	4.1×10^{-2}	6000	Plyasunov et al. (2004)	L	
(ethyl propionate)	4.1×10^{-2}	5900	Fenclová et al. (2014)	M	1
[105-37-3]	3.9×10^{-2}		Duchowicz et al. (2020)	V	186
FKRCODPIKNYEAC-UHFFFAOYSA-N	3.9×10^{-2}		HSDB (2015)	V	
	3.8×10^{-2}		Mackay et al. (2006c)	V	
	3.8×10^{-2}		Mackay et al. (1995)	V	
	3.7×10^{-2}		Abraham (1984)	V	
	4.5×10^{-2}		Hine and Mookerjee (1975)	V	
	4.5×10^{-2}		Yaws (2003)	X	258
	4.5×10^{-2}		Yaws (2003)	X	237
	4.1×10^{-2}		Dupeux et al. (2022)	Q	259
	7.7×10^{-2}		Duchowicz et al. (2020)	Q	
	4.5×10^{-2}		Li et al. (2014)	Q	241
	2.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.6×10^{-2}		Hilal et al. (2008)	Q	
	4.4×10^{-2}		Modarresi et al. (2007)	Q	67
	4.6×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	3.5×10^{-2}		Yao et al. (2002)	Q	229
	4.0×10^{-2}		English and Carroll (2001)	Q	230, 231
	3.9×10^{-2}		Katritzky et al. (1998)	Q	
	3.4×10^{-2}		Suzuki et al. (1992)	Q	232
	3.5×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	4.5×10^{-2}		Yaws (1999)	?	21
	3.8×10^{-2}		Abraham et al. (1990)	?	
propyl propanoate	2.6×10^{-2}	6400	Brockbank (2013)	L	1, 510
$C_2H_5COOC_3H_7$	2.9×10^{-2}	6200	Plyasunov et al. (2004)	L	
(propyl propionate)	2.5×10^{-2}		Duchowicz et al. (2020)	V	186
[106-36-5]	2.5×10^{-2}		Abraham (1984)	V	
MCSINKKTEDDPNK-UHFFFAOYSA-N	2.5×10^{-2}		Hine and Mookerjee (1975)	V	
	8.2×10^{-2}		Duchowicz et al. (2020)	Q	
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-2}		Hilal et al. (2008)	Q	
	3.6×10^{-2}		Modarresi et al. (2007)	Q	67
	2.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.6×10^{-2}		Yao et al. (2002)	Q	229
	3.1×10^{-2}		English and Carroll (2001)	Q	230, 274
	3.9×10^{-2}		Katritzky et al. (1998)	Q	
	2.6×10^{-2}		Suzuki et al. (1992)	Q	232
	2.8×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.1×10^{-2}		Yaws (1999)	?	21

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.5×10^{-2}		Abraham et al. (1990)	?	
isopropyl propanoate	1.8×10^{-2}		Plyasunov et al. (2004)	L	
$C_2H_5COOC_3H_7$	1.7×10^{-2}		Duchowicz et al. (2020)	V	186
(isopropyl propionate)	1.7×10^{-2}		Meylan and Howard (1991)	V	
[637-78-5]	1.7×10^{-2}		Hine and Mookerjee (1975)	V	
IJMWOMHMDSDKGK-UHFFFAOYSA-N	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	1.7×10^{-2}		Hilal et al. (2008)	Q	
	3.1×10^{-2}		Modarresi et al. (2007)	Q	67
	2.3×10^{-2}		Suzuki et al. (1992)	Q	232
	2.4×10^{-2}		Meylan and Howard (1991)	Q	
	2.5×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.7×10^{-2}		Abraham et al. (1990)	?	
butyl propanoate	2.2×10^{-2}	6900	Brockbank (2013)	L	1
$C_7H_{14}O_2$	2.0×10^{-2}	7000	Plyasunov et al. (2004)	L	
(butyl propionate)	2.0×10^{-2}		Duchowicz et al. (2020)	V	186
[590-01-2]	3.3×10^{-2}		Yaws (2003)	X	258
BTMVHUNTONAYDX-UHFFFAOYSA-N	3.3×10^{-2}		Yaws (2003)	X	237, 12
	2.6×10^{-2}		Dupeux et al. (2022)	Q	259
	8.6×10^{-2}		Duchowicz et al. (2020)	Q	
	8.9×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
	3.2×10^{-2}		Modarresi et al. (2007)	Q	67
	6.2×10^{-3}		Yaffe et al. (2003)	Q	248, 272
	2.3×10^{-2}		Yao et al. (2002)	Q	229
	3.7×10^{-2}		Katritzky et al. (1998)	Q	
	1.4×10^{-2}		Yaws (1999)	?	21
(2-methylpropyl)-propanoate	1.5×10^{-2}	6600	Plyasunov et al. (2004)	L	
$C_7H_{14}O_2$	1.5×10^{-2}		Duchowicz et al. (2020)	V	186
(isobutyl propionate)	3.3×10^{-2}		Duchowicz et al. (2020)	Q	
[540-42-1]	1.8×10^{-2}		Hilal et al. (2008)	Q	
FZXRXKLUIMKDEL-UHFFFAOYSA-N		5900	Kühne et al. (2005)	Q	
	6.2×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.9×10^{-2}		Nirmalakhandan et al. (1997)	Q	
		7300	Kühne et al. (2005)	?	
tert-butyl propanoate	7.5×10^{-3}		Ebert et al. (2023)	?	365
$C_7H_{14}O_2$					
[20487-40-5]					
JAELLLITIZHOGQ-UHFFFAOYSA-N					
pentyl propanoate	1.9×10^{-2}		Plyasunov et al. (2004)	L	
$C_2H_5COOC_5H_{11}$	1.2×10^{-2}		Duchowicz et al. (2020)	V	186
(amyl propionate)	1.4×10^{-2}		Abraham (1984)	V	
[624-54-4]	1.2×10^{-2}		Hine and Mookerjee (1975)	V	
TWSRVQVEYJNFKQ-UHFFFAOYSA-N	8.9×10^{-2}		Duchowicz et al. (2020)	Q	
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	2.6×10^{-2}		Modarresi et al. (2007)	Q	67
	1.2×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.7×10^{-2}		English and Carroll (2001)	Q	230, 231
	3.4×10^{-2}		Katritzky et al. (1998)	Q	
	2.2×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	1.5×10^{-2}		Suzuki et al. (1992)	Q	232
	1.8×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.4×10^{-2}		Abraham et al. (1990)	?	
propanoic acid, 2-hydroxy-, ethyl ester $C_5H_{10}O_3$ (ethyl lactate) [97-64-3] LZCLXQDLBQLTDK-UHFFFAOYSA-N	1.7×10^{1}		Duchowicz et al. (2020)	V	186
	1.7×10^{1}		HSDB (2015)	V	
	3.1		Duchowicz et al. (2020)	Q	
ethyl 3-ethoxypropanoate $C_7H_{14}O_3$ (ethyl 3-ethoxypropionate) [763-69-9] BHXIWUJLHYHGSJ-UHFFFAOYSA-N	1.5×10^{-2}		Yaws (1999)	?	21
propanoic acid, 2-phenylethyl ester $C_{11}H_{14}O_2$ [122-70-3] HVGZQCSMLUDISR-UHFFFAOYSA-N	3.9×10^{-1}		HSDB (2015)	Q	99
methyl butanoate $C_3H_7COOCH_3$ (methyl butyrate) [623-42-7] UUIQMZJEGPQKFD-UHFFFAOYSA-N	3.9×10^{-2}	5700	Brockbank (2013)	L	1, 511
	4.2×10^{-2}	5700	Plyasunov et al. (2004)	L	
	3.7×10^{-2}		Aprea et al. (2007)	M	
	3.6×10^{-2}		Ioffe et al. (1984)	M	
	4.8×10^{-2}		Buttery et al. (1969)	M	
	3.6×10^{-1}	4400	Djerki and Laub (1988)	V	
	3.7×10^{-2}		Amoore and Buttery (1978)	V	
		5800	Della Gatta et al. (1981)	T	
	3.5×10^{-2}		Yaws (2003)	X	258
	3.6×10^{-2}		Nahon et al. (2000)	C	14
	4.4×10^{-2}		Dupeux et al. (2022)	Q	259
	2.9×10^{-2}		Keshavarz et al. (2022)	Q	
	2.3×10^{-1}		Duchowicz et al. (2020)	Q	299
	4.8×10^{-2}		Li et al. (2014)	Q	241
	1.2×10^{-2}		Ghargheizi et al. (2012)	Q	
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.8×10^{-2}		Hilal et al. (2008)	Q	
	4.0×10^{-2}		Modarresi et al. (2007)	Q	67

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.6×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	3.2×10^{-2}		Yao et al. (2002)	Q	229
	4.0×10^{-2}		English and Carroll (2001)	Q	230, 231
	3.9×10^{-2}		Katritzky et al. (1998)	Q	
	1.5×10^{-1}		Russell et al. (1992)	Q	279
	3.4×10^{-2}		Suzuki et al. (1992)	Q	232
	3.2×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	4.8×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	3.5×10^{-2}		Yaws (1999)	?	21
	4.8×10^{-2}		Abraham et al. (1990)	?	
ethyl butanoate $C_3H_7COOC_2H_5$ (ethyl butyrate) [105-54-4] OBNCKNCVKJNDBV-UHFFFAOYSA-N	2.5×10^{-2}	6100	Brockbank (2013)	L	1
	2.9×10^{-2}	6300	Plyasunov et al. (2004)	L	
	2.9×10^{-2}	6400	Fenclová et al. (2014)	M	1
	2.4×10^{-2}		Aprea et al. (2007)	M	
	2.6×10^{-2}		Souchon et al. (2004)	M	
	2.1×10^{-2}		van Ruth et al. (2002)	M	14
	2.1×10^{-2}		van Ruth and Villeneuve (2002)	M	14, 361
	1.6×10^{-2}		van Ruth et al. (2001)	M	14
	4.0×10^{-2}		Landy et al. (1996)	M	
	2.4×10^{-2}		Landy et al. (1995)	M	
	2.5×10^{-2}		HSDB (2015)	V	
	2.4×10^{-2}		Mackay et al. (2006c)	V	
	1.2×10^{-2}		Philippe et al. (2003)	V	14
	2.4×10^{-2}		Mackay et al. (1995)	V	
	2.8×10^{-2}		Abraham (1984)	V	
	2.7×10^{-2}		Hine and Mookerjee (1975)	V	
	2.8×10^{-2}		Yaws (2003)	X	258
	2.8×10^{-2}		Yaws (2003)	X	237, 87
	2.7×10^{-2}		Nahon et al. (2000)	C	14
	4.5×10^{-2}		Dupeux et al. (2022)	Q	259
	3.4		Abney (2021)	Q	399
	2.4×10^{-2}		Savary et al. (2014)	Q	
	1.6×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.0×10^{-2}		Hilal et al. (2008)	Q	
	3.1×10^{-2}		Modarresi et al. (2007)	Q	67
	2.7×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	2.8×10^{-2}		Yao et al. (2002)	Q	229
	3.1×10^{-2}		English and Carroll (2001)	Q	230, 231
	3.9×10^{-2}		Katritzky et al. (1998)	Q	
	2.6×10^{-2}		Suzuki et al. (1992)	Q	232
	2.8×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.4×10^{-2}		Yaws (1999)	?	21, 87
	2.7×10^{-2}		Abraham et al. (1990)	?	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
propyl butanoate	1.8×10^{-2}	6400	Brockbank (2013)	L	1
$C_3H_7COOC_3H_7$	2.2×10^{-2}	6600	Plyasunov et al. (2004)	L	
(propyl butyrate)	1.6×10^{-2}		Duchowicz et al. (2020)	V	186
[105-66-8]	1.6×10^{-2}		Meylan and Howard (1991)	V	
HUAZGNHGCJGYNP-UHFFFAOYSA-N	1.9×10^{-2}		Hine and Mookerjee (1975)	V	
	2.6×10^{-2}		Yaws (2003)	X	237, 154
	8.6×10^{-2}		Duchowicz et al. (2020)	Q	
	8.1×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
	1.4×10^{-2}		Hilal et al. (2008)	Q	
	2.8×10^{-2}		Modarresi et al. (2007)	Q	67
	2.2×10^{-2}		Yao et al. (2002)	Q	229
	2.3×10^{-2}		English and Carroll (2001)	Q	230, 260
	3.6×10^{-2}		Katritzky et al. (1998)	Q	
	2.0×10^{-2}		Suzuki et al. (1992)	Q	232
	1.8×10^{-2}		Meylan and Howard (1991)	Q	
	2.2×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.6×10^{-2}		Yaws (1999)	?	21, 154
	1.9×10^{-2}		Abraham et al. (1990)	?	
2-propyl butanoate	1.8×10^{-2}		Plyasunov et al. (2004)	L	
$C_7H_{14}O_2$	1.9×10^{-2}		Dupeux et al. (2022)	Q	259
(isopropyl butyrate)					
[638-11-9]					
FFOPEPMHKILNIT-UHFFFAOYSA-N					
butyl butanoate	1.7×10^{-2}	7600	Brockbank (2013)	L	1
$C_8H_{16}O_2$	1.6×10^{-2}	7600	Plyasunov et al. (2004)	L	
(butyl butyrate)	1.4×10^{-2}		Duchowicz et al. (2020)	V	186
[109-21-7]	1.0×10^{-2}		Dupeux et al. (2022)	Q	259
XUPYJHCZDLZNFP-UHFFFAOYSA-N	8.9×10^{-2}		Duchowicz et al. (2020)	Q	
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.3×10^{-2}		Modarresi et al. (2007)	Q	67
	3.4×10^{-2}		Katritzky et al. (1998)	Q	
	1.1×10^{-2}		Yaws (1999)	?	21
2-methylpropyl butanoate	1.3×10^{-2}		Hilal et al. (2008)	Q	
$C_8H_{16}O_2$					
(2-methylpropyl butyrate)					
[539-90-2]					
RGFNRWTWDWVHDD-UHFFFAOYSA-N					

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methylpropyl 2-methylpropanoate	7.4×10^{-3}	6900	Brockbank (2013)	L	1, 512
$C_8H_{16}O_2$	7.8×10^{-3}	6700	Plyasunov et al. (2004)	L	
(isobutyl isobutyrate)	1.0×10^{-2}		Amoore and Buttery (1978)	M	
[97-85-8]	1.2×10^{-2}		Duchowicz et al. (2020)	V	186
RXGUIWHIADMCFC-UHFFFAOYSA-N	7.2×10^{-3}		Amoore and Buttery (1978)	V	
	1.4×10^{-2}		Duchowicz et al. (2020)	Q	
	1.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	1.0×10^{-2}		Modarresi et al. (2007)	Q	67
	7.5×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.4×10^{-2}		English and Carroll (2001)	Q	230, 231
	1.3×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	6.9×10^{-3}		Yaws (1999)	?	21
	7.0×10^{-3}		Abraham et al. (1990)	?	
pentyl butanoate	1.7×10^{-2}	6400	Brockbank (2013)	L	1
$C_9H_{18}O_2$	9.8×10^{-3}		Dupeux et al. (2022)	Q	259
(pentyl butyrate)					
[540-18-1]					
CFNJLPHOBMVMNS-UHFFFAOYSA-N					
3-methylbutyl butanoate	1.1×10^{-2}	7500	Brockbank (2013)	L	1
$C_9H_{18}O_2$					
(isopentyl butyrate)					
[106-27-4]					
PQLMXFQTAMDXIZ-UHFFFAOYSA-N					
methyl 2-methylpropanoate	2.6×10^{-2}	5600	Brockbank (2013)	L	1
$C_5H_{10}O_2$	2.6×10^{-2}	5500	Plyasunov et al. (2004)	L	
(methyl isobutyrate)	3.3×10^{-2}	5700	Bagno et al. (1991)	T	473
[547-63-7]		5700	Della Gatta et al. (1981)	T	
BHIWKHZACMWKOJ-UHFFFAOYSA-N					
ethyl 2-methylpropanoate	1.5×10^{-2}	6000	Brockbank (2013)	L	1
$C_6H_{12}O_2$	1.7×10^{-2}	6200	Plyasunov et al. (2004)	L	
(ethyl isobutyrate)	2.0×10^{-2}		Hilal et al. (2008)	Q	
[97-62-1]	1.8×10^{-2}		Yao et al. (2002)	Q	229
WDAXFOBOLVPGLV-UHFFFAOYSA-N	2.4×10^{-2}		Yaws (1999)	?	21
hexyl butanoate	1.1×10^{-2}		Dupeux et al. (2022)	Q	259
$C_{10}H_{20}O_2$					
(hexyl butyrate)					
[2639-63-6]					
XAPCMTMQBXLDBB-UHFFFAOYSA-N					

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyclohexyl butanoate		6500	Kühne et al. (2005)	Q	
$C_{10}H_{18}O_2$		5600	Kühne et al. (2005)	?	
(cyclohexyl butyrate)					
[1551-44-6]					
VZHUBBUZNIULNM-UHFFFAOYSA-N					
3-oxobutanoic acid, methyl ester	6.4		Hovorka et al. (2002)	M	38
$C_5H_8O_3$	3.6×10^{1}		Duchowicz et al. (2020)	V	186
(methylacetoacetate)	3.7×10^{1}		HSDB (2015)	V	
[105-45-3]	1.2×10^{1}		Duchowicz et al. (2020)	Q	
WRQNANDWMGAFTP-UHFFFAOYSA-N	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	245
	1.7×10^{1}		Hilal et al. (2008)	Q	
	7.9		Modarresi et al. (2007)	Q	67
3-oxobutanoic acid, ethyl ester	9.0	7200	Brockbank (2013)	L	1
$C_6H_{10}O_3$	5.8		Hovorka et al. (2002)	M	38
(ethylacetoacetate)	8.2		Duchowicz et al. (2020)	V	186
[141-97-9]	1.7×10^{1}		Yaws (2003)	X	258
XYIBRDXRRQCHLP-UHFFFAOYSA-N	1.7×10^{1}		Yaws (2003)	X	237, 154
	2.4×10^{1}		Dupeux et al. (2022)	Q	259
	4.5		Duchowicz et al. (2020)	Q	
	7.8		Raventos-Duran et al. (2010)	Q	271, 243
	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{1}		Raventos-Duran et al. (2010)	Q	245
	1.7×10^{1}		Gharagheizi et al. (2010)	Q	246
	1.1×10^{1}		Hilal et al. (2008)	Q	
	5.6		Modarresi et al. (2007)	Q	67
	9.1		Yaws (1999)	?	21, 154
methyl pentanoate	3.0×10^{-2}	6100	Plyasunov et al. (2004)	L	
$C_4H_9COOCH_3$	3.1×10^{-2}		Buttery et al. (1969)	M	
(methyl valerate)	9.7×10^{-1}	5000	Djerki and Laub (1988)	V	
[624-24-8]		6200	Della Gatta et al. (1981)	T	
HNBDRPTVWVGKBR-UHFFFAOYSA-N	3.9×10^{-2}		Keshavarz et al. (2022)	Q	
	2.4×10^{-1}		Duchowicz et al. (2020)	Q	299
	2.9×10^{-2}		Li et al. (2014)	Q	241
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.2×10^{-2}		Hilal et al. (2008)	Q	
	3.6×10^{-2}		Modarresi et al. (2007)	Q	67
	3.1×10^{-2}		English and Carroll (2001)	Q	230, 231
	3.8×10^{-2}		Katritzky et al. (1998)	Q	
	2.6×10^{-2}		Suzuki et al. (1992)	Q	232
	2.5×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	3.1×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	3.1×10^{-2}		Abraham et al. (1990)	?	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethyl pentanoate	2.3×10^{-2}	6800	Plyasunov et al. (2004)	L	
$C_4H_9COOC_2H_5$	1.4×10^{-1}	4800	Meynier et al. (2003)	M	38
(ethyl valerate)	2.7×10^{-2}		Duchowicz et al. (2020)	V	186
[539-82-2]	2.8×10^{-2}		Meylan and Howard (1991)	V	
ICMAFTSLXCXHRK-UHFFFAOYSA-N	2.8×10^{-2}		Abraham (1984)	V	
	2.9×10^{-2}		Hine and Mookerjee (1975)	V	
	2.7×10^{-2}		Meynier et al. (2003)	C	
	8.6×10^{-2}		Duchowicz et al. (2020)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.5×10^{-2}		Hilal et al. (2008)	Q	
	2.6×10^{-2}		Modarresi et al. (2007)	Q	67
	2.3×10^{-2}		English and Carroll (2001)	Q	230, 231
	2.0×10^{-2}		Suzuki et al. (1992)	Q	232
	1.8×10^{-2}		Meylan and Howard (1991)	Q	
	2.2×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.7×10^{-2}		Abraham et al. (1990)	?	
methyl 2,2-dimethylpropanoate	9.5×10^{-3}	5600	Plyasunov et al. (2004)	L	
$C_6H_{12}O_2$	2.3×10^{-2}	6000	Bagno et al. (1991)	T	473
(methyl pivalate)		6000	Della Gatta et al. (1981)	T	
[598-98-1]	3.9×10^{-2}		Keshavarz et al. (2022)	Q	
CNMFHDIDIMZHKY-UHFFFAOYSA-N	4.1×10^{-2}		Duchowicz et al. (2020)	Q	
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.7×10^{-2}		Hilal et al. (2008)	Q	
	3.7×10^{-2}		Modarresi et al. (2007)	Q	67
	1.8×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	2.3×10^{-2}		English and Carroll (2001)	Q	230, 231
	1.8×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	2.3×10^{-2}		Duchowicz et al. (2020)	?	185, 21
ethyl 2-methylbutanoate	1.4×10^{-2}	6700	Plyasunov et al. (2004)	L	
$C_7H_{14}O_2$	8.9×10^{-3}		Pollien et al. (2003)	M	
[7452-79-1]	2.7×10^{-2}		Roberts and Pollien (1997)	M	
HCRBXQFHJMCTLF-UHFFFAOYSA-N					
ethyl 3-methylbutanoate	1.4×10^{-2}	6500	Brockbank (2013)	L	1
$C_7H_{14}O_2$	1.4×10^{-2}	6700	Plyasunov et al. (2004)	L	
(ethyl isovalerate)	1.1×10^{-2}	5900	Wieland et al. (2015)	M	513
[108-64-5]	1.4×10^{-2}		Duchowicz et al. (2020)	V	186
PPXUHEORWJQRHJ-UHFFFAOYSA-N	2.2×10^{-2}		Dupeux et al. (2022)	Q	259
	3.3×10^{-2}		Duchowicz et al. (2020)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{-2}		Hilal et al. (2008)	Q	
	2.8×10^{-2}		Modarresi et al. (2007)	Q	67
	1.5×10^{-2}		Yao et al. (2002)	Q	229
	1.6×10^{-2}		Yaws (1999)	?	21
ethyl 2,2-dimethylpropanoate	6.4×10^{-3}	6700	Brockbank (2013)	L	1
$C_7H_{14}O_2$	5.7×10^{-3}	6100	Plyasunov et al. (2004)	L	
(ethyl pivalate)					
[3938-95-2]					
HHEIMYAXCOIQCJ-UHFFFAOYSA-N					
butyl pentanoate	9.8×10^{-3}		Plyasunov et al. (2004)	L	
$C_9H_{18}O_2$	2.3×10^{-2}		Dupeux et al. (2022)	Q	259
(butyl valerate)	2.0×10^{-2}		Yao et al. (2002)	Q	229
[591-68-4]	1.5×10^{-2}		Yaws (1999)	?	21
OKJADYKTJJGKDX-UHFFFAOYSA-N					
3-methylbutyl 3-methylbutanoate	4.0×10^{-3}		Yaws (1999)	?	21
$C_{10}H_{20}O_2$					
(isoamyl isovalerate)					
[659-70-1]					
XINCECQTMHSORG-UHFFFAOYSA-N					
methyl hexanoate	2.6×10^{-2}	6600	Plyasunov et al. (2004)	L	
$C_5H_{11}COOCH_3$	1.9×10^{-2}		Aprea et al. (2007)	M	
(methyl caproate)	2.7×10^{-2}		Buttery et al. (1969)	M	
[106-70-7]	2.6	5600	Djerki and Laub (1988)	V	
NUKZAGXMHTUAFE-UHFFFAOYSA-N	5.3×10^{-2}		Keshavarz et al. (2022)	Q	
	2.5×10^{-1}		Duchowicz et al. (2020)	Q	299
	2.7×10^{-2}		Li et al. (2014)	Q	241
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.8×10^{-2}		Hilal et al. (2008)	Q	
	2.9×10^{-2}		Modarresi et al. (2007)	Q	67
	2.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.3×10^{-2}		English and Carroll (2001)	Q	230, 274
	3.6×10^{-2}		Katritzky et al. (1998)	Q	
	2.0×10^{-2}		Suzuki et al. (1992)	Q	232
	2.0×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.7×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	2.7×10^{-2}		Abraham et al. (1990)	?	
ethyl hexanoate	1.9×10^{-2}	7200	Plyasunov et al. (2004)	L	
$C_5H_{11}COOC_2H_5$	1.4×10^{-2}		Aprea et al. (2007)	M	
(ethyl caproate)	1.6×10^{-2}		Landy et al. (1996)	M	
[123-66-0]	9.4×10^{-3}		Landy et al. (1995)	M	
SHZIWNPUGXLXDT-UHFFFAOYSA-N	6.9×10^{-3}		Philippe et al. (2003)	V	14
	1.8×10^{-2}		Abraham (1984)	V	
	3.0		Abney (2021)	Q	399

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.4×10^{-2}		Savary et al. (2014)	Q	
	1.1×10^{-2}		Hilal et al. (2008)	Q	
	1.7×10^{-2}		English and Carroll (2001)	Q	230, 260
	1.7×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	1.8×10^{-2}		Abraham et al. (1990)	?	
2-ethylbutanoic acid, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester $C_{18}H_{34}O_6$ [95-08-9] JEYLQCXBYFQJRO-UHFFFAOYSA-N	9.9×10^{5}		HSDB (2015)	Q	99
methyl heptanoate $C_8H_{16}O_2$ [106-73-0] XNCNNDVCAUWAIT-UHFFFAOYSA-N	1.8×10^{-2}		Plyasunov et al. (2004)	L	
ethyl heptanoate $C_6H_{13}COOC_2H_5$ [106-30-9] TVQGDYNRXLTQAP-UHFFFAOYSA-N	2.0×10^{-2}		Meylan and Howard (1991)	V	
	2.0×10^{-2}		Abraham (1984)	V	
	2.0×10^{-2}		Hine and Mookerjee (1975)	V	
	9.6×10^{-2}		Keshavarz et al. (2022)	Q	
	9.1×10^{-2}		Duchowicz et al. (2020)	Q	299
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	9.2×10^{-3}		Hilal et al. (2008)	Q	
	1.9×10^{-2}		Modarresi et al. (2007)	Q	67
	1.2×10^{-2}		Suzuki et al. (1992)	Q	232
	1.0×10^{-2}		Meylan and Howard (1991)	Q	
	2.1×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.0×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	2.0×10^{-2}		Abraham et al. (1990)	?	
methyl octanoate $C_6H_{13}COOCH_3$ [111-11-5] JGHZJRVDZXSNKQ-UHFFFAOYSA-N	1.2×10^{-2}		Plyasunov et al. (2004)	L	
	9.9×10^{-3}		Aprea et al. (2007)	M	
	1.3×10^{-2}		Buttery et al. (1969)	M	
	9.6×10^{-2}		Keshavarz et al. (2022)	Q	
	2.7×10^{-1}		Duchowicz et al. (2020)	Q	299
	1.3×10^{-2}		Li et al. (2014)	Q	241
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	67
	4.7×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	1.2×10^{-2}		Suzuki et al. (1992)	Q	232
	1.1×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.3×10^{-2}		Duchowicz et al. (2020)	?	185, 21

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethyl octanoate $C_7H_{15}COOC_2H_5$ [106-32-1] YYZUSRORWSJGET-UHFFFAOYSA-N	1.7×10^{-2} 1.1×10^{-2} 1.2×10^{-2} 7.8×10^{-3}		Plyasunov et al. (2004) Aprea et al. (2007) Abraham (1984) Savary et al. (2014)	L M V Q	
octadecanoic acid, 2-methylpropyl ester $C_{22}H_{44}O_2$ (isobutyl stearate) [646-13-9] ORFWYUFLWUWSFM-UHFFFAOYSA-N	2.6×10^{-4}		HSDB (2015)	Q	99
octadecanoic acid, butyl ester $C_{22}H_{44}O_2$ [123-95-5] ULBTUVJTXULMLP-UHFFFAOYSA-N	2.6×10^{-4}		HSDB (2015)	Q	99
methyl nonanoate $C_{10}H_{20}O_2$ [1731-84-6] IJXHLVMUNBOGRR-UHFFFAOYSA-N	8.2×10^{-3} 7.0×10^{-3}		Plyasunov et al. (2004) Abraham (1984)	L V	
ethyl nonanoate $C_8H_{17}COOC_2H_5$ [123-29-5] BYEVBITUADOIGY-UHFFFAOYSA-N	1.3×10^{-2}		Abraham (1984)	V	
nonanedioic acid, bis(2-ethylhexyl) ester $C_{25}H_{48}O_4$ (di-2-ethylhexyl azelate) [103-24-2] ZDWGXBPVPXVXMQ-UHFFFAOYSA-N	8.2×10^{-2}		HSDB (2015)	Q	99
methyl decanoate $C_{11}H_{22}O_2$ (methyl caprate) [110-42-9] YRHYCMZPEVDGFQ-UHFFFAOYSA-N	1.1×10^{-2} 4.8×10^{-3} 1.4×10^{-2} 3.2×10^{-3} 2.8×10^{-1} 5.8×10^{-3} 7.7×10^{-3}		Aprea et al. (2007) Duchowicz et al. (2020) Krop et al. (1997) Abraham (1984) Duchowicz et al. (2020) HSDB (2015) Hilal et al. (2008)	M V V V Q Q Q	 186 99
ethyl decanoate $C_9H_{19}COOC_2H_5$ [110-38-3] RGXWDWUGBIJHDO-UHFFFAOYSA-N	1.2×10^{-2} 1.4×10^{-2} 1.7×10^{-2}		Plyasunov et al. (2004) Aprea et al. (2007) Abraham (1984)	L M V	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
decanedioic acid, diethyl ester $C_{14}H_{26}O_4$ (diethyl sebacate) [110-40-7] ONKUXPIBXRRIDU-UHFFFAOYSA-N	2.7		Bartelt-Hunt et al. (2008)	?	21
methyl dodecanoate $C_{13}H_{26}O_2$ (methyl laurate) [111-82-0] UQDUPQYQJKYHQI-UHFFFAOYSA-N	8.3×10^{-3} 7.5×10^{-3} 3.3×10^{-3} 4.8×10^{-3}		Krop et al. (1997) Dupeux et al. (2022) HSDB (2015) Hilal et al. (2008)	V Q Q Q	 259 99
ethyl dodecanoate $C_{14}H_{28}O_2$ (ethyl laurate) [106-33-2] MMXKVMNBHPAILY-UHFFFAOYSA-N	7.7×10^{-3} 3.1×10^{-3}		Krop et al. (1997) Hilal et al. (2008)	V Q	
propyl dodecanoate $C_{15}H_{30}O_2$ (propyl laurate) [3681-78-5] FTBUKOLPOATXGV-UHFFFAOYSA-N	7.7×10^{-3} 2.1×10^{-3}		Krop et al. (1997) Hilal et al. (2008)	V Q	
2-hydroxypropyl dodecanoate $C_{15}H_{30}O_3$ [142-55-2] BHIZVZJETFVJMJ-UHFFFAOYSA-N	9.5×10^{-2}		Ebert et al. (2023)	?	318
dodecanoic acid, 2-hydroxy-1-methylethyl ester $C_{15}H_{30}O_3$ [107328-11-0] SVWZGNLBKFWCMV-UHFFFAOYSA-N	2.6×10^{1}		Ebert et al. (2023)	?	318
butyl dodecanoate $C_{16}H_{32}O_2$ (butyl laurate) [106-18-3] NDKYEUQMPZIGFN-UHFFFAOYSA-N	7.1×10^{-3} 1.5×10^{-3}		Krop et al. (1997) Hilal et al. (2008)	V Q	
2-ethylhexyl dodecanoate $C_{20}H_{40}O_2$ (2-ethylhexyl laurate) [20292-08-4] LWLRMRFJCCMNML-UHFFFAOYSA-N	3.0×10^{-3} 8.6×10^{-4}		Krop et al. (1997) Hilal et al. (2008)	V Q	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl tetradecanoate $C_{15}H_{30}O_2$ (methyl myristate) [124-10-7] ZAZKJZBWRNNLDS-UHFFFAOYSA-N	5.0×10^{-3} 1.9×10^{-3} 3.1×10^{-3}		Krop et al. (1997) HSDB (2015) Hilal et al. (2008)	V Q Q	 99
methyl hexadecanoate $C_{17}H_{34}O_2$ (methyl palmitate) [112-39-0] FLIACVVOZYBSBS-UHFFFAOYSA-N	2.9×10^{-3} 1.1×10^{-3} 1.8×10^{-3}		Krop et al. (1997) HSDB (2015) Hilal et al. (2008)	V Q Q	 99
isopropyl palmitate $C_{19}H_{38}O_2$ [142-91-6] XUGNVMKQXJXZCD-UHFFFAOYSA-N	2.1×10^{-4}		HSDB (2015)	Q	447
ascorbic palmitate $C_{22}H_{38}O_7$ [137-66-6] QAQJMLQRFWZOBN-LAUBAEHRSA-N	7.0×10^{1}		HSDB (2015)	Q	99
methyl octadecanoate $C_{19}H_{38}O_2$ (methyl stearate) [112-61-8] HPEUJPJOZXNMSJ-UHFFFAOYSA-N	1.7×10^{-3} 6.2×10^{-4} 1.1×10^{-3}		Krop et al. (1997) HSDB (2015) Hilal et al. (2008)	V Q Q	 99
methyl eicosanoate $C_{21}H_{42}O_2$ (methyl arachidate) [1120-28-1] QGBRLVONZXHAKJ-UHFFFAOYSA-N	1.0×10^{-3}		Krop et al. (1997)	V	
methyl docosanoate $C_{23}H_{46}O_2$ (methyl behenate) [929-77-1] QSQLTHHMFHEFIY-UHFFFAOYSA-N	5.9×10^{-4}		Krop et al. (1997)	V	
cyclopropanecarboxylic acid, methyl ester $C_5H_8O_2$ [2868-37-3] PKAHQJNJPDVTDP-UHFFFAOYSA-N	4.1×10^{-1} 1.1×10^{-1} 1.4×10^{-1}	6100	Bagno et al. (1991) Hilal et al. (2008) English and Carroll (2001)	T Q Q	473 230, 231
cyclohexanecarboxylic acid, methyl ester $C_6H_{11}COOCH_3$ [4630-82-4] ZQWPRMPSCMSAJU-UHFFFAOYSA-N	1.1×10^{-1} 1.1×10^{-1}	7200	Bagno et al. (1991) English and Carroll (2001)	T Q	473 230, 231

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(*Z*,*Z*,*Z*)-9,12,15-octadecatrienoic acid, methyl ester $C_{19}H_{32}O_2$ (methyl linolenate) [301-00-8] DVWSXZIHSUZZKJ-YSTUJMKBSA-N	2.8×10^{-1} 7.2×10^{-3}		Krop et al. (1997) Hilal et al. (2008)	V Q	
(*Z*,*Z*)-9,12-octadecadienoic acid, methyl ester $C_{19}H_{34}O_2$ (methyl linolate) [112-63-0] WTTJVINHCBCLGX-NQLNTKRDSA-N	6.2×10^{-2} 4.8×10^{-3}		Krop et al. (1997) Hilal et al. (2008)	V Q	
(*Z*)-9-octadecenoic acid, methyl ester $C_{19}H_{36}O_2$ (methyl oleate) [112-62-9] QYDYPVFESGNLHU-KHPPLWFESA-N	1.3×10^{-2} 7.0×10^{-4} 2.5×10^{-3}		Krop et al. (1997) HSDB (2015) Hilal et al. (2008)	V Q Q	 99
(*Z*)-13-docosenoic acid, methyl ester $C_{23}H_{44}O_2$ (methyl erucate) [1120-34-9] ZYNDJIBBPLNPOW-KHPPLWFESA-N	5.3×10^{-3} 8.2×10^{-4}		Krop et al. (1997) Hilal et al. (2008)	V Q	
trans-quercus lactone $C_9H_{16}O_2$ (*trans*-whisky lactone) [105119-22-0] WNVCMFHPRIBNCW-SFYZADRCSA-N	3.5×10^{1}		Abney (2021)	Q	399
γ-decalactone $C_{10}H_{18}O_2$ [706-14-9] IFYYFLINQYPWGJ-UHFFFAOYSA-N	5.3×10^{1}		Abney (2021)	Q	399
γ-dodecalactone $C_{12}H_{22}O_2$ [2305-05-7] WGPCZPLRVAWXPW-UHFFFAOYSA-N	3.7×10^{1}		Abney (2021)	Q	399
oxacyclohexadecan-2-one $C_{15}H_{28}O_2$ (pentadecalactone) [106-02-5] FKUPPRZPSYCDRS-UHFFFAOYSA-N	4.0×10^{-3} 7.6×10^{-2}		Amoore and Buttery (1978) Amoore and Buttery (1978)	M V	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-*tert*-butylcyclohexyl acetate	9.9×10^{-3}		Zhang et al. (2010)	Q	287, 288
$C_{12}H_{22}O_2$	3.8×10^{-2}		Zhang et al. (2010)	Q	287, 289
[88-41-5]	5.3×10^{-1}		Zhang et al. (2010)	Q	287, 290
FINOAUDUYKVGDS-UHFFFAOYSA-N	7.0×10^{-3}		Zhang et al. (2010)	Q	287, 291
hedione	7.0×10^{1}		Dupeux et al. (2022)	Q	259
$C_{13}H_{22}O_3$					
[24851-98-7]					
KVWWIYGFBYDJQC-UHFFFAOYSA-N					
ethylene brassylate	5.3×10^{1}		Dupeux et al. (2022)	Q	259
$C_{15}H_{26}O_4$					
[105-95-3]					
XRHCAGNSDHCHFJ-UHFFFAOYSA-N					
propyl 3-oxo-2-pentylcyclopentaneacetate	1.4×10^{1}		Ebert et al. (2023)	?	318
$C_{15}H_{26}O_3$					
[158474-72-7]					
IPDFPNNPBMREIF-UHFFFAOYSA-N					
2-ethyl-3-oxo-butanoic acid, ethyl ester	3.4		Hilal et al. (2008)	Q	
$C_8H_{14}O_3$					
[607-97-6]					
OKANYBNORCUPKZ-UHFFFAOYSA-N					
2-hydroxypropanoic acid, butyl ester	4.9		HSDB (2015)	V	
$C_7H_{14}O_3$	2.7		Wang et al. (2017)	Q	80, 238
[138-22-7]	2.9×10^{1}		Wang et al. (2017)	Q	80, 239
MRABAEUHTLLEML-UHFFFAOYSA-N	2.6		Wang et al. (2017)	Q	80, 240
	1.6		Raventos-Duran et al. (2010)	Q	271, 243
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	6.4×10^{1}		Hilal et al. (2008)	Q	
	4.3×10^{1}		Modarresi et al. (2007)	Q	67
methyl propenoate	5.0×10^{-2}		Duchowicz et al. (2020)	V	186
$C_4H_6O_2$	4.9×10^{-2}		HSDB (2015)	V	
(methyl acrylate)	5.2×10^{-2}		Mackay et al. (2006c)	V	
[96-33-3]	5.2×10^{-2}		Mackay et al. (1995)	V	
BAPJBEWLBFYGME-UHFFFAOYSA-N	5.8×10^{-2}		Yaws (2003)	X	237, 72
	6.3×10^{-1}		Duchowicz et al. (2020)	Q	
	7.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
	5.4×10^{-2}		Hilal et al. (2008)	Q	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.4×10^{-2}		Modarresi et al. (2007)	Q	67
	5.2×10^{-2}		Yaws (1999)	?	21, 72
ethyl propenoate	3.9×10^{-2}	4400	Brockbank (2013)	L	1
$C_5H_8O_2$	2.9×10^{-2}		Duchowicz et al. (2020)	V	186
(ethyl acrylate)	2.9×10^{-2}		HSDB (2015)	V	
[140-88-5]	2.9×10^{-2}		Mackay et al. (2006c)	V	
JIGUQPWFLRLWPJ-UHFFFAOYSA-N	2.9×10^{-2}		Mackay et al. (1995)	V	
	3.9×10^{-2}		Yaws (2003)	X	258
	4.7×10^{-2}		Dupeux et al. (2022)	Q	259
	2.5×10^{-1}		Duchowicz et al. (2020)	Q	
	8.8×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.5×10^{-2}		Hilal et al. (2008)	Q	
	5.3×10^{-2}		Modarresi et al. (2007)	Q	67
	8.8×10^{-2}		Yao et al. (2002)	Q	229
	4.0×10^{-2}		Yaws (1999)	?	21
2-propenoic acid, butyl ester	1.5×10^{-2}		Duchowicz et al. (2020)	V	186
$C_7H_{12}O_2$	2.1×10^{-2}		HSDB (2015)	V	
(butyl acrylate)	2.9×10^{-1}		Duchowicz et al. (2020)	Q	
[141-32-2]	2.6×10^{-2}		Gharagheizi et al. (2012)	Q	
CQEYYJKEWSMYFG-UHFFFAOYSA-N	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-2}		Hilal et al. (2008)	Q	
	4.4×10^{-2}		Modarresi et al. (2007)	Q	67
	5.2×10^{-2}		Yao et al. (2002)	Q	229, 267
	1.7×10^{-2}		Yaws (1999)	?	21, 12
2-propenoic acid, 2-methylpropyl ester	1.3×10^{-2}		Duchowicz et al. (2020)	V	186
$C_7H_{12}O_2$	1.6×10^{-2}		HSDB (2015)	V	
(isobutyl acrylate)	1.1×10^{-1}		Duchowicz et al. (2020)	Q	
[106-63-8]	1.4×10^{-2}		Gharagheizi et al. (2012)	Q	
CFVWNXQPGQOHRJ-UHFFFAOYSA-N	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.4×10^{-2}		Hilal et al. (2008)	Q	
	3.4×10^{-2}		Modarresi et al. (2007)	Q	67
	3.9×10^{-2}		Yao et al. (2002)	Q	229
	1.5×10^{-2}		Yaws (1999)	?	21, 72

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-propenoic acid, 2-ethylhexyl ester	2.3×10^{-2}		Duchowicz et al. (2020)	V	186
$C_{11}H_{20}O_2$	2.3×10^{-2}		HSDB (2015)	V	
(2-ethylhexyl acrylate)	2.7×10^{-2}		Yaws (2003)	X	237, 72
[103-11-7]	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
GOXQRTZXKQZDDN-UHFFFAOYSA-N	6.2×10^{-3}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	67
	2.0×10^{-2}		Yao et al. (2002)	Q	229
	2.3×10^{-2}		Yaws (1999)	?	21, 72
2-propenoic acid, 2-hydroxyethyl ester $C_5H_8O_3$ (2-hydroxyethyl acrylate) [818-61-1] OMIGHNLMNHATMP-UHFFFAOYSA-N	1.2×10^{3}		HSDB (2015)	V	
2-methyl-2-propenoic acid, ethyl ester	1.7×10^{-2}		Duchowicz et al. (2020)	V	186
$C_6H_{10}O_2$	1.7×10^{-2}		HSDB (2015)	V	
[97-63-2]	1.6×10^{-2}		Hilal et al. (2008)	C	
SUPCQIBBMFXVTL-UHFFFAOYSA-N	8.9×10^{-2}		Duchowicz et al. (2020)	Q	
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.9×10^{-2}		Hilal et al. (2008)	Q	
	3.5×10^{-2}		Modarresi et al. (2007)	Q	67
2-methyl-2-propenoic acid, 2-propenyl ester $C_7H_{10}O_2$ (allyl methacrylate) [96-05-9] FBCQUCJYYPMKRO-UHFFFAOYSA-N	2.4×10^{-2}		HSDB (2015)	Q	99
2-methyl-2-propenoic acid, oxiranylmethyl ester $C_7H_{10}O_3$ (glycidyl methacrylate) [106-91-2] VOZRXNHHFUQHIL-UHFFFAOYSA-N	3.2×10^{1}		HSDB (2015)	Q	99

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
allyl acetoacetate $C_7H_{10}O_3$ [1118-84-9] AXLMPTNTPOWPLT-UHFFFAOYSA-N	1.2×10^{1}		Ebert et al. (2023)	?	318
2-methyl-2-propenoic acid, propyl ester $C_7H_{12}O_2$ (propyl methacrylate) [2210-28-8] NHARPDSAXCBDDR-UHFFFAOYSA-N	1.8×10^{-2}		HSDB (2015)	Q	99
2-methyl-2-propenoic acid, butyl ester	2.0×10^{-2}		Duchowicz et al. (2020)	V	186
$C_8H_{14}O_2$	2.0×10^{-2}		HSDB (2015)	V	
(butyl methacrylate)	9.9×10^{-2}		Duchowicz et al. (2020)	Q	
[97-88-1]	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
SOGAXMICEFXMKE-UHFFFAOYSA-N	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.8×10^{-2}		Hilal et al. (2008)	Q	
	4.0×10^{-2}		Modarresi et al. (2007)	Q	67
2-methyl-2-propenoic acid, 2-methylpropyl ester	1.9×10^{-2}		Duchowicz et al. (2020)	V	186
$C_8H_{14}O_2$	1.9×10^{-2}		HSDB (2015)	V	
[97-86-9]	3.9×10^{-2}		Duchowicz et al. (2020)	Q	
RUMACXVDVNRZJZ-UHFFFAOYSA-N	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.1×10^{-2}		Hilal et al. (2008)	Q	
	2.7×10^{-2}		Modarresi et al. (2007)	Q	67
2-methyl-2-propenoic acid, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester $C_{14}H_{22}O_6$ [109-16-0] HWSSEYVMGDIFMH-UHFFFAOYSA-N	5.8×10^{6}		HSDB (2015)	Q	99
methyl methacrylate	2.9×10^{-2}	5300	Brockbank (2013)	L	1
$C_5H_8O_2$	4.3×10^{-2}	7700	Hiatt (2013)	M	
[80-62-6]	3.1×10^{-2}		Duchowicz et al. (2020)	V	186
VVQNEPGJFQJSBK-UHFFFAOYSA-N	3.1×10^{-2}		HSDB (2015)	V	
	3.1×10^{-2}	5300	Dohnal et al. (2010)	V	1
	3.1×10^{-2}		Mackay et al. (2006c)	V	
	3.0×10^{-2}		Lide and Frederikse (1995)	V	
	3.1×10^{-2}		Mackay et al. (1995)	V	
	2.4×10^{-1}		Duchowicz et al. (2020)	Q	
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.4×10^{-2}		Hilal et al. (2008)	Q	
	3.5×10^{-2}		Modarresi et al. (2007)	Q	67
			Burkholder et al. (2019)	W	514
			Burkholder et al. (2015)	W	515
(E)-3-hexenyl ethanoate $C_8H_{14}O_2$ [3681-82-1] NPFVOOAXDOBMCE-SNAWJCMRSA-N	3.3×10^{-2}		Karl et al. (2003)	M	
(Z)-3-hexenyl ethanoate $C_8H_{14}O_2$ [3681-71-8] NPFVOOAXDOBMCE-PLNGDYQASA-N	3.1×10^{-2}		Karl et al. (2003)	M	
ethenyl ethanoate $CH_3COOCHCH_2$ (vinyl acetate) [108-05-4] XTXRWKRVRITETP-UHFFFAOYSA-N	2.0×10^{-2}	4500	Burkholder et al. (2019)	L	
	2.0×10^{-2}	4500	Burkholder et al. (2015)	L	
	2.0×10^{-2}	4600	Brockbank (2013)	L	1
	2.0×10^{-2}	4400	Böhme et al. (2008)	M	
	1.9×10^{-2}		HSDB (2015)	V	
	2.0×10^{-2}	4600	Dohnal et al. (2010)	V	1
	1.6×10^{-2}		Mackay et al. (2006c)	V	
	2.0×10^{-2}		Lide and Frederikse (1995)	V	
	1.6×10^{-2}		Mackay et al. (1995)	V	
	2.0×10^{-2}		Yaws (2003)	X	258
	2.0×10^{-2}		Yaws (2003)	X	237
	1.7×10^{-2}		Goldstein (1982)	X	446
	1.7×10^{-2}	2600	Goldstein (1982)	X	298
	1.2×10^{-2}		Dupeux et al. (2022)	Q	259
	5.8×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	2.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
	6.9×10^{-2}		Hilal et al. (2008)	Q	
	6.6×10^{-2}		Modarresi et al. (2007)	Q	67
	2.0×10^{-2}		Yaws (1999)	?	21
($7E$,$9Z$)-dodecadienyl acetate $C_{14}H_{24}O_2$ [54364-62-4] LLRZUAWETKPZJO-SCFJQAPRSA-N	1.2×10^{-2}		Ebert et al. (2023)	?	318
($9Z$,$12E$)-9,12-tetradecadienyl acetate $C_{16}H_{28}O_2$ [30507-70-1] ZZGJZGSVLNSDPG-FDTUMDBZSA-N	1.7×10^{-1}		Ebert et al. (2023)	?	318

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
isoambrettolide $C_{16}H_{28}O_2$ [28645-51-4] QILMAYXCYBTEDM-IWQZZHSRSA-N	2.5		Dupeux et al. (2022)	Q	259
vetyveryl acetate $C_{17}H_{26}O_2$ [117-98-6] UAVFEMBKDRODDE-UHFFFAOYSA-N	2.2		Dupeux et al. (2022)	Q	259
hydroprene $C_{17}H_{30}O_2$ [41096-46-2] FYQGBXGJFWXIPP-UEVLXMDPSA-N	5.1×10^{-2}		Ebert et al. (2023)	?	316
empenthrin $C_{18}H_{26}O_2$ [54406-48-3] YUGWDVYLFSETPE-UHFFFAOYSA-N	2.9×10^{-2}		Ebert et al. (2023)	?	316
3-(4-methoxyphenyl)-2-propenoic acid, 2-ethylhexyl ester $C_{18}H_{26}O_3$ (octinoxate) [5466-77-3] YBGZDTIWKVFICR-JLHYYAGUSA-N	1.2		HSDB (2015)	Q	447
kinoprene $C_{18}H_{28}O_2$ [42588-37-4] FZRBKIRIBLNOAM-WHVZTFIZSA-N	1.8×10^{-1}		Ebert et al. (2023)	?	316
allethrin $C_{19}H_{26}O_3$ [584-79-2] ZCVAOQKBXKSDMS-UHFFFAOYSA-N	6.0×10^{1}		Ebert et al. (2023)	?	318
S-methoprene $C_{19}H_{34}O_3$ [65733-16-6] NFGXHKASABOEEW-GYMWBFJFSA-N	1.5		Ebert et al. (2023)	?	318
methyl benzoate $C_6H_5COOCH_3$ [93-58-3] QPJVMBTYPHYUOC-UHFFFAOYSA-N	2.9×10^{-1}	6400	Brockbank (2013)	L	1
	3.0×10^{-1}		Duchowicz et al. (2020)	V	186
	3.0×10^{-1}		HSDB (2015)	V	
	3.0×10^{-1}		Mackay et al. (2006c)	V	
	3.0×10^{-1}		Mackay et al. (1995)	V	
	2.8×10^{-1}		Meylan and Howard (1991)	V	
	5.6×10^{-1}		Hine and Mookerjee (1975)	V	
	3.1×10^{-1}		Abraham et al. (1994a)	R	
	5.8×10^{-1}	6300	Bagno et al. (1991)	T	473

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.8×10^{-1}		Yaws (2003)	X	258
	2.6×10^{-1}		Dupeux et al. (2022)	Q	259
	1.4		Duchowicz et al. (2020)	Q	
	2.9×10^{-1}		Zhang et al. (2010)	Q	287, 288
	3.6×10^{-1}		Zhang et al. (2010)	Q	287, 289
	9.5×10^{-1}		Zhang et al. (2010)	Q	287, 290
	6.1×10^{-1}		Zhang et al. (2010)	Q	287, 291
	2.9×10^{-1}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Modarresi et al. (2007)	Q	67
		5100	Kühne et al. (2005)	Q	
	3.2×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	6.8×10^{-1}		Yao et al. (2002)	Q	229
	1.1		English and Carroll (2001)	Q	230, 274
	3.0×10^{-1}		Katritzky et al. (1998)	Q	
	5.6×10^{-1}		Suzuki et al. (1992)	Q	232
	2.8×10^{-1}		Meylan and Howard (1991)	Q	
	2.7×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
		3500	Kühne et al. (2005)	?	
	2.8×10^{-1}		Yaws (1999)	?	21
	5.6×10^{-1}		Abraham et al. (1990)	?	
ethyl benzoate $C_6H_5COOC_2H_5$ [93-89-0] MTZQAGJQAFMTAQ-UHFFFAOYSA-N	1.7×10^{-1}	6300	Brockbank (2013)	L	1
	1.3×10^{-1}		Duchowicz et al. (2020)	V	186
	9.7×10^{-2}		Mackay et al. (2006c)	V	
	9.7×10^{-2}		Mackay et al. (1995)	V	
	1.9×10^{-1}		Abraham et al. (1994a)	R	
	1.4×10^{-1}		Yaws (2003)	X	258
	1.5×10^{-1}		Dupeux et al. (2022)	Q	259
	5.2×10^{-1}		Duchowicz et al. (2020)	Q	
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.1×10^{-1}		Zhang et al. (2010)	Q	287, 288
	2.1×10^{-1}		Zhang et al. (2010)	Q	287, 289
	5.1×10^{-1}		Zhang et al. (2010)	Q	287, 290
	4.8×10^{-1}		Zhang et al. (2010)	Q	287, 291
	1.9×10^{-1}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Modarresi et al. (2007)	Q	67
	1.9×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	6.7×10^{-1}		English and Carroll (2001)	Q	230, 231
	5.1×10^{-1}		Katritzky et al. (1998)	Q	
	2.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.4×10^{-1}		Yaws (1999)	?	21
	1.9×10^{-1}		Abraham et al. (1990)	?	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-hydroxybenzoic acid methyl ester	1.6	9500	Brockbank (2013)	L	1
$C_8H_8O_3$	3.3×10^{-1}		Karl et al. (2008)	M	
(methyl salicylate)	1.0×10^{-1}		Duchowicz et al. (2020)	V	186
[119-36-8]	1.1×10^{1}		HSDB (2015)	V	
OSWPMRLSEDHDFF-UHFFFAOYSA-N	7.8		Duchowicz et al. (2020)	Q	
	1.8×10^{1}		Hilal et al. (2008)	Q	
	9.3		Modarresi et al. (2007)	Q	67
	1.0×10^{-1}		Bartelt-Hunt et al. (2008)	?	21
	1.0		Yaws (1999)	?	21, 38
benzoic acid, 4-methyl-, methyl ester	2.6×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_9H_{10}O_2$	3.9×10^{-1}		Zhang et al. (2010)	Q	287, 289
[99-75-2]	1.7		Zhang et al. (2010)	Q	287, 290
QSSJZLPUHJDYKF-UHFFFAOYSA-N	3.5×10^{-1}		Zhang et al. (2010)	Q	287, 291
acetylsalicylic acid	7.6×10^{3}		Duchowicz et al. (2020)	V	186
$C_9H_8O_4$	1.5×10^{4}		Duchowicz et al. (2020)	Q	
(aspirin)	1.5×10^{5}		Abraham et al. (2019)	Q	
[50-78-2]	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	271, 243
BSYNRYMUTXBXSQ-UHFFFAOYSA-N	4.9×10^{4}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{3}		Raventos-Duran et al. (2010)	Q	245
1,4-benzenedicarboxylic acid, dimethyl ester	7.4×10^{-2}		Duchowicz et al. (2020)	V	186
$C_{10}H_{10}O_4$	7.6×10^{-2}		HSDB (2015)	V	
[120-61-6]	2.2×10^{2}		Duchowicz et al. (2020)	Q	
WOZVHXUHUFLZGK-UHFFFAOYSA-N	4.4×10^{1}		Zhang et al. (2010)	Q	287, 288
	1.3×10^{2}		Zhang et al. (2010)	Q	287, 289
	5.3×10^{1}		Zhang et al. (2010)	Q	287, 290
	9.2×10^{1}		Zhang et al. (2010)	Q	287, 291
	2.4		Modarresi et al. (2007)	Q	67
butyl benzoate	2.5×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{11}H_{14}O_2$	1.0×10^{-1}		Dupeux et al. (2022)	Q	259
[136-60-7]	5.7×10^{-1}		Duchowicz et al. (2020)	Q	
XSIFPSYPOVKYCO-UHFFFAOYSA-N	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-1}		Zhang et al. (2010)	Q	287, 288
	1.0×10^{-1}		Zhang et al. (2010)	Q	287, 289
	5.2×10^{-1}		Zhang et al. (2010)	Q	287, 290
	3.2×10^{-1}		Zhang et al. (2010)	Q	287, 291
	8.3×10^{-2}		Modarresi et al. (2007)	Q	67

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
diphenyl carbonate	1.2×10^{-1}		HSDB (2015)	Q	99
$C_{13}H_{10}O_3$	1.2×10^{-1}		Zhang et al. (2010)	Q	287, 288
[102-09-0]	1.6×10^{1}		Zhang et al. (2010)	Q	287, 289
ROORDVPLFPIABK-UHFFFAOYSA-N	9.5×10^{-1}		Zhang et al. (2010)	Q	287, 290
	1.2×10^{2}		Zhang et al. (2010)	Q	287, 291
benzyl benzoate	1.8		Mackay et al. (2006c)	V	
$C_{14}H_{12}O_2$	1.8		Mackay et al. (1995)	V	
[120-51-4]	1.7		Dupeux et al. (2022)	Q	259
SESFRYSPDFLNCH-UHFFFAOYSA-N					
trans-ethylcinnamate	2.3		Duchowicz et al. (2020)	V	186
$C_{11}H_{12}O_2$	1.4		Abney (2021)	Q	399
[103-36-6]	6.5×10^{-1}		Duchowicz et al. (2020)	Q	
KBEBGUQPQBELIU-CMDGGOBGSA-N					
dipropylene glycol dibenzoate	7.2×10^{2}		Duchowicz et al. (2020)	V	186
$C_{20}H_{22}O_5$	9.4×10^{2}		Duchowicz et al. (2020)	Q	
[27138-31-4]					
CGLQOIMEUPORRI-UHFFFAOYSA-N					
dimethyl phthalate	5.1×10^{1}	8000	Brockbank (2013)	L	1
$C_{10}H_{10}O_4$	2.3×10^{1}		Chao et al. (2017)	M	
[131-11-3]	5.0×10^{1}		Duchowicz et al. (2020)	V	186
NIQCNGHVCWTJSM-UHFFFAOYSA-N	4.9×10^{1}		HSDB (2015)	V	
	9.3×10^{1}		Mackay et al. (2006c)	V	
	2.0×10^{1}		Saçan et al. (2005)	V	
	1.0×10^{2}		Cousins and Mackay (2000)	V	
	8.1×10^{1}		Staples et al. (1997)	V	
	9.1×10^{1}		Lide and Frederikse (1995)	V	
	9.1×10^{1}		Mackay et al. (1995)	V	
	5.0×10^{1}		Hwang et al. (1992)	V	
	9.0		Wolfe et al. (1980)	V	
	8.8×10^{1}		Yaws (2003)	X	237, 12
	2.9×10^{1}		Goldstein (1982)	X	446
	3.0×10^{1}	5700	Goldstein (1982)	X	298
	2.3×10^{1}		McCarty (1980)	X	368
	5.0×10^{1}		Ryan et al. (1988)	C	
	2.2×10^{2}		Duchowicz et al. (2020)	Q	
	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{2}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	8.2×10^{1}		Gharagheizi et al. (2010)	Q	246
	1.7×10^{2}		Hilal et al. (2008)	Q	
	9.6		Saçan et al. (2005)	Q	
	5.4×10^{1}		Yaws (1999)	?	21, 12

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,4-cyclohexanedicarboxylic acid, dimethyl ester $C_{10}H_{16}O_4$ (dimethyl hexahydroterephthalate) [94-60-0] LNGAGQAGYITKCW-UHFFFAOYSA-N	1.0×10^{2}		HSDB (2015)	V	
1,3-benzenedicarboxylic acid, dimethyl ester $C_{10}H_{10}O_4$ (dimethyl isophthalate) [1459-93-4] VNGOYPQMJFJDLV-UHFFFAOYSA-N	1.6×10^{2}		HSDB (2015)	Q	99
diethyl phthalate $C_{12}H_{14}O_4$ [84-66-2] FLKPEMZONWLCSK-UHFFFAOYSA-N	6.0×10^{1}	10000	Brockbank (2013)	L	1
	2.2×10^{1}		Chao et al. (2017)	M	
	1.6×10^{1}		Duchowicz et al. (2020)	V	186
	1.6×10^{1}		HSDB (2015)	V	
	2.2×10^{1}		Mackay et al. (2006c)	V	
	4.1×10^{1}		Cousins and Mackay (2000)	V	
	3.7×10^{1}		Staples et al. (1997)	V	
	2.1×10^{1}		Lide and Frederikse (1995)	V	
	1.0×10^{2}		Mackay et al. (1995)	V	
	4.9×10^{2}		Wolfe et al. (1980)	V	
	6.9×10^{1}		Yaws (2003)	X	237
	1.2×10^{1}		Goldstein (1982)	X	446
	1.2×10^{1}	5600	Goldstein (1982)	X	298
	2.1×10^{-1}		Ryan et al. (1988)	C	
	5.8×10^{-1}		Petrasek et al. (1983)	C	
	3.4×10^{1}		Duchowicz et al. (2020)	Q	
	1.5×10^{1}		Gharagheizi et al. (2012)	Q	
	2.5×10^{1}		Zhang et al. (2010)	Q	287, 288
	1.5×10^{2}		Zhang et al. (2010)	Q	287, 289
	2.7×10^{2}		Zhang et al. (2010)	Q	287, 290
	5.6×10^{1}		Zhang et al. (2010)	Q	287, 291
	6.5×10^{1}		Gharagheizi et al. (2010)	Q	246
	7.7×10^{1}		Hilal et al. (2008)	Q	
		12000	Kühne et al. (2005)	Q	
	5.8		Saçan et al. (2005)	Q	
	2.1×10^{1}		Yao et al. (2002)	Q	229
	1.6×10^{1}		Bartelt-Hunt et al. (2008)	?	21
		12000	Kühne et al. (2005)	?	
	6.9×10^{1}		Yaws (1999)	?	21

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dipropyl phthalate	2.2×10^{1}		Brockbank (2013)	L	
$C_{14}H_{18}O_4$	2.4×10^{1}		Duchowicz et al. (2020)	V	186
[131-16-8]	1.8×10^{1}		Cousins and Mackay (2000)	V	516
MQHNKCZKNAJROC-UHFFFAOYSA-N	3.3		Cousins and Mackay (2000)	V	516
	3.2×10^{1}		Staples et al. (1997)	V	
	4.1×10^{1}		Duchowicz et al. (2020)	Q	
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	271, 243
	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	245
	2.4×10^{1}		Saçan et al. (2005)	Q	
diallyl phthalate	3.5×10^{1}		Saçan et al. (2005)	V	
$C_{14}H_{14}O_4$	2.3×10^{1}		Cousins and Mackay (2000)	V	
[131-17-9]	3.5×10^{1}		Staples et al. (1997)	V	
QUDWYFHPNIMBFC-UHFFFAOYSA-N	2.5×10^{1}		HSDB (2015)	Q	99
	1.7×10^{1}		Saçan et al. (2005)	Q	
bis(2-methoxyethyl) phthalate	2.3×10^{1}		Fishbein and Albro (1972)	V	12
$C_{14}H_{18}O_5$	3.5×10^{7}		HSDB (2015)	Q	99
[117-82-8]					
HSUIVCLOAAJSRE-UHFFFAOYSA-N					
dibutyl phthalate	1.1×10^{1}	12000	Brockbank (2013)	L	1, 517
$C_{16}H_{22}O_4$	9.3		Lee et al. (2012)	M	
[84-74-2]	5.5		Atlas et al. (1983)	M	72
DOIRQSBPFJWKBE-UHFFFAOYSA-N	2.2×10^{1}		Mackay et al. (2006c)	V	
	2.7×10^{1}		Saçan et al. (2005)	V	
	7.5		Cousins and Mackay (2000)	V	
	1.1×10^{1}		Staples et al. (1997)	V	
	2.2×10^{1}		Lide and Frederikse (1995)	V	
	2.0×10^{1}		Mackay et al. (1995)	V	
	2.6×10^{2}		Hwang et al. (1992)	V	
	7.6		Wolfe et al. (1980)	V	
	5.6×10^{1}		Yaws (2003)	X	237, 12
	1.6×10^{-1}		McCarty (1980)	X	368
	3.4×10^{1}		Ryan et al. (1988)	C	
	5.6×10^{1}		Gharagheizi et al. (2010)	Q	246
	2.9×10^{1}		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	67
		14000	Kühne et al. (2005)	Q	
	3.7×10^{1}		Saçan et al. (2005)	Q	
		13000	Kühne et al. (2005)	?	
	2.7×10^{1}		Yaws (1999)	?	21, 12
diisobutyl phthalate	3.5		HSDB (2015)	V	
$C_{16}H_{22}O_4$	7.5		Cousins and Mackay (2000)	V	
[84-69-5]	5.4×10^{1}		Staples et al. (1997)	V	
MGWAVDBGNNKXQV-UHFFFAOYSA-N	3.1×10^{1}		Saçan et al. (2005)	Q	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-benzenedicarboxylic acid, butyl cyclohexyl ester $C_{18}H_{24}O_4$ (butyl cyclohexyl phthalate) [84-64-0] BHKLONWXRPJNAE-UHFFFAOYSA-N	1.0×10^{1}		HSDB (2015)	Q	99
butyl glycolyl butyl phthalate $C_{18}H_{24}O_6$ [85-70-1] GOJCZVPJCKEBQV-UHFFFAOYSA-N	4.7×10^{2}		HSDB (2015)	Q	99
diamyl phthalate $C_{18}H_{26}O_4$ [131-18-0] IPKKHRVROFYTEK-UHFFFAOYSA-N	1.1×10^{1}		HSDB (2015)	Q	99
butyl benzyl phthalate	1.0×10^{2}		Lee et al. (2012)	M	
$C_{19}H_{20}O_4$	7.8		Duchowicz et al. (2020)	V	186
[85-68-7]	7.6		HSDB (2015)	V	
IRIAEXORFWYRCZ-UHFFFAOYSA-N	7.5		Mackay et al. (2006c)	V	
	1.9×10^{1}		Saçan et al. (2005)	V	
	4.9		Cousins and Mackay (2000)	V	
	1.3×10^{1}		Staples et al. (1997)	V	
	7.8		Mackay et al. (1995)	V	
	9.6		Ryan et al. (1988)	C	
	2.9×10^{2}		Duchowicz et al. (2020)	Q	
	3.2×10^{1}		Saçan et al. (2005)	Q	
	>9.9		Petrasek et al. (1983)	E	
dihexyl phthalate	8.3		Brockbank (2013)	L	
$C_{20}H_{30}O_4$	3.8×10^{-1}		Duchowicz et al. (2020)	V	186
[84-75-3]	3.8×10^{-1}		HSDB (2015)	V	
KCXZNSGUUQJJTR-UHFFFAOYSA-N	1.4		Cousins and Mackay (2000)	V	
	2.2×10^{-1}		Staples et al. (1997)	V	
	5.5×10^{1}		Duchowicz et al. (2020)	Q	
	1.6×10^{1}		Saçan et al. (2005)	Q	
butyl 2-ethylhexyl phthalate	2.1		Cousins and Mackay (2000)	V	
$C_{20}H_{30}O_4$	2.5×10^{1}		Staples et al. (1997)	V	
[85-69-8]	4.7		HSDB (2015)	Q	99
AVOLBYOSCILFLL-UHFFFAOYSA-N	6.9×10^{1}		Saçan et al. (2005)	Q	
diphenyl terephthalate	3.2×10^{2}		Zhang et al. (2010)	Q	287, 288
$C_{20}H_{14}O_4$	4.3×10^{4}		Zhang et al. (2010)	Q	287, 289
[1539-04-4]	2.7×10^{4}		Zhang et al. (2010)	Q	287, 290
HPGJOUYGWKFYQW-UHFFFAOYSA-N	7.7×10^{4}		Zhang et al. (2010)	Q	287, 291

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dicyclohexyl phthalate $C_{20}H_{26}O_4$ [84-61-7] VOWAEIGWURALJQ-UHFFFAOYSA-N	9.9×10^{1} 9.9×10^{1} 4.8×10^{2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
bis(2-butoxyethyl) phthalate $C_{20}H_{30}O_6$ [117-83-9] CMCJNODIWQEOAI-UHFFFAOYSA-N	4.9×10^{6}		HSDB (2015)	Q	99
diheptyl phthalate $C_{22}H_{34}O_4$ [3648-21-3] JQCXWCOOWVGKMT-UHFFFAOYSA-N	5.9×10^{-1} 2.8 8.9×10^{-1}		Cousins and Mackay (2000) HSDB (2015) Saçan et al. (2005)	V Q Q	 99
dioctyl phthalate $C_{24}H_{38}O_4$ [117-84-0] MQIUGAXCHLFZKX-UHFFFAOYSA-N	3.8 3.8 9.6×10^{-2} 2.5×10^{-1} 9.6×10^{-2} 1.8 1.8 8.9×10^{1} 3.4×10^{1} 6.2×10^{1} 7.2×10^{1} 6.4 >9.9 7.6×10^{1}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006c) Cousins and Mackay (2000) Staples et al. (1997) Mackay et al. (1995) Wolfe et al. (1980) Yaws (2003) Ryan et al. (1988) Duchowicz et al. (2020) Gharagheizi et al. (2010) Saçan et al. (2005) Petrasek et al. (1983) Yaws (1999)	V V V V V V V X C Q Q Q E ?	186 237, 79 246 21, 79
diisooctyl phthalate $C_{24}H_{38}O_4$ [27554-26-3] IJFPVINAQGWBRJ-UHFFFAOYSA-N	3.1×10^{-1} 3.2×10^{-1} 2.5×10^{-1} 9.5 1.5×10^{2}		Duchowicz et al. (2020) HSDB (2015) Cousins and Mackay (2000) Duchowicz et al. (2020) Saçan et al. (2005)	V V V Q Q	186
decyl hexyl phthalate $C_{24}H_{38}O_4$ [25724-58-7] OMQBXAQAHHFSST-UHFFFAOYSA-N	1.6×10^{2}		Saçan et al. (2005)	Q	
bis(2-ethylhexyl)-phthalate $C_{24}H_{38}O_4$ (DEHP) [117-81-7] BJQHLKABXJIVAM-UHFFFAOYSA-N	3.7×10^{1} 3.7×10^{1} 5.8×10^{-1} 1.4×10^{1} 2.5×10^{-1} 5.8×10^{-1} 3.7×10^{1} 6.7×10^{-1} 5.4×10^{-2}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006c) Saçan et al. (2005) Cousins and Mackay (2000) Staples et al. (1997) Mackay et al. (1995) Meylan and Howard (1991) Riederer (1990)	V V V V V V V V V	186

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{1}		Wolfe et al. (1980)	V	
	3.4×10^{1}		Ryan et al. (1988)	C	
	8.2×10^{1}		Petrasek et al. (1983)	C	
	9.5		Duchowicz et al. (2020)	Q	
	2.5×10^{1}		Saçan et al. (2005)	Q	
	8.4×10^{-1}		Meylan and Howard (1991)	Q	
	3.7×10^{1}		Bartelt-Hunt et al. (2008)	?	21
bis(2-ethylhexyl) terephthalate $C_{24}H_{38}O_4$ [6422-86-2] RWPICVVBGZBXNA-UHFFFAOYSA-N	9.9×10^{-1}		HSDB (2015)	Q	99
dinonyl phthalate $C_{26}H_{42}O_4$ [84-76-4] DROMNWUQASBTFM-UHFFFAOYSA-N	1.1×10^{-1}		Cousins and Mackay (2000)	V	
	7.0×10^{-1}		HSDB (2015)	Q	99
	3.0×10^{1}		Saçan et al. (2005)	Q	
diisononyl phthalate $C_{26}H_{42}O_4$ [28553-12-0] HBGGXOJOCNVPFY-UHFFFAOYSA-N	6.6		Duchowicz et al. (2020)	V	186
	6.6		HSDB (2015)	V	
	1.1×10^{-1}		Cousins and Mackay (2000)	V	
	9.9		Duchowicz et al. (2020)	Q	
	3.3×10^{1}		Saçan et al. (2005)	Q	
didecyl phthalate $C_{28}H_{46}O_4$ [84-77-5] PGIBJVOPLXHHGS-UHFFFAOYSA-N	4.6×10^{-2}		Cousins and Mackay (2000)	V	
	3.5×10^{-1}		HSDB (2015)	Q	99
diisodecyl phthalate $C_{28}H_{46}O_4$ [26761-40-0] ZVFDTKUVRCTHQE-UHFFFAOYSA-N	8.9		Duchowicz et al. (2020)	V	186
	9.0		HSDB (2015)	V	
	3.8×10^{1}		Saçan et al. (2005)	V	
	4.6×10^{-2}		Cousins and Mackay (2000)	V	
	1.1×10^{1}		Yaws (2003)	X	237, 79
	1.0×10^{1}		Duchowicz et al. (2020)	Q	
	1.3×10^{1}		Gharagheizi et al. (2010)	Q	246
	2.4×10^{1}		Saçan et al. (2005)	Q	
	8.9		Yaws (1999)	?	21, 79
diundecyl phthalate $C_{30}H_{50}O_4$ [3648-20-2] QQVHEQUEHCEAKS-UHFFFAOYSA-N	3.3×10^{1}		Saçan et al. (2005)	V	
	2.0×10^{-2}		Cousins and Mackay (2000)	V	
	1.8×10^{-1}		HSDB (2015)	Q	99
	1.4×10^{1}		Saçan et al. (2005)	Q	
ditridecyl phthalate $C_{34}H_{58}O_4$ [119-06-2] YCZJVRCZIPDYHH-UHFFFAOYSA-N	3.6×10^{-3}		Cousins and Mackay (2000)	V	
	4.5×10^{-2}		HSDB (2015)	Q	99
	7.9×10^{1}		Saçan et al. (2005)	Q	

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethanedioic acid, dimethyl ester	3.4		Duchowicz et al. (2020)	V	186
$C_4H_6O_4$	2.6×10^{1}		Duchowicz et al. (2020)	Q	
(dimethyl oxalate)	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
[553-90-2]	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	244
LOMVENUNSWAXEN-UHFFFAOYSA-N	3.9		Raventos-Duran et al. (2010)	Q	245
	6.9		Hilal et al. (2008)	Q	
	4.6×10^{-1}		Modarresi et al. (2007)	Q	67
ethanedioic acid, diethyl ester	4.5		Duchowicz et al. (2020)	V	186
$C_6H_{10}O_4$	6.4		Duchowicz et al. (2020)	Q	
[95-92-1]					
WYACBZDAHNBPPB-UHFFFAOYSA-N					
propanedioic acid, dimethyl ester	3.8×10^{1}	11000	Katrib et al. (2003)	M	
$C_5H_8O_4$					
(dimethyl malonate)					
[108-59-8]					
BEPAFCGSDWSTEL-UHFFFAOYSA-N					
propanedioic acid, diethyl ester	3.9	7500	Brockbank (2013)	L	1
$C_7H_{12}O_4$	4.7		Duchowicz et al. (2020)	V	186
(diethyl malonate)	7.9		Duchowicz et al. (2020)	Q	
[105-53-3]	2.0		Raventos-Duran et al. (2010)	Q	242, 243
IYXGSMUGOJNHAZ-UHFFFAOYSA-N	4.9		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	245
	3.9		Hilal et al. (2008)	Q	
	5.0×10^{-1}		Modarresi et al. (2007)	Q	67
		5900	Kühne et al. (2005)	Q	
	4.2		Bartelt-Hunt et al. (2008)	?	21
		6400	Kühne et al. (2005)	?	
	4.1		Yaws (1999)	?	21, 14
butanedioic acid, dimethyl ester	3.0×10^{1}	8500	Katrib et al. (2003)	M	
$C_6H_{10}O_4$	1.5×10^{2}		HSDB (2015)	Q	99
(dimethyl succinate)		7100	Kühne et al. (2005)	Q	
[106-65-0]		7000	Kühne et al. (2005)	?	
MUXOBHXGJLMRAB-UHFFFAOYSA-N					
diethyl succinate	1.9×10^{1}		Duchowicz et al. (2020)	V	186
$C_8H_{14}O_4$	9.3		Duchowicz et al. (2020)	Q	
[123-25-1]	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
DKMROQRQHGEIOW-UHFFFAOYSA-N	4.9		Raventos-Duran et al. (2010)	Q	244
	9.9		Raventos-Duran et al. (2010)	Q	245
	4.0		Hilal et al. (2008)	Q	
	1.3		Modarresi et al. (2007)	Q	67

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(Z)-2-butenedioic acid dimethyl ester	1.4×10^{1}		Duchowicz et al. (2020)	V	186
$C_6H_8O_4$	5.2×10^{1}		Duchowicz et al. (2020)	Q	
(dimethyl maleate)	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	271, 243
[624-48-6]	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	244
LDCRTTXIJACKKU-ARJAWSKDSA-N	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	245
	2.3×10^{1}		Hilal et al. (2008)	Q	
	1.6		Modarresi et al. (2007)	Q	67
(E)-2-butenedioic acid dimethyl ester	1.4×10^{1}		HSDB (2015)	Q	99
$C_6H_8O_4$					
(dimethyl fumarate)					
[624-49-7]					
LDCRTTXIJACKKU-ONEGZZNKSA-N					
pentanedioic acid, dimethyl ester	1.5×10^{1}		Duchowicz et al. (2020)	V	186
$C_7H_{12}O_4$	6.9×10^{1}		Duchowicz et al. (2020)	Q	
[1119-40-0]					
XTDYIOOONNVFMA-UHFFFAOYSA-N					
diethyl glutarate	1.7×10^{1}		Ebert et al. (2023)	?	316
$C_9H_{16}O_4$					
[818-38-2]					
OUWSNHWQZPEFEX-UHFFFAOYSA-N					
diethyl pimelate	2.2×10^{1}		Duchowicz et al. (2020)	V	186
$C_{11}H_{20}O_4$	1.3×10^{1}		Duchowicz et al. (2020)	Q	
[2050-20-6]	1.5		Hilal et al. (2008)	Q	
LKKOGZVQGQUVHF-UHFFFAOYSA-N	8.6×10^{-1}		Modarresi et al. (2007)	Q	67
	2.2×10^{1}		Bartelt-Hunt et al. (2008)	?	21
1,3-benzenedicarboxylic acid, diethyl ester	2.5×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_{12}H_{14}O_4$	1.9×10^{1}		Zhang et al. (2010)	Q	287, 289
[636-53-3]	2.9×10^{7}		Zhang et al. (2010)	Q	287, 290
JLVWYWVLMFVCDI-UHFFFAOYSA-N	5.6×10^{1}		Zhang et al. (2010)	Q	287, 291
dibutyl maleate	2.6×10^{1}		Duchowicz et al. (2020)	V	186
$C_{12}H_{20}O_4$	1.5×10^{1}		Duchowicz et al. (2020)	Q	
[105-76-0]	2.5		Raventos-Duran et al. (2010)	Q	271, 243
JBSLOWBPDRZSMB-FPLPWBNLSA-N	4.9		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	245
dimethyl sebacate	1.8×10^{1}		Ebert et al. (2023)	?	316
$C_{12}H_{22}O_4$					
(decanedioic acid, dimethyl ester)					
[106-79-6]					
ALOUNLDAKADEEB-UHFFFAOYSA-N					

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,6-naphthalenedicarboxylic acid, dimethyl ester	4.5×10^{2}		Zhang et al. (2010)	Q	287, 288
$C_{14}H_{12}O_4$	2.5×10^{3}		Zhang et al. (2010)	Q	287, 289
[840-65-3]	2.6×10^{7}		Zhang et al. (2010)	Q	287, 290
GYUVMLBYMPKZAZ-UHFFFAOYSA-N	1.3×10^{3}		Zhang et al. (2010)	Q	287, 291
diisooctyl adipate	1.9×10^{-1}		HSDB (2015)	Q	99
$C_{22}H_{42}O_4$					
[1330-86-5]					
CJFLBOQMPJCWLR-UHFFFAOYSA-N					
di-(2-ethylhexyl)-adipate	2.3×10^{1}		Felder et al. (1986)	M	87
$C_{22}H_{42}O_4$	4.3×10^{-1}		Hilal et al. (2008)	Q	
[103-23-1]	4.0×10^{-1}		Modarresi et al. (2007)	Q	67
SAOKZLXYCUGLFA-UHFFFAOYSA-N					
peroxybenzoic acid, *tert*-butyl ester	4.7×10^{-2}		HSDB (2015)	Q	99
$C_{11}H_{14}O_3$	4.7×10^{-2}		Zhang et al. (2010)	Q	287, 288
[614-45-9]	1.8×10^{-1}		Zhang et al. (2010)	Q	287, 289
GJBRNHKUVLOCEB-UHFFFAOYSA-N	8.2		Zhang et al. (2010)	Q	287, 290
	5.4		Zhang et al. (2010)	Q	287, 291
neodecaneperoxoic acid, 1,1-dimethylethyl ester	9.9×10^{-4}		Zhang et al. (2010)	Q	287, 288
$C_{14}H_{28}O_3$	4.7×10^{-3}		Zhang et al. (2010)	Q	287, 289
[26748-41-4]	1.2×10^{-1}		Zhang et al. (2010)	Q	287, 290
NMOALOSNPWTWRH-UHFFFAOYSA-N	2.3×10^{-2}		Zhang et al. (2010)	Q	287, 291
neoheptaneperoxoic acid, 1-methyl-1-phenylethyl ester	3.8×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{16}H_{24}O_3$	9.0×10^{-2}		Zhang et al. (2010)	Q	287, 289
[130097-36-8]	2.5		Zhang et al. (2010)	Q	287, 290
WFAUFYAGXAXBEG-UHFFFAOYSA-N	1.3		Zhang et al. (2010)	Q	287, 291
hydroxypropyl acrylate	5.8×10^{3}		HSDB (2015)	Q	99
$C_6H_{10}O_3$					
[25584-83-2]					
AYEFIAVHMUFQPZ-UHFFFAOYSA-N					
2-hydroxyethyl methacrylate	4.6×10^{1}		Duchowicz et al. (2020)	V	186
$C_6H_{10}O_3$	6.6×10^{1}		Duchowicz et al. (2020)	Q	
[868-77-9]	2.1×10^{3}		HSDB (2015)	Q	99
WOBHKFSMXKNTIM-UHFFFAOYSA-N					
2-hydroxypropyl acrylate	1.6×10^{3}		HSDB (2015)	Q	99
$C_6H_{10}O_3$					
[999-61-1]					
GWZMWHWAWHPNHN-UHFFFAOYSA-N					

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexanedioic acid, dimethyl ester $C_8H_{14}O_4$ (dimethyl adipate) [627-93-0] UDSFAEKRVUSQDD-UHFFFAOYSA-N	4.3 8.1×10^{1} 1.0×10^{1} 6.0		Duchowicz et al. (2020) Duchowicz et al. (2020) HSDB (2015) Bartelt-Hunt et al. (2008)	V Q Q ?	186 99 21
methyl 4-hydroxybenzoate $C_8H_8O_3$ (methylparaben) [99-76-3] LXCFILQKKLGQFO-UHFFFAOYSA-N	4.5×10^{3}		HSDB (2015)	Q	99
diethyl fumarate $C_8H_{12}O_4$ [623-91-6] IEPRKVQEAMIZSS-AATRIKPKSA-N	4.1×10^{2}		HSDB (2015)	Q	99
diethyl adipate $C_{10}H_{18}O_4$ [141-28-6] VIZORQUEIQEFRT-UHFFFAOYSA-N	2.7 2.7 1.2×10^{1} 3.7		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Bartelt-Hunt et al. (2008)	V V Q ?	186 21
propyl 4-hydroxybenzoate $C_{10}H_{12}O_3$ (propylparaben) [94-13-3] QELSKZZBTMNZEB-UHFFFAOYSA-N	1.5×10^{3}		HSDB (2015)	Q	99
diethylene glycol diacrylate $C_{10}H_{14}O_5$ [4074-88-8] LEJBBGNFPAFPKQ-UHFFFAOYSA-N	1.0×10^{4}		HSDB (2015)	Q	99
(2,2-dimethyl-3-prop-2-enoyloxypropyl) prop-2-enoate $C_{11}H_{16}O_4$ (2,2-dimethyltrimethylene acrylate) [2223-82-7] MXFQRSUWYYSPOC-UHFFFAOYSA-N	2.7×10^{1}		HSDB (2015)	Q	447
methyl jasmonate $C_{13}H_{20}O_3$ [1211-29-6] GEWDNTWNSAZUDX-NNOMMRTBSA-N	5.0×10^{1} 7.0×10^{2}		Karl et al. (2008) HSDB (2015)	M Q	 99
cinoxate $C_{14}H_{18}O_4$ [104-28-9] CMDKPGRTAQVGFQ-RMKNXTFCSA-N	1.9×10^{3}		HSDB (2015)	Q	447

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
trimethylolpropane triacrylate $C_{15}H_{20}O_6$ [15625-89-5] DAKWPKUUDNSNPN-UHFFFAOYSA-N	1.6×10^{4}		HSDB (2015)	Q	447
benzyl cinnamate $C_{16}H_{14}O_2$ [103-41-3] NGHOLYJTSCBCGC-VAWYXSNFSA-N	3.0×10^{1}		HSDB (2015)	Q	99
2,2,4-trimethyl-1,3-pentanediol diisobutyrate $C_{16}H_{30}O_4$ [6846-50-0] OMVSWZDEEGIJJI-UHFFFAOYSA-N	9.0×10^{-1}		HSDB (2015)	Q	99
nonanedioic acid, dibutyl ester $C_{17}H_{32}O_4$ (dibutyl azelate) [2917-73-9] RISLXYINQFKFRL-UHFFFAOYSA-N	8.2×10^{-1}		HSDB (2015)	Q	99
isopropyl myristate $C_{17}H_{34}O_2$ [110-27-0] AXISYYRBXTVTFY-UHFFFAOYSA-N	4.2×10^{-4}		HSDB (2015)	Q	99
decanedioic acid, dibutyl ester $C_{18}H_{34}O_4$ [109-43-3] PYGXAGIECVVIOZ-UHFFFAOYSA-N	2.0×10^{2} 2.1×10^{2} 1.8×10^{1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
diethylene glycol dibenzoate $C_{18}H_{18}O_5$ [120-55-8] NXQMCAOPTPLPRL-UHFFFAOYSA-N	3.3×10^{6}		HSDB (2015)	Q	99
12-hydroxy-9-octadecenoic acid, methyl ester $C_{19}H_{36}O_3$ (ricinoleic acid, methyl ester) [141-24-2] XKGDWZQXVZSXAO-RAXLEYEMSA-N	6.7×10^{1}		HSDB (2015)	Q	99
chrysanthemumic acid 2,4-dimethylbenzyl ester $C_{19}H_{26}O_2$ (dimethrin) [70-38-2] FHNKBSDJERHDHZ-UHFFFAOYSA-N	1.3×10^{-1}		HSDB (2015)	Q	99

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tributyl acetylcitrate $C_{20}H_{34}O_8$ (acetyl tributyl citrate) [77-90-7] QZCLKYGREBVARF-UHFFFAOYSA-N	2.6×10^{4}		HSDB (2015)	Q	99
hexanedioic acid, bis[2-(2-butoxyethoxy)ethyl] ester $C_{22}H_{42}O_8$ (bis(2-(2-butoxyethoxy)ethyl) adipate) [141-17-3] SCABKEBYDRTODC-UHFFFAOYSA-N	3.2×10^{7}		HSDB (2015)	Q	99
1,2-benzenedicarboxylic acid, decyl octyl ester $C_{26}H_{42}O_4$ [119-07-3] LVAGMBHLXLZJKZ-UHFFFAOYSA-N	4.7×10^{-1}		HSDB (2015)	Q	99
phthalic acid, isodecyl octyl ester $C_{26}H_{42}O_4$ [1330-96-7] UXLBXTIBYMXRNX-UHFFFAOYSA-N	4.7×10^{-1}		HSDB (2015)	Q	99
diisononyl hexahydrophthalate $C_{26}H_{48}O_4$ [166412-78-8] HORIEOQXBKUKGQ-UHFFFAOYSA-N	1.4×10^{-1}		HSDB (2015)	Q	99
decanedioic acid, bis(2-ethylhexyl) ester $C_{26}H_{50}O_4$ (bis(2-ethylhexyl) sebacate) [122-62-3] VJHINFRRDQUWOJ-UHFFFAOYSA-N	1.2×10^{-1}		HSDB (2015)	Q	99
glycerol tricaprylate $C_{27}H_{50}O_6$ (tricaprylin) [538-23-8] VLPFTAMPNXLGLX-UHFFFAOYSA-N	3.9×10^{2}		HSDB (2015)	Q	99
tris(2-ethylhexyl) trimellitate $C_{33}H_{54}O_6$ [3319-31-1] KRADHMIOFJQKEZ-UHFFFAOYSA-N	2.2×10^{1}		HSDB (2015)	Q	99
MCM:CHOOCH2OOH $C_2H_4O_4$ RHCLSHTZJFAXOU-UHFFFAOYSA-N	3.8×10^{3} 7.4×10^{2} 6.3×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CHOOCHO	3.3		Wang et al. (2017)	Q	80, 238
$C_2H_2O_3$	2.5×10^{1}		Wang et al. (2017)	Q	80, 239
VGGRCVDNFAQIKO-UHFFFAOYSA-N	1.1×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:CHOOMCO3H	4.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_3H_4O_5$	2.0×10^{3}		Wang et al. (2017)	Q	80, 239
NYMJKVCDMUPZFI-UHFFFAOYSA-N	3.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ETHFORMOOH	3.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_4$	2.9×10^{2}		Wang et al. (2017)	Q	80, 239
DJECRZORXDSOEF-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MECOFOROOH	1.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_3H_4O_5$	3.6×10^{4}		Wang et al. (2017)	Q	80, 239
TUWVUCWHUYJQAO-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:METACETHO	2.2		Wang et al. (2017)	Q	80, 238
$C_3H_4O_3$	4.4×10^{1}		Wang et al. (2017)	Q	80, 239
ORWKVZNEPHTCQE-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:METACETO2H	2.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_4$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
AIBRVUZTVKELQP-UHFFFAOYSA-N	4.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MMCF	1.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_3H_4O_4$	7.8×10^{1}		Wang et al. (2017)	Q	80, 239
IIHOUWJOSQHHHH-UHFFFAOYSA-N	3.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:MMCFOOH	1.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_3H_4O_6$	5.9×10^{5}		Wang et al. (2017)	Q	80, 239
LQGPNTLGGGGYKM-UHFFFAOYSA-N	4.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MOCOCH2OOH	2.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_4$	2.5×10^{2}		Wang et al. (2017)	Q	80, 239
OQIIXPHPHGKJRP-UHFFFAOYSA-N	5.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ACEC2H4OOH	2.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	2.0×10^{3}		Wang et al. (2017)	Q	80, 239
JNHNRXKAKFYQGM-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ACETMECO3H	3.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_5$	3.5×10^{3}		Wang et al. (2017)	Q	80, 239
UCKKJLQTXHILBL-UHFFFAOYSA-N	7.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:COO2C3CO3H	3.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_5$	2.9×10^{3}		Wang et al. (2017)	Q	80, 239
CKNWOSHDVKEZAO-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:COO2C4OOH	2.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	1.6×10^{3}		Wang et al. (2017)	Q	80, 239
KATJWBCCJXQUDM-UHFFFAOYSA-N	4.4×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

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MCM:EOCOCH2OOH	2.1×10^3		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	1.1×10^2		Wang et al. (2017)	Q	80, 239
ZDXGLRBKCRTGQP-UHFFFAOYSA-N	3.3×10^1		Wang et al. (2017)	Q	80, 240
MCM:ETHACETOOH	2.4×10^3		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	2.7×10^2		Wang et al. (2017)	Q	80, 239
FITNUWWXWGTMFO-UHFFFAOYSA-N	2.8×10^1		Wang et al. (2017)	Q	80, 240
MCM:IPRFORMOOH	2.0×10^3		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	5.1×10^1		Wang et al. (2017)	Q	80, 239
DHNDYBGDIQCRQB-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	80, 240
maleic anhydride	1.9×10^1		Wang et al. (2017)	Q	80, 238
$C_4H_2O_3$	1.2×10^5		Wang et al. (2017)	Q	80, 239
(MCM:MALANHY)	9.6		Wang et al. (2017)	Q	80, 240
[108-31-6]					
FPYJFEHAWHCUMM-UHFFFAOYSA-N					
MCM:MECOACEOOH	1.1×10^5		Wang et al. (2017)	Q	80, 238
$C_4H_6O_5$	6.6×10^4		Wang et al. (2017)	Q	80, 239
ZCPJTWSQAFRVMG-UHFFFAOYSA-N	5.3×10^2		Wang et al. (2017)	Q	80, 240
MCM:ACCOETOOH	8.7×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	5.8×10^5		Wang et al. (2017)	Q	80, 239
MRPVYADEHOUTJI-UHFFFAOYSA-N	8.1×10^3		Wang et al. (2017)	Q	80, 240
MCM:ACCOMECO3H	1.3×10^6		Wang et al. (2017)	Q	80, 238
$C_5H_6O_6$	8.5×10^5		Wang et al. (2017)	Q	80, 239
OSZJUWKUAMKWAM-UHFFFAOYSA-N	1.3×10^3		Wang et al. (2017)	Q	80, 240
MCM:ACETC2CO3H	2.5×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	3.2×10^3		Wang et al. (2017)	Q	80, 239
LEMDJBHCHPODAJ-UHFFFAOYSA-N	5.0×10^1		Wang et al. (2017)	Q	80, 240
MCM:ACETCOC2H5	1.2		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	2.5×10^1		Wang et al. (2017)	Q	80, 239
KLUDQUOLAFVLOL-UHFFFAOYSA-N	2.4		Wang et al. (2017)	Q	80, 240
MCM:BUFORMOOH	2.6×10^3		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	9.8×10^1		Wang et al. (2017)	Q	80, 239
HTFWPRQCJNWCFL-UHFFFAOYSA-N	1.3×10^1		Wang et al. (2017)	Q	80, 240
MCM:COO2C4CO3H	2.5×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	2.5×10^3		Wang et al. (2017)	Q	80, 239
XFYUESMQFXHHIL-UHFFFAOYSA-N	1.6×10^2		Wang et al. (2017)	Q	80, 240
MCM:IPRACBCO3H	2.8×10^4		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	6.9×10^2		Wang et al. (2017)	Q	80, 239
IEXBKLGSFAHQBW-UHFFFAOYSA-N	6.6		Wang et al. (2017)	Q	80, 240
MCM:IPRACBOOH	1.9×10^3		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	7.3×10^2		Wang et al. (2017)	Q	80, 239
HJBGHGSQOFAQDB-UHFFFAOYSA-N	5.3		Wang et al. (2017)	Q	80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

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MCM:IPRACOOH	1.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	5.9×10^{1}		Wang et al. (2017)	Q	80, 239
UMMAXRSQAGVERV-UHFFFAOYSA-N	1.8		Wang et al. (2017)	Q	80, 240
MCM:MMALANHY	1.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_4O_3$	2.1×10^{5}		Wang et al. (2017)	Q	80, 239
AYKYXWQEBUNJCN-UHFFFAOYSA-N	8.7		Wang et al. (2017)	Q	80, 240
MCM:MTBEAALOOH	1.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	2.3×10^{2}		Wang et al. (2017)	Q	80, 239
OJPAWJIXAIXDOD-UHFFFAOYSA-N	5.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MTBEALCO3H	2.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
GVHAIIVWIJOUAR-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NPRACAOOH	1.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	7.4×10^{2}		Wang et al. (2017)	Q	80, 239
BAISPQOWBPLMQI-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NPRACBOOH	1.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	1.5×10^{2}		Wang et al. (2017)	Q	80, 239
KUTULJFZWKOEBJ-UHFFFAOYSA-N	9.8		Wang et al. (2017)	Q	80, 240
MCM:NPRACCOOH	1.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	1.0×10^{3}		Wang et al. (2017)	Q	80, 239
GYDFEBDSBUDYEN-UHFFFAOYSA-N	5.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PRCOFORM	1.6		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	1.4×10^{1}		Wang et al. (2017)	Q	80, 239
JKMPLJUAEDQBOK-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:PRCOFOROOH	1.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	2.4×10^{5}		Wang et al. (2017)	Q	80, 239
VVRRHCGIFBEYON-UHFFFAOYSA-N	9.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PRCOOMOOH	1.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	4.9×10^{2}		Wang et al. (2017)	Q	80, 239
JALZRJAYIBRIKJ-UHFFFAOYSA-N	2.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:TLFUONE	3.2×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_2$	1.4×10^{2}		Wang et al. (2017)	Q	80, 239
BGLUXFNVVSVEET-UHFFFAOYSA-N	8.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:ACCOPROOH	8.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	2.1×10^{5}		Wang et al. (2017)	Q	80, 239
HNMHVARGKGGINS-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:ACETCOC3H7	1.0		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	1.3×10^{1}		Wang et al. (2017)	Q	80, 239
BVQHHUQLZPXYAQ-UHFFFAOYSA-N	2.4		Wang et al. (2017)	Q	80, 240

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MCM:BOCOCH2OOH	1.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	3.5×10^{1}		Wang et al. (2017)	Q	80, 239
DQCMTBDKSIDVDF-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DMMALANHY	8.1		Wang et al. (2017)	Q	80, 238
$C_6H_6O_3$	1.7×10^{5}		Wang et al. (2017)	Q	80, 239
MFGALGYVFGDXIX-UHFFFAOYSA-N	8.7		Wang et al. (2017)	Q	80, 240
MCM:EBFUONE	3.0×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_2$	7.8×10^{1}		Wang et al. (2017)	Q	80, 239
GOUILHYTHSOMQJ-UHFFFAOYSA-N	4.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:EMALANHY	1.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_3$	1.1×10^{5}		Wang et al. (2017)	Q	80, 239
AXGOOCLYBPQWNG-UHFFFAOYSA-N	5.8		Wang et al. (2017)	Q	80, 240
MCM:MCOOTBOOH	1.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	2.8×10^{2}		Wang et al. (2017)	Q	80, 239
GZZAVFPVGHHZEL-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MXYFUONE	2.2×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_2$	9.1×10^{1}		Wang et al. (2017)	Q	80, 239
SAXRUMLUKZBSTO-UHFFFAOYSA-N	3.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NBUACAOOH	1.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	5.9×10^{2}		Wang et al. (2017)	Q	80, 239
VUJYCIVMLKMZJB-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NBUACBOOH	1.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	4.4×10^{2}		Wang et al. (2017)	Q	80, 239
ZDNJENJHBNLWSZ-UHFFFAOYSA-N	6.9		Wang et al. (2017)	Q	80, 240
MCM:NBUACCOOH	1.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
CCXFYGGLIMLVCI-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PRCOOMCO3H	2.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	8.7×10^{2}		Wang et al. (2017)	Q	80, 239
NIESGQMUWIIUQP-UHFFFAOYSA-N	2.1		Wang et al. (2017)	Q	80, 240
MCM:SBUACAOOH	1.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	3.6×10^{1}		Wang et al. (2017)	Q	80, 239
XEFYSNUZBIEBQZ-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	80, 240
MCM:SBUACBOOH	1.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	3.6×10^{2}		Wang et al. (2017)	Q	80, 239
SHPWQWOSZRJPCY-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:TBUACCO3H	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	1.2×10^{2}		Wang et al. (2017)	Q	80, 239
CTLNPRHGCLAPPZ-UHFFFAOYSA-N	2.7		Wang et al. (2017)	Q	80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

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MCM:TMB1FUONE	2.2×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_2$	1.3×10^{2}		Wang et al. (2017)	Q	80, 239
GLCOTRLUPUIAFI-UHFFFAOYSA-N	3.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:IPBFUONE	2.8×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_2$	6.9×10^{1}		Wang et al. (2017)	Q	80, 239
LWFKYUIZWLTJCA-UHFFFAOYSA-N	4.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:IPMALANHY	9.3		Wang et al. (2017)	Q	80, 238
$C_7H_8O_3$	6.3×10^{4}		Wang et al. (2017)	Q	80, 239
QSWLSAYLEATCSH-UHFFFAOYSA-N	2.8		Wang et al. (2017)	Q	80, 240
MCM:MEBFUONE	2.0×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_2$	5.4×10^{1}		Wang et al. (2017)	Q	80, 239
UVERQUDHQJYTIT-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PBFUONE	2.3×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_2$	5.5×10^{1}		Wang et al. (2017)	Q	80, 239
CLCLZCBNFSGUOD-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PMALANHY	8.7		Wang et al. (2017)	Q	80, 238
$C_7H_8O_3$	6.0×10^{4}		Wang et al. (2017)	Q	80, 239
LPFJFXRQANKTRA-UHFFFAOYSA-N	4.2		Wang et al. (2017)	Q	80, 240
MCM:TMB2FUONE	1.5×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_2$	9.1×10^{1}		Wang et al. (2017)	Q	80, 239
OSFZDFIHIYXIEL-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C1013OOH	2.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_4$	9.8×10^{2}		Wang et al. (2017)	Q	80, 239
BQYOGPDLQGPEQM-UHFFFAOYSA-N	2.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C1013CO3H	2.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_5$	6.3×10^{2}		Wang et al. (2017)	Q	80, 239
ZWRGNVXICSEPNH-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PXYFUONE	2.3×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_2$	3.0×10^{2}		Wang et al. (2017)	Q	80, 239
VGHBEMPMIVEGJP-UHFFFAOYSA-N	4.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:OXYFUONE	1.6×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_2$	2.8×10^{2}		Wang et al. (2017)	Q	80, 239
QHQDWCHELGHSTO-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:CHOOCH2OH	1.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_4O_3$	6.5×10^{1}		Wang et al. (2017)	Q	80, 239
APUQIHKCZFWODD-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ETHFORMOH	1.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_3$	6.2×10^{1}		Wang et al. (2017)	Q	80, 239
JRUKHAIVAGVYRP-UHFFFAOYSA-N	7.3		Wang et al. (2017)	Q	80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:ETOHOCHO	1.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_3$	3.3×10^{2}		Wang et al. (2017)	Q	80, 239
UKQJDWBNQNAJHB-UHFFFAOYSA-N	2.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:METACETOH	9.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_3$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
JYVNDCLJHKQUHE-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MMCFOH	4.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_3H_4O_5$	1.4×10^{5}		Wang et al. (2017)	Q	80, 239
XDYLYGBFMHJJOW-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MOXCOCH2OH	5.0		Wang et al. (2017)	Q	80, 238
$C_3H_6O_3$	1.5×10^{2}		Wang et al. (2017)	Q	80, 239
GSJFXBNYJCXDGI-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ACEETOHOOH	8.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_5$	2.9×10^{4}		Wang et al. (2017)	Q	80, 239
QQYYYRFGUJQKRH-UHFFFAOYSA-N	2.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:BZFUOH	4.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_4$	3.3×10^{7}		Wang et al. (2017)	Q	80, 239
SGMJBNSHAZVGMC-UHFFFAOYSA-N	1.7×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:BZFUOOH	7.8×10^{9}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_5$	8.9×10^{7}		Wang et al. (2017)	Q	80, 239
LZJWYIKGTDPLAQ-UHFFFAOYSA-N	3.2×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:EOX2COMEOH	4.0		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	7.1×10^{1}		Wang et al. (2017)	Q	80, 239
ZANNOFHADGWOLI-UHFFFAOYSA-N	1.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ETACETOH	9.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	3.6×10^{2}		Wang et al. (2017)	Q	80, 239
HXDLWJWIAHWIKI-UHFFFAOYSA-N	3.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:ETHACETOH	8.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	7.1×10^{1}		Wang et al. (2017)	Q	80, 239
MLAFRLBDNVSLPE-UHFFFAOYSA-N	7.4		Wang et al. (2017)	Q	80, 240
MCM:HOACETEOOH	3.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_5$	5.6×10^{5}		Wang et al. (2017)	Q	80, 239
QWYGOSGRTMPWCI-UHFFFAOYSA-N	5.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:IPRFORMOH	7.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	3.2×10^{1}		Wang et al. (2017)	Q	80, 239
SVJMGLNDGCVDIT-UHFFFAOYSA-N	2.9		Wang et al. (2017)	Q	80, 240
MCM:MALANHY2OH	7.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_5$	4.8×10^{8}		Wang et al. (2017)	Q	80, 239
BOGVTNYNTGOONP-UHFFFAOYSA-N	3.9×10^{6}		Wang et al. (2017)	Q	80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MALANHYOOH	1.2×10^{12}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_6$	1.0×10^{9}		Wang et al. (2017)	Q	80, 239
UPSCPEYLZZUIND-UHFFFAOYSA-N	1.3×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:PROL2FORM	1.5×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	2.6×10^{2}		Wang et al. (2017)	Q	80, 239
CRMUFGZQBODVGS-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:BUOHFORM	8.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	3.0×10^{1}		Wang et al. (2017)	Q	80, 239
KIZCCPGSHHAFRX-UHFFFAOYSA-N	4.6		Wang et al. (2017)	Q	80, 240
MCM:IPRACBOH	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	2.0×10^{2}		Wang et al. (2017)	Q	80, 239
YJNKLTDJZSXVHQ-UHFFFAOYSA-N	2.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:IPRACOH	5.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	4.1×10^{1}		Wang et al. (2017)	Q	80, 239
MYOAZFOMGTTYOD-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	80, 240
MCM:MMALNHY2OH	3.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_5$	6.8×10^{8}		Wang et al. (2017)	Q	80, 239
DGWWNMWYNUWPBC-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:MMALNHYOOH	6.3×10^{11}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_6$	6.8×10^{8}		Wang et al. (2017)	Q	80, 239
JNCHKPBVXWMPAJ-UHFFFAOYSA-N	7.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:MTBEACHOHO	8.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	7.6×10^{1}		Wang et al. (2017)	Q	80, 239
GQMJADBSHHFADW-UHFFFAOYSA-N	8.3		Wang et al. (2017)	Q	80, 240
MCM:NPRACAOH	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	3.2×10^{2}		Wang et al. (2017)	Q	80, 239
PPPFYBPQAPISCT-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NPRACBOH	7.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	4.7×10^{1}		Wang et al. (2017)	Q	80, 239
VEGXEWGKYMMJKP-UHFFFAOYSA-N	3.2		Wang et al. (2017)	Q	80, 240
MCM:NPRACCOH	6.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	6.3×10^{2}		Wang et al. (2017)	Q	80, 239
DOUBAFNWVFAWEC-UHFFFAOYSA-N	9.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PXYFUOH	2.7×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	4.3×10^{7}		Wang et al. (2017)	Q	80, 239
OHTGZAWPVDWARE-UHFFFAOYSA-N	3.0×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:PXYFUOOH	4.5×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	4.9×10^{7}		Wang et al. (2017)	Q	80, 239
IEFDVDGOIVKGRZ-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

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MCM:TLFUOH	4.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	3.7×10^{7}		Wang et al. (2017)	Q	80, 239
JYHWQRJRDKSSIF-UHFFFAOYSA-N	7.4×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:TLFUOOH	7.3×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	1.0×10^{8}		Wang et al. (2017)	Q	80, 239
GNXADMJANDYCAE-UHFFFAOYSA-N	2.9×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:BOX2COMOH	2.9		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	2.9×10^{1}		Wang et al. (2017)	Q	80, 239
VFGRALUHHHDIQI-UHFFFAOYSA-N	9.8		Wang et al. (2017)	Q	80, 240
MCM:DMMALYOH	2.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	1.2×10^{9}		Wang et al. (2017)	Q	80, 239
KIOPGGAGDHZEGB-UHFFFAOYSA-N	4.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:DMMALYOOH	3.5×10^{11}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_6$	8.9×10^{8}		Wang et al. (2017)	Q	80, 239
VRKLPKITGMCVQP-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:EBFUOH	4.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	3.5×10^{7}		Wang et al. (2017)	Q	80, 239
AQSJHOPJZAKOAP-UHFFFAOYSA-N	3.7×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:EBFUOOH	6.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	8.5×10^{7}		Wang et al. (2017)	Q	80, 239
KIZOVCBYCQGADC-UHFFFAOYSA-N	7.6×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:EMALNHY2OH	3.6×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	8.3×10^{8}		Wang et al. (2017)	Q	80, 239
GPJQUVLKFIAXFZ-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:EMALNHYOOH	5.0×10^{11}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_6$	8.5×10^{8}		Wang et al. (2017)	Q	80, 239
LSSHMOINJMVLHQ-UHFFFAOYSA-N	6.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:MXYFUOH	2.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	3.7×10^{7}		Wang et al. (2017)	Q	80, 239
WCMYKJKBZGIGND-UHFFFAOYSA-N	3.0×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:MXYFUOOH	4.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	2.8×10^{7}		Wang et al. (2017)	Q	80, 239
WCIMCWKIICZLLM-UHFFFAOYSA-N	3.6×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:NBUACAOH	5.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	6.5×10^{2}		Wang et al. (2017)	Q	80, 239
KLUHZXMBIDAHSJ-UHFFFAOYSA-N	6.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NBUACBOH	8.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	2.1×10^{2}		Wang et al. (2017)	Q	80, 239
BZLQSYFOTWOIDC-UHFFFAOYSA-N	5.1×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

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MCM:NBUACCOH	5.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	3.6×10^{1}		Wang et al. (2017)	Q	80, 239
BMNRJWUOBYYCRX-UHFFFAOYSA-N	2.7		Wang et al. (2017)	Q	80, 240
MCM:OXYFUOH	1.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	3.2×10^{7}		Wang et al. (2017)	Q	80, 239
GZKXVWYDQQSODI-UHFFFAOYSA-N	1.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:OXYFUOOH	2.4×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	2.3×10^{7}		Wang et al. (2017)	Q	80, 239
DHHFHIZBMAEZJT-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:PRCOOETOH	6.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.3×10^{2}		Wang et al. (2017)	Q	80, 239
GIOCILWWMFZESP-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:SBUACAOH	4.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	3.2×10^{1}		Wang et al. (2017)	Q	80, 239
WAXXMBOGFVJIHX-UHFFFAOYSA-N	7.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:SBUACBOH	9.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.7×10^{2}		Wang et al. (2017)	Q	80, 239
BCWWODMTUXMSAB-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:TBOCOCH2OH	2.0		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.7×10^{1}		Wang et al. (2017)	Q	80, 239
WINGEFIITRDOLJ-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	80, 240
MCM:TBUACOH	4.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	9.1×10^{1}		Wang et al. (2017)	Q	80, 239
GWOKHTMCBUZSOP-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:TMB1FUOH	2.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	2.2×10^{7}		Wang et al. (2017)	Q	80, 239
AUTABLFJFWRKGZ-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:TMB1FUOOH	1.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	7.4×10^{7}		Wang et al. (2017)	Q	80, 239
NFODFJMABSYJFC-UHFFFAOYSA-N	4.2×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:BOXCOOLOOH	2.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_5$	2.4×10^{5}		Wang et al. (2017)	Q	80, 239
PDOIGHDIMNJPNL-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:IPBFUOH	3.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	3.0×10^{7}		Wang et al. (2017)	Q	80, 239
ZIPHTXAVHSYMQR-UHFFFAOYSA-N	5.3×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:IPBFUOOH	5.4×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	7.8×10^{7}		Wang et al. (2017)	Q	80, 239
HVQWCSPFZPPNOE-UHFFFAOYSA-N	2.1×10^{6}		Wang et al. (2017)	Q	80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

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MCM:IPMLNHY2OH	3.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	1.2×10^{9}		Wang et al. (2017)	Q	80, 239
RBIJYTIBBLMIRU-UHFFFAOYSA-N	4.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:IPMLNHYOOH	4.7×10^{11}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_6$	1.1×10^{9}		Wang et al. (2017)	Q	80, 239
LGGLTRMSNOIPLU-UHFFFAOYSA-N	9.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:MEBFUOH	2.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	2.2×10^{7}		Wang et al. (2017)	Q	80, 239
SYHJYGJIPQZFIO-UHFFFAOYSA-N	1.6×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:MEBFUOOH	3.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	1.7×10^{7}		Wang et al. (2017)	Q	80, 239
VRHMFTJWRSNJLN-UHFFFAOYSA-N	2.2×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:PBFUOH	3.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	2.4×10^{7}		Wang et al. (2017)	Q	80, 239
DMMDFVMQHRHVSU-UHFFFAOYSA-N	5.6×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:PBFUOOH	5.3×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	6.2×10^{7}		Wang et al. (2017)	Q	80, 239
KAMUACRVJWJEFX-UHFFFAOYSA-N	6.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PMALNHY2OH	2.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	8.9×10^{8}		Wang et al. (2017)	Q	80, 239
PVDNZCIFUUKKBS-UHFFFAOYSA-N	1.3×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:PMALNHYOOH	4.1×10^{11}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_6$	8.0×10^{8}		Wang et al. (2017)	Q	80, 239
VKSMRBCXNQEUFP-UHFFFAOYSA-N	4.4×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PRCOOPROL	6.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_3$	1.3×10^{2}		Wang et al. (2017)	Q	80, 239
QXXGFEMAULVMST-UHFFFAOYSA-N	4.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:TMB2FUOH	1.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_4$	1.8×10^{7}		Wang et al. (2017)	Q	80, 239
YEQCQVSGZKCWAA-UHFFFAOYSA-N	1.3×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:TMB2FUOOH	2.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	1.2×10^{7}		Wang et al. (2017)	Q	80, 239
MINPHQZFUPUEBD-UHFFFAOYSA-N	3.6×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C1013OH	7.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_3$	5.4×10^{2}		Wang et al. (2017)	Q	80, 239
OYGVMQZTRRRABW-UHFFFAOYSA-N	3.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ALCOMOXOOH	2.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_3H_4O_5$	1.6×10^{5}		Wang et al. (2017)	Q	80, 239
DRQRCDXSDDWNEU-UHFFFAOYSA-N	9.3×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DFC	1.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_2O_5$	6.9×10^{3}		Wang et al. (2017)	Q	80, 239
DOMHJQJKOPZSOM-UHFFFAOYSA-N	1.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:MOXY2CHO	3.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_3H_4O_3$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
MFRMAQFRVTUENW-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MOXYCOCHO	3.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_3H_4O_3$	3.2×10^{1}		Wang et al. (2017)	Q	80, 239
KFKXSMSQHIOMSO-UHFFFAOYSA-N	6.5×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:ACETETCHO	2.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_3$	1.8×10^{2}		Wang et al. (2017)	Q	80, 239
GUPGZURVZDIQPM-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO14O3CHO	2.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_4$	1.2×10^{4}		Wang et al. (2017)	Q	80, 239
ZFWWLKBCHQUFEJ-UHFFFAOYSA-N	8.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:COO2C3CHO	2.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_3$	5.4×10^{1}		Wang et al. (2017)	Q	80, 239
AGADEVQOWQDDFX-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:EOCOCHO	2.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_3$	1.7×10^{1}		Wang et al. (2017)	Q	80, 239
DBPFRRFGLYGEJI-UHFFFAOYSA-N	8.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:ACCOMECHO	1.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_4$	1.6×10^{4}		Wang et al. (2017)	Q	80, 239
GRUDDVNYUQQBCU-UHFFFAOYSA-N	9.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ACEC2CHO	2.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	1.7×10^{2}		Wang et al. (2017)	Q	80, 239
PRSPLAWXBFRHKV-UHFFFAOYSA-N	7.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:COO2C4CHO	2.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	1.3×10^{2}		Wang et al. (2017)	Q	80, 239
DLZVZNAPRCRXEG-UHFFFAOYSA-N	3.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:IPRACBCHO	2.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	3.9×10^{1}		Wang et al. (2017)	Q	80, 239
FXPPNKAYSGWCQG-UHFFFAOYSA-N	5.0		Wang et al. (2017)	Q	80, 240
MCM:MTBEACHO13	1.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	5.8		Wang et al. (2017)	Q	80, 239
MDWWHOIDIKOPHH-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	80, 240
MCM:BOXCOALOOH	1.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	2.0×10^{4}		Wang et al. (2017)	Q	80, 239
MZUJTBRWESAMQA-UHFFFAOYSA-N	4.4×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:BOXCOCHO	1.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	6.0		Wang et al. (2017)	Q	80, 239
NRYDRJHYTRBBEA-UHFFFAOYSA-N	1.5×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C14O3ECHO	1.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	3.3×10^{3}		Wang et al. (2017)	Q	80, 239
FVLOJCOPOCRBFF-UHFFFAOYSA-N	5.6		Wang et al. (2017)	Q	80, 240
MCM:PRCOOMCHO	1.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	4.7×10^{1}		Wang et al. (2017)	Q	80, 239
YEBNSRBQIIWQQC-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:TBOCOCHO	1.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	3.6		Wang et al. (2017)	Q	80, 239
WDPZTIFGRQKSEN-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:TBUACCO	1.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	6.6		Wang et al. (2017)	Q	80, 239
BYYPPVMBDPUHHR-UHFFFAOYSA-N	5.5		Wang et al. (2017)	Q	80, 240
MCM:C14O3IPCHO	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	2.3×10^{3}		Wang et al. (2017)	Q	80, 239
NPPWDFRKAMDHMM-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	80, 240
MCM:C14O3PCHO	1.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	2.1×10^{3}		Wang et al. (2017)	Q	80, 239
GNODSIBUYMXKGR-UHFFFAOYSA-N	3.6		Wang et al. (2017)	Q	80, 240
MCM:C1014OOH	5.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_5$	8.3×10^{4}		Wang et al. (2017)	Q	80, 239
REYZAYCUYYNPLJ-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:BCALBOC	2.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{24}O_3$	3.0×10^{1}		Wang et al. (2017)	Q	80, 239
FEPYZLRQFOQWRK-UHFFFAOYSA-N	8.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CHOOMCO2H	4.7×10^{5}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_4$	1.9×10^{5}		Wang et al. (2017)	Q	80, 239
CBNAABWGSNQFTA-UHFFFAOYSA-N	8.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C1014OH	1.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{18}O_4$	2.1×10^{5}		Wang et al. (2017)	Q	80, 239
IJPJFXOOJHUBTK-UHFFFAOYSA-N	9.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C152OH	2.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{26}O_5$	1.0×10^{8}		Wang et al. (2017)	Q	80, 239
XZXFZFZFZSKVDT-UHFFFAOYSA-N	1.7×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C152OOH	2.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{26}O_6$	2.2×10^{8}		Wang et al. (2017)	Q	80, 239
PKQOWOPWICZSPN-UHFFFAOYSA-N	5.1×10^{7}		Wang et al. (2017)	Q	80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C23O3CHO	1.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_4$	7.3×10^{3}		Wang et al. (2017)	Q	80, 239
RULCSXTUAHNYHJ-UHFFFAOYSA-N	6.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:MCOCOMOOOH	1.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_5$	2.5×10^{5}		Wang et al. (2017)	Q	80, 239
BJTKGFWDIAZUGI-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:MCOCOMOX	2.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_3$	3.0×10^{1}		Wang et al. (2017)	Q	80, 239
CWKLZLBVOJRSOM-UHFFFAOYSA-N	4.3		Wang et al. (2017)	Q	80, 240
MCM:PRNFORMOOH	2.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_5$	5.4×10^{3}		Wang et al. (2017)	Q	80, 239
LIFMXPSJWIBAGH-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PRONFORM	2.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_6O_3$	1.5×10^{2}		Wang et al. (2017)	Q	80, 239
WNVAJGCMEDTLIE-UHFFFAOYSA-N	3.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ACCOCOMOOH	6.8×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_6$	3.2×10^{6}		Wang et al. (2017)	Q	80, 239
WKJHUBLAYZIBAJ-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:ACECOCOCH3	8.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_4$	9.1×10^{3}		Wang et al. (2017)	Q	80, 239
OBTVATRSWTWNGS-UHFFFAOYSA-N	8.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:ACEPROPONE	1.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	1.8×10^{2}		Wang et al. (2017)	Q	80, 239
DBERHVIZRVGDFO-UHFFFAOYSA-N	8.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ACPRONEOOH	1.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	5.5×10^{3}		Wang et al. (2017)	Q	80, 239
FOWIMBLOPIOWII-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C23O3CCO3H	1.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_6$	5.5×10^{5}		Wang et al. (2017)	Q	80, 239
SPYAIQASSDQEIX-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C23O3MCOOH	1.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	6.6×10^{4}		Wang et al. (2017)	Q	80, 239
RVGUYYZMHBERKG-UHFFFAOYSA-N	6.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PRNOCOMOOH	1.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	2.2×10^{5}		Wang et al. (2017)	Q	80, 239
GJTAOZDAMDVHTP-UHFFFAOYSA-N	8.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:ACBUOAOOH	1.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	1.1×10^{5}		Wang et al. (2017)	Q	80, 239
BDHJVYCZNHBETI-UHFFFAOYSA-N	3.8×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:ACBUONBOOH	1.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	2.5×10^{3}		Wang et al. (2017)	Q	80, 239
RISONYRIGLPILV-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:ACCOCOC2H5	6.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	4.7×10^{3}		Wang et al. (2017)	Q	80, 239
WZGYRWNUCYXCFD-UHFFFAOYSA-N	3.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:ACCOCOEOOH	6.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_6$	1.5×10^{6}		Wang et al. (2017)	Q	80, 239
RKPSGJVLERUIIG-UHFFFAOYSA-N	2.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:ACCOPRONE	6.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	1.6×10^{4}		Wang et al. (2017)	Q	80, 239
RYLHMXPGTMYTTF-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:ACEBUTBONE	1.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	8.1×10^{1}		Wang et al. (2017)	Q	80, 239
LHGWJCBYBIICPP-UHFFFAOYSA-N	4.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ACEBUTONE	1.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	1.8×10^{2}		Wang et al. (2017)	Q	80, 239
NWCYECXHIYEBJE-UHFFFAOYSA-N	5.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:ACOMCOMOOH	5.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_6$	5.4×10^{6}		Wang et al. (2017)	Q	80, 239
NKXSSYAJYGYQPN-UHFFFAOYSA-N	4.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C23O3ECOOH	1.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	3.0×10^{4}		Wang et al. (2017)	Q	80, 239
NLYPTRYHUBHKKI-UHFFFAOYSA-N	4.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C23O3EHO	6.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	4.6×10^{3}		Wang et al. (2017)	Q	80, 239
AIDIMUPPUNPUTI-UHFFFAOYSA-N	3.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C23O3MCO3H	1.5×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_6$	1.1×10^{5}		Wang et al. (2017)	Q	80, 239
FIPISRZHVPVVNA-UHFFFAOYSA-N	9.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C6O4KETOOH	3.6×10^{10}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_7$	3.8×10^{8}		Wang et al. (2017)	Q	80, 239
LLKUMVBDCSCXDR-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C6OTKETCO	5.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_5$	1.0×10^{6}		Wang et al. (2017)	Q	80, 239
GAPVBMQBWAUBHC-UHFFFAOYSA-N	3.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C6OTKETOOH	7.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_6$	8.3×10^{5}		Wang et al. (2017)	Q	80, 239
USMDUVUWRKQXQG-UHFFFAOYSA-N	6.8×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C6OTRIKET	1.0×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	2.4×10^4		Wang et al. (2017)	Q	80, 239
XAHWCAXZWOTSBC-UHFFFAOYSA-N	5.1×10^2		Wang et al. (2017)	Q	80, 240
MCM:CO356OCOOH	6.0×10^7		Wang et al. (2017)	Q	80, 238
$C_6H_8O_6$	4.5×10^6		Wang et al. (2017)	Q	80, 239
MVKXXKVCXUKLOS-UHFFFAOYSA-N	1.6×10^2		Wang et al. (2017)	Q	80, 240
MCM:SBUACCOOH	8.1×10^5		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_5$	5.3×10^2		Wang et al. (2017)	Q	80, 239
DTGNYNGASXJUMP-UHFFFAOYSA-N	1.3×10^1		Wang et al. (2017)	Q	80, 240
MCM:SBUACEONE	1.6×10^1		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_3$	3.3×10^1		Wang et al. (2017)	Q	80, 239
ZKPTYCJWRHHBOW-UHFFFAOYSA-N	2.0×10^1		Wang et al. (2017)	Q	80, 240
MCM:BOX2COMOOH	9.1×10^5		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	2.1×10^4		Wang et al. (2017)	Q	80, 239
YCDXONIQHOVSSF-UHFFFAOYSA-N	3.2×10^2		Wang et al. (2017)	Q	80, 240
MCM:BOXCOCOME	1.2×10^1		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_3$	6.3		Wang et al. (2017)	Q	80, 239
ZAZUOXBHFXAWMD-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	80, 240
MCM:C23O3ECO3H	1.4×10^7		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_6$	5.1×10^4		Wang et al. (2017)	Q	80, 239
FWVKIPPVGIEQRB-UHFFFAOYSA-N	8.1×10^1		Wang et al. (2017)	Q	80, 240
MCM:MC6OTKTOOH	4.5×10^8		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_6$	9.3×10^4		Wang et al. (2017)	Q	80, 239
DJTBKMNUYULRIV-UHFFFAOYSA-N	1.4×10^3		Wang et al. (2017)	Q	80, 240
MCM:MC6OTRIKET	9.6×10^3		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	5.9×10^3		Wang et al. (2017)	Q	80, 239
FJYCWZCSXDGURV-UHFFFAOYSA-N	2.6×10^2		Wang et al. (2017)	Q	80, 240
MCM:PRCOOPRONE	1.2×10^1		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_3$	5.0×10^1		Wang et al. (2017)	Q	80, 239
AIJLJYUDTAJRDN-UHFFFAOYSA-N	3.8×10^1		Wang et al. (2017)	Q	80, 240
MCM:PRNOCOPOOH	9.1×10^5		Wang et al. (2017)	Q	80, 238
$C_7H_{12}O_5$	6.8×10^5		Wang et al. (2017)	Q	80, 239
RGEURRORAZXRIV-UHFFFAOYSA-N	1.7×10^4		Wang et al. (2017)	Q	80, 240
MCM:C1013CO	1.6×10^1		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_3$	8.3×10^1		Wang et al. (2017)	Q	80, 239
DPRGOCIPALHGLN-UHFFFAOYSA-N	6.5×10^2		Wang et al. (2017)	Q	80, 240
MCM:BZFUCO	1.2×10^4		Wang et al. (2017)	Q	80, 238
$C_4H_4O_4$	4.2×10^6		Wang et al. (2017)	Q	80, 239
MFFNSLKCUZEAFI-UHFFFAOYSA-N	1.1×10^5		Wang et al. (2017)	Q	80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MALNHYOHCO	2.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_4H_2O_5$	1.0×10^{9}		Wang et al. (2017)	Q	80, 239
DBWAPECJPVXLJZ-UHFFFAOYSA-N	1.1×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:ACPRONEOH	2.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	1.3×10^{4}		Wang et al. (2017)	Q	80, 239
LBOLMEABDOYQGX-UHFFFAOYSA-N	7.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C23O3MOH	4.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	2.0×10^{4}		Wang et al. (2017)	Q	80, 239
WHFDSTOTVFOUIH-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:ACBUONAOH	4.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	5.1×10^{4}		Wang et al. (2017)	Q	80, 239
UGJVDYQVVBKWGL-UHFFFAOYSA-N	2.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:ACBUONBOH	2.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	6.8×10^{3}		Wang et al. (2017)	Q	80, 239
GYQPXJWBTJDNGC-UHFFFAOYSA-N	7.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C23O3EOH	4.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
BVDDSYZMRAYYIJ-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C6OTKETOH	4.4×10^{4}	16000	Wieser et al. (2023)	Q	437
$C_6H_8O_5$	1.5×10^{6}		Wang et al. (2017)	Q	80, 238
NOUUUBJIFPBZMZ-UHFFFAOYSA-N	2.0×10^{6}		Wang et al. (2017)	Q	80, 239
	6.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:EBFUCO	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	5.0×10^{6}		Wang et al. (2017)	Q	80, 239
QFGGPABGKQEYQI-UHFFFAOYSA-N	7.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:SBUACCOH	1.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}O_4$	4.5×10^{3}		Wang et al. (2017)	Q	80, 239
SUDJMSTXSVVFNQ-UHFFFAOYSA-N	5.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:IPBFUCO	9.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	4.6×10^{6}		Wang et al. (2017)	Q	80, 239
NHSFIZKDULUUEP-UHFFFAOYSA-N	6.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:MC6OTKETOH	8.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	7.1×10^{5}		Wang et al. (2017)	Q	80, 239
GQVIXHCRVNFYGI-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:PBFUCO	8.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	3.6×10^{6}		Wang et al. (2017)	Q	80, 239
PKKIVTPUHZVJRM-UHFFFAOYSA-N	7.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C23O3CCHO	1.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_4$	2.1×10^{4}		Wang et al. (2017)	Q	80, 239
JQZIMULKJBYVEJ-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C23O3MCHO	1.4×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	6.0×10^3		Wang et al. (2017)	Q	80, 239
KNKMVXKCHLTCEX-UHFFFAOYSA-N	8.1×10^1		Wang et al. (2017)	Q	80, 240
MCM:C5OCO3M	1.4×10^4		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	5.6×10^3		Wang et al. (2017)	Q	80, 239
MFFVRQLCBYBQSQ-UHFFFAOYSA-N	4.8×10^1		Wang et al. (2017)	Q	80, 240
MCM:C23O3ECHO	1.1×10^4		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	3.2×10^3		Wang et al. (2017)	Q	80, 239
RCPFVGJRKWBYKE-UHFFFAOYSA-N	4.6×10^1		Wang et al. (2017)	Q	80, 240
MCM:C1014CO	4.6×10^3		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_4$	2.0×10^4		Wang et al. (2017)	Q	80, 239
MPJVRMHYAPYGFM-UHFFFAOYSA-N	4.8×10^3		Wang et al. (2017)	Q	80, 240
MCM:BCLKBOC	7.8×10^3		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_4$	3.6×10^4		Wang et al. (2017)	Q	80, 239
YETGIZICMMLUOK-UHFFFAOYSA-N	5.6×10^4		Wang et al. (2017)	Q	80, 240
MCM:C148CO	5.8×10^6		Wang et al. (2017)	Q	80, 238
$C_{14}H_{20}O_5$	3.5×10^5		Wang et al. (2017)	Q	80, 239
WKRISEJACIFSSJ-UHFFFAOYSA-N	1.5×10^3		Wang et al. (2017)	Q	80, 240
MCM:C148OOH	6.8×10^8		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_6$	3.0×10^6		Wang et al. (2017)	Q	80, 239
QNGFZXSUHFZFIE-UHFFFAOYSA-N	4.4×10^4		Wang et al. (2017)	Q	80, 240
MCM:C148OH	1.3×10^6		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_5$	7.6×10^6		Wang et al. (2017)	Q	80, 239
LXDPLKVHKWYPKP-UHFFFAOYSA-N	9.8×10^4		Wang et al. (2017)	Q	80, 240
MCM:ACETC2CO2H	2.9×10^3		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	4.8×10^4		Wang et al. (2017)	Q	80, 239
RFEXARYJXBYPLD-UHFFFAOYSA-N	6.5×10^4		Wang et al. (2017)	Q	80, 240
MCM:C24O3CCO2H	1.6×10^5		Wang et al. (2017)	Q	80, 238
$C_5H_6O_5$	3.5×10^6		Wang et al. (2017)	Q	80, 239
HSSKPURIBYAXCO-UHFFFAOYSA-N	7.3×10^4		Wang et al. (2017)	Q	80, 240
MCM:IPRACBCO2H	3.5×10^3		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	6.9×10^3		Wang et al. (2017)	Q	80, 239
WTLNOANVTIKPEE-UHFFFAOYSA-N	5.0×10^3		Wang et al. (2017)	Q	80, 240
MCM:MTBEALCO2H	2.8×10^3		Wang et al. (2017)	Q	80, 238
$C_5H_8O_4$	2.1×10^3		Wang et al. (2017)	Q	80, 239
BXXOFUQIACXFIW-UHFFFAOYSA-N	2.0×10^3		Wang et al. (2017)	Q	80, 240
MCM:C1013CO2H	3.0×10^3		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_4$	3.1×10^4		Wang et al. (2017)	Q	80, 239
QWGCLZMSSSTRLX-UHFFFAOYSA-N	5.0×10^4		Wang et al. (2017)	Q	80, 240

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Table A3.8: Esters (RCOOR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CO14O3CO2H	3.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_5$	5.4×10^{4}		Wang et al. (2017)	Q	80, 239
OPFWUCMVKDVVTF-UHFFFAOYSA-N	1.7×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C23O3CCO2H	2.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_5$	9.1×10^{6}		Wang et al. (2017)	Q	80, 239
WRKCXTWVOWDGBE-UHFFFAOYSA-N	1.7×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C23O3MCO2H	2.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	1.6×10^{6}		Wang et al. (2017)	Q	80, 239
OGSBZWITKXVLIV-UHFFFAOYSA-N	9.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C23O3ECO2H	1.7×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	6.0×10^{5}		Wang et al. (2017)	Q	80, 239
OEONINCNUUTEPU-UHFFFAOYSA-N	2.5×10^{4}		Wang et al. (2017)	Q	80, 240

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A3.9 Ethers (ROR)

Table A3.9: Ethers (ROR)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dimethyl ether	9.9×10^{-3}		Duchowicz et al. (2020)	V	186
CH_3OCH_3	1.7×10^{-3}		HSDB (2015)	V	
[115-10-6]	7.6×10^{-2}		Mackay et al. (2006c)	V	
LCGLNKUTAGEVQW-UHFFFAOYSA-N	1.3×10^{-1}		Mackay et al. (1993)	V	
	9.9×10^{-3}		Hine and Mookerjee (1975)	V	
	9.8×10^{-3}		Hine and Weimar (1965)	R	
	1.0×10^{-2}	4900	Bagno et al. (1991)	T	473
	1.5×10^{-2}		Yaws (2003)	X	237, 28
	6.5×10^{-3}		Hayer et al. (2022)	Q	20
	5.1×10^{-2}		Duchowicz et al. (2020)	Q	
	3.0×10^{-3}		Wang et al. (2017)	Q	80, 238
	3.0×10^{-2}		Wang et al. (2017)	Q	80, 239
	1.1×10^{-2}		Wang et al. (2017)	Q	80, 240
	7.1×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
	1.8×10^{-2}		Hilal et al. (2008)	Q	
	1.4×10^{-2}		Modarresi et al. (2007)	Q	67
	7.5×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	8.4×10^{-3}		Katritzky et al. (1998)	Q	
	2.2×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	5.3×10^{-2}		Russell et al. (1992)	Q	358
	1.2×10^{-2}		Suzuki et al. (1992)	Q	232
	1.5×10^{-2}		Yaws (1999)	?	21, 28
	6.2×10^{-3}		Abraham and Weathersby (1994)	?	21
	9.9×10^{-3}		Abraham et al. (1990)	?	
ethyl methyl ether	8.2×10^{-3}		Duchowicz et al. (2020)	V	186
$C_2H_5OCH_3$	1.4×10^{-2}		Bagno et al. (1991)	T	473
[540-67-0]	1.9×10^{-2}		Duchowicz et al. (2020)	Q	
XOBKSJJDNFUZPF-UHFFFAOYSA-N	1.5×10^{-2}		HSDB (2015)	Q	99
	1.5×10^{-2}		Hilal et al. (2008)	Q	
	3.0×10^{-2}		English and Carroll (2001)	Q	230, 231
	9.7×10^{-3}		Katritzky et al. (1998)	Q	
	1.9×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	8.9×10^{-3}		Saxena and Hildemann (1996)	E	401
	1.8×10^{-2}		Yaws (1999)	?	21
diethyl ether	9.9×10^{-3}	5800	Burkholder et al. (2019)	L	1
$C_2H_5OC_2H_5$	2.0×10^{-2}	5800	Burkholder et al. (2015)	L	
[60-29-7]	9.9×10^{-3}	5800	Brockbank (2013)	L	1
RTZKZFJDLAIYFH-UHFFFAOYSA-N	5.0×10^{-3}		Steward et al. (1973)	L	14
	9.6×10^{-3}	5000	Allott et al. (1973)	L	
	1.1×10^{-2}	6600	Hiatt (2013)	M	
	9.5×10^{-2}		Helburn et al. (2008)	M	
	1.0×10^{-2}	5700	Ondo and Dohnal (2007)	M	1
	1.1×10^{-2}		Nielsen et al. (1994)	M	

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.3×10^{-3}		Yu (1992)	M	12
	7.0×10^{-3}	3900	Lamarche and Droste (1989)	M	345
	6.3×10^{-3}		Guitart et al. (1989)	M	14
	1.3×10^{-2}	7400	Bachofen and Farhi (1971)	M	
	6.3×10^{-3}		Brody et al. (1971)	M	14
	7.8×10^{-3}		Signer et al. (1969)	M	
	5.1×10^{-3}		Eger et al. (1963)	M	14
	1.1×10^{-2}		Mackay et al. (2006c)	V	
	1.0×10^{-2}	5800	Fukuchi et al. (2002)	V	
	1.1×10^{-2}		Mackay et al. (1993)	V	
	8.7×10^{-3}		Hwang et al. (1992)	V	
	1.1×10^{-2}		Hine and Weimar (1965)	V	
	1.1×10^{-2}		Butler and Ramchandani (1935)	V	
	6.0×10^{-3}	5700	Bagno et al. (1991)	T	473
	1.2×10^{-2}		Yaws (2003)	X	237
	4.3×10^{-3}		Keshavarz et al. (2022)	Q	
	6.8×10^{-3}		Duchowicz et al. (2020)	Q	184
	2.1×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.6×10^{-2}		Wang et al. (2017)	Q	80, 239
	2.2×10^{-3}		Wang et al. (2017)	Q	80, 240
	7.7×10^{-3}		Li et al. (2014)	Q	241
	1.3×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
	7.0×10^{-3}		Hilal et al. (2008)	Q	
	1.3×10^{-2}		Modarresi et al. (2007)	Q	67
		5300	Kühne et al. (2005)	Q	
	8.6×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	2.4×10^{-2}		English and Carroll (2001)	Q	230, 231
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
	1.7×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	4.6×10^{-2}		Russell et al. (1992)	Q	279
	7.3×10^{-3}		Suzuki et al. (1992)	Q	232
	8.0×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		5700	Kühne et al. (2005)	?	
	1.2×10^{-2}		Yaws (1999)	?	21
	5.8×10^{-3}		Abraham and Weathersby (1994)	?	21
	7.7×10^{-3}		Hoff et al. (1993)	?	21
	6.0×10^{-3}		Abraham et al. (1990)	?	
diethyl ether-d10 $C_2D_5OC_2D_5$ [2679-89-2] RTZKZFJDLAIYFH-MWUKXHIBSA-N	1.3×10^{-2}	6500	Hiatt (2013)	M	

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl propyl ether	6.6×10^{-3}		Duchowicz et al. (2020)	V	186
$CH_3OC_3H_7$	6.7×10^{-3}		Meylan and Howard (1991)	V	
[557-17-5]	6.7×10^{-3}		Hine and Mookerjee (1975)	V	
VNKYTQGIUYNRMY-UHFFFAOYSA-N	6.9×10^{-3}		Yaws (2003)	X	237
	2.0×10^{-2}		Duchowicz et al. (2020)	Q	
	5.2×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	8.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.1×10^{-2}		Hilal et al. (2008)	Q	
	6.9×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.1×10^{-2}		Katritzky et al. (1998)	Q	
	1.5×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	7.3×10^{-3}		Suzuki et al. (1992)	Q	232
	6.5×10^{-3}		Meylan and Howard (1991)	Q	
	6.9×10^{-3}		Yaws (1999)	?	21
methyl 2-propyl ether	1.1×10^{-2}		Duchowicz et al. (2020)	V	186
$CH_3OC_3H_7$	1.2×10^{-2}		Hine and Mookerjee (1975)	V	
(methyl isopropyl ether)	1.2×10^{-2}		Yaws (2003)	X	258
[598-53-8]	1.1×10^{-2}		Yaws (2003)	X	237
RMGHERXMTMUMMV-UHFFFAOYSA-N	7.1×10^{-3}		Dupeux et al. (2022)	Q	259
	7.8×10^{-3}		Duchowicz et al. (2020)	Q	
	1.4×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
	8.2×10^{-3}		Hilal et al. (2008)	Q	
	1.2×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.1×10^{-2}		Katritzky et al. (1998)	Q	
	6.5×10^{-3}		Suzuki et al. (1992)	Q	232
	1.1×10^{-2}		Yaws (1999)	?	21
divinyl ether	5.4×10^{-4}		Steward et al. (1973)	L	14
C_4H_6O	5.4×10^{-4}		Allott et al. (1973)	L	14
[109-93-3]	1.2×10^{-3}		Duchowicz et al. (2020)	V	186
QYKIQEUNHZKYBP-UHFFFAOYSA-N	5.6×10^{-4}		Yaws (2003)	X	237, 14
	7.3×10^{-2}		Duchowicz et al. (2020)	Q	
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	6.0×10^{-4}		Gharagheizi et al. (2010)	Q	246
	3.8×10^{-4}		Hilal et al. (2008)	Q	
	2.0×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	5.8×10^{-4}		Abraham and Weathersby (1994)	?	21

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl butyl ether	6.6×10^{-3}	6100	Brockbank (2013)	L	1, 518
$C_5H_{12}O$	5.5×10^{-3}		Duchowicz et al. (2020)	V	186
[628-28-4]	4.4×10^{-3}		Amoore and Buttery (1978)	V	
CXBDYQVECUFKRK-UHFFFAOYSA-N	7.1×10^{-3}		Yaws (2003)	X	237
	2.1×10^{-2}		Duchowicz et al. (2020)	Q	
	4.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	5.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
	9.6×10^{-3}		Modarresi et al. (2007)	Q	67
	5.6×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.1×10^{-2}		Katritzky et al. (1998)	Q	
2-methoxybutane	6.7×10^{-3}		Duchowicz et al. (2020)	V	186
$C_5H_{12}O$	7.1×10^{-3}		Yaws (2003)	X	237
(methyl *sec*-butyl ether)	8.1×10^{-3}		Duchowicz et al. (2020)	Q	
[6795-87-5]	7.3×10^{-3}		Gharagheizi et al. (2012)	Q	
FVNIMHIOIXPIQT-UHFFFAOYSA-N	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	7.2×10^{-3}		Gharagheizi et al. (2010)	Q	246
	6.2×10^{-3}		Hilal et al. (2008)	Q	
	1.6×10^{-2}		Modarresi et al. (2007)	Q	67
	8.6×10^{-3}		Yaws (1999)	?	21
methyl isobutyl ether	4.3×10^{-3}	6700	Brockbank (2013)	L	1
$C_5H_{12}O$	4.5×10^{-3}		Duchowicz et al. (2020)	V	186
[625-44-5]	7.2×10^{-3}		Yaws (2003)	X	237
ZYVYEJXMYBUCMN-UHFFFAOYSA-N	8.1×10^{-3}		Duchowicz et al. (2020)	Q	
	2.3×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
	7.1×10^{-3}		Modarresi et al. (2007)	Q	67
	5.6×10^{-3}		Yaffe et al. (2003)	Q	248, 272
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
	8.6×10^{-3}		Yaws (1999)	?	21
methyl *tert*-butyl ether	1.2×10^{-2}	5100	Schwardt et al. (2021)	L	1
$CH_3OC(CH_3)_3$	1.3×10^{-2}	5900	Brockbank (2013)	L	1
(MTBE)	1.7×10^{-2}	9100	Hiatt (2013)	M	
[1634-04-4]	2.4×10^{-2}	18000	Zhang et al. (2013)	M	324
BZLVMXJERCGZMT-UHFFFAOYSA-N	3.2×10^{-2}		Zhang et al. (2013)	M	325
	1.9×10^{-2}	5300	Hwang et al. (2010)	M	33, 519, 11
	1.1×10^{-2}	4800	Sieg et al. (2009)	M	326
	1.1×10^{-2}	4400	Falabella and Teja (2008)	M	11, 338
	1.5×10^{-2}	5900	Böhme et al. (2008)	M	
	1.2×10^{-2}	5100	Haimi et al. (2006)	M	520
	1.2×10^{-2}	5000	Arp and Schmidt (2004)	M	521

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.4×10^{-2}	4500	Fischer et al. (2004)	M	
	7.2×10^{-3}	3200	Bierwagen and Keller (2001)	M	
	1.7×10^{-2}		Miller and Stuart (2000)	M	72
	2.3×10^{-2}		Park et al. (1997)	M	
	1.9×10^{-2}	15000	Robbins et al. (1993)	M	522
	1.4×10^{-2}		Mackay et al. (2006c)	V	
	1.0×10^{-1}	3700	Fukuchi et al. (2002)	V	
	1.6×10^{-2}		Park et al. (1997)	V	
	1.4×10^{-2}		Mackay et al. (1993)	V	
	2.0×10^{-2}		Hwang et al. (1992)	V	
	1.7×10^{-2}		Guthrie (1973)	V	
	1.7×10^{-2}		Bagno et al. (1991)	T	473
	1.8×10^{-2}		Yaws (2003)	X	258
	1.0×10^{-2}		Dupeux et al. (2022)	Q	259
	5.7×10^{-3}		Keshavarz et al. (2022)	Q	
	3.5×10^{-3}		Duchowicz et al. (2020)	Q	184
	1.3×10^{-3}		Wang et al. (2017)	Q	80, 238
	6.0×10^{-3}		Wang et al. (2017)	Q	80, 239
	1.5×10^{-2}		Wang et al. (2017)	Q	80, 240
	2.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-3}		Hilal et al. (2008)	Q	
	1.3×10^{-2}		Modarresi et al. (2007)	Q	67
		6300	Kühne et al. (2005)	Q	
	1.8×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.4×10^{-2}		English and Carroll (2001)	Q	230, 231
	1.1×10^{-2}		Katritzky et al. (1998)	Q	
	8.6×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	4.3×10^{-3}		Suzuki et al. (1992)	Q	232
	1.7×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		6000	Kühne et al. (2005)	?	
	1.8×10^{-2}		Yaws (1999)	?	21
ethyl propyl ether $C_2H_5OC_3H_7$ [628-32-0] NVJUHMXYKCUMQA-UHFFFAOYSA-N	8.7×10^{-3}		Duchowicz et al. (2020)	V	186
	8.6×10^{-3}		Hine and Mookerjee (1975)	V	
	8.6×10^{-3}		Butler and Ramchandani (1935)	V	
	6.4×10^{-3}		Yaws (2003)	X	237
	7.7×10^{-3}		Howard and Meylan (1997)	X	446
	7.0×10^{-3}		Duchowicz et al. (2020)	Q	
	8.2×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	7.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
	7.9×10^{-3}		Hilal et al. (2008)	Q	
	1.4×10^{-2}		Modarresi et al. (2007)	Q	67

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.6×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
	5.7×10^{-3}		Suzuki et al. (1992)	Q	232
	7.9×10^{-3}		Yaws (1999)	?	21
ethyl isopropyl ether $C_5H_{12}O$ [625-54-7] XSJVWZAETSBXKU-UHFFFAOYSA-N	8.1×10^{-3}		Yaws (2003)	X	237
	2.0×10^{-2}		Gharagheizi et al. (2012)	Q	
	9.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
2,2-dimethoxypropane $C_5H_{12}O_2$ [77-76-9] HEWZVZIVELJPQZ-UHFFFAOYSA-N	1.4×10^{-1}		Ebert et al. (2023)	?	316
methyl 1,2-dimethylpropyl ether $C_6H_{14}O$ [62016-49-3] JPUDLQKLSRSRGN-UHFFFAOYSA-N	4.6×10^{-3}		Yaws (2003)	X	237
	3.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	5.7×10^{-3}		Gharagheizi et al. (2010)	Q	246
methyl 1-ethylpropyl ether $C_6H_{14}O$ [36839-67-5] CQRFEDVNTJTKFU-UHFFFAOYSA-N	4.4×10^{-3}		Yaws (2003)	X	237
	4.3×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.2×10^{-3}		Gharagheizi et al. (2010)	Q	246
methyl 1-methylbutyl ether $C_6H_{14}O$ [6795-88-6] XSAJCGUYMQTAHL-UHFFFAOYSA-N	4.2×10^{-3}		Yaws (2003)	X	237
	6.9×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
methyl 2,2-dimethylpropyl ether $C_6H_{14}O$ [1118-00-9] JILHZKWLEAKYRC-UHFFFAOYSA-N	4.5×10^{-3}		Yaws (2003)	X	237
	1.2×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
methyl 2-methylbutyl ether $C_6H_{14}O$ [62016-48-2] XGLHRCWEOMNVKS-UHFFFAOYSA-N	4.3×10^{-3}		Yaws (2003)	X	237
	2.1×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
methyl 3-methylbutyl ether $C_6H_{14}O$ [626-91-5] ZQAYBCWERYRAMF-UHFFFAOYSA-N	4.3×10^{-3}		Yaws (2003)	X	237
	3.1×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
methyl pentyl ether $C_6H_{14}O$ [628-80-8] DBUJFULDVAZULB-UHFFFAOYSA-N	3.8×10^{-3}		Yaws (2003)	X	237
	3.9×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.0×10^{-3}		Gharagheizi et al. (2010)	Q	246

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methoxy-2-methylbutane	9.7×10^{-3}	6600	Brockbank (2013)	L	1
$C_6H_{14}O$	5.3×10^{-2}	9400	Hwang et al. (2010)	M	519, 11
(*tert*-amyl methyl ether)	1.0×10^{-2}	7000	Haimi et al. (2006)	M	523
[994-05-8]	8.6×10^{-3}	6500	Arp and Schmidt (2004)	M	
HVZJRWJGKQPSFL-UHFFFAOYSA-N	5.2×10^{-3}		Miller and Stuart (2000)	M	72
	1.0×10^{-2}		Dohnal and Hovorka (1999)	M	
	7.0×10^{-3}		Park et al. (1997)	M	
	8.1×10^{-3}		Park et al. (1997)	V	
	4.2×10^{-3}		Yaws (2003)	X	237
	3.9×10^{-3}		Yaws (2003)	X	237
	4.7×10^{-2}		Keshavarz et al. (2022)	Q	
	3.6×10^{-3}		Duchowicz et al. (2020)	Q	299
	1.3×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.8×10^{-3}		Gharagheizi et al. (2010)	Q	246
	3.8×10^{-3}		Gharagheizi et al. (2010)	Q	246
		6600	Kühne et al. (2005)	Q	
	7.5×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		6900	Kühne et al. (2005)	?	
	5.4×10^{-3}		Yaws (1999)	?	21
	5.0×10^{-3}	7600	Pankow et al. (1996)	?	
1-ethoxy-butane	7.6×10^{-3}	5700	Brockbank (2013)	L	1
$C_6H_{14}O$	6.4×10^{-3}		Miller and Stuart (2000)	M	72
(ethyl butyl ether)	7.8×10^{-3}		Mackay et al. (2006c)	V	
[628-81-9]	7.8×10^{-3}		Mackay et al. (1993)	V	
PZHIWRCQKBBTOW-UHFFFAOYSA-N	4.0×10^{-3}		Yaws (2003)	X	237
	6.7×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
		5900	Kühne et al. (2005)	Q	
		5000	Kühne et al. (2005)	?	
ethyl isobutyl ether	4.9×10^{-3}		Yaws (2003)	X	237
$C_6H_{14}O$	3.5×10^{-3}		Gharagheizi et al. (2012)	Q	
[627-02-1]	4.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
RQUBQBFVDOLUKC-UHFFFAOYSA-N					
ethyl *sec*-butyl ether	4.9×10^{-3}		Yaws (2003)	X	237
$C_6H_{14}O$	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[2679-87-0]	5.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
VSCUCHUDCLERMY-UHFFFAOYSA-N					
ethyl *tert*-butyl ether	7.2×10^{-3}	6900	Brockbank (2013)	L	1
$C_2H_5OC(CH_3)_3$	1.2×10^{-1}	13000	Hwang et al. (2010)	M	519, 11
(ETBE)	6.3×10^{-3}	6600	Sieg et al. (2009)	M	326
[637-92-3]	4.4×10^{-3}	4300	Falabella and Teja (2008)	M	11, 338
NUMQCACRALPSHD-UHFFFAOYSA-N	6.4×10^{-3}	7300	Haimi et al. (2006)	M	524
	6.1×10^{-3}	6500	Arp and Schmidt (2004)	M	
	4.2×10^{-3}		Miller and Stuart (2000)	M	72
	5.2×10^{-3}		Yaws (2003)	X	237

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Table A3.9: Ethers (ROR) (. . . continued)

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	7.8×10^{-3}		Keshavarz et al. (2022)	Q	
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	299
	1.1×10^{-3}		Wang et al. (2017)	Q	80, 238
	4.1×10^{-3}		Wang et al. (2017)	Q	80, 239
	1.5×10^{-2}		Wang et al. (2017)	Q	80, 240
	2.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	5.2×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
	6.0×10^{-3}		Duchowicz et al. (2020)	?	185, 21
	3.7×10^{-3}	7600	Pankow et al. (1996)	?	
dipropyl ether $C_3H_7OC_3H_7$ [111-43-3] POLCUAVZOMRGSN-UHFFFAOYSA-N	2.9×10^{-3}	6400	Brockbank (2013)	L	1
	3.0×10^{-3}		Li and Carr (1993)	M	
	2.9×10^{-3}		Li et al. (1993)	M	
	2.2×10^{-3}	9100	Hartkopf and Karger (1973)	M	
	3.9×10^{-3}		Mackay et al. (2006c)	V	
	3.9×10^{-3}		Mackay et al. (1993)	V	
	5.7×10^{-3}		Hwang et al. (1992)	V	
	2.9×10^{-3}		Hine and Mookerjee (1975)	V	
	2.8×10^{-3}		Butler and Ramchandani (1935)	V	
	4.5×10^{-3}		Yaws (2003)	X	258
	4.5×10^{-3}		Yaws (2003)	X	237
	1.2×10^{-3}		Dupeux et al. (2022)	Q	259
	7.8×10^{-3}		Keshavarz et al. (2022)	Q	
	7.2×10^{-3}		Duchowicz et al. (2020)	Q	184
	4.4×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	4.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
	6.0×10^{-3}		Hilal et al. (2008)	Q	
	7.5×10^{-3}		Modarresi et al. (2007)	Q	67
		5900	Kühne et al. (2005)	Q	
	4.5×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.1×10^{-2}		Katritzky et al. (1998)	Q	
	1.0×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	4.3×10^{-3}		Suzuki et al. (1992)	Q	232
	4.5×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		7300	Kühne et al. (2005)	?	
	4.5×10^{-3}		Yaws (1999)	?	21
	1.9×10^{-3}		Hoff et al. (1993)	?	21
	4.5×10^{-3}		Yaws and Yang (1992)	?	21
	2.9×10^{-3}		Abraham et al. (1990)	?	

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
diisopropyl ether	4.5×10^{-3}	6600	Brockbank (2013)	L	1
$C_3H_7OC_3H_7$	1.5×10^{-2}	8400	Hwang et al. (2010)	M	519, 11
[108-20-3]	3.9×10^{-3}	6400	Arp and Schmidt (2004)	M	
ZAFNJMIOTHYJRJ-UHFFFAOYSA-N	4.3×10^{-3}		Miller and Stuart (2000)	M	72
	4.7×10^{-3}		Dohnal and Hovorka (1999)	M	
	4.8×10^{-3}		Nielsen et al. (1994)	M	
	4.2×10^{-3}		Li and Carr (1993)	M	
	4.4×10^{-3}		Li et al. (1993)	M	
	2.8×10^{-3}		Guitart et al. (1989)	M	14
	4.3×10^{-3}		HSDB (2015)	V	
	3.9×10^{-3}		Mackay et al. (2006c)	V	
	4.8×10^{-3}	6200	Fukuchi et al. (2002)	V	
	3.1×10^{-3}	6400	Pankow et al. (1996)	V	
	3.9×10^{-3}		Mackay et al. (1993)	V	
	9.9×10^{-4}		Hine and Mookerjee (1975)	V	
	9.8×10^{-4}		Hine and Weimar (1965)	V	
	5.7×10^{-3}		Yaws (2003)	X	258
	5.6×10^{-3}		Yaws (2003)	X	237
	5.7×10^{-3}		Dupeux et al. (2022)	Q	259
	7.8×10^{-3}		Keshavarz et al. (2022)	Q	
	1.1×10^{-3}		Duchowicz et al. (2020)	Q	
	1.8×10^{-3}		Wang et al. (2017)	Q	80, 238
	6.2×10^{-3}		Wang et al. (2017)	Q	80, 239
	1.2×10^{-2}		Wang et al. (2017)	Q	80, 240
	2.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	5.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
	3.7×10^{-3}		Hilal et al. (2008)	Q	
	9.6×10^{-3}		Modarresi et al. (2007)	Q	67
		6600	Kühne et al. (2005)	Q	
	4.5×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
	8.0×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	3.5×10^{-3}		Suzuki et al. (1992)	Q	232
	3.9×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		7200	Kühne et al. (2005)	?	
	5.6×10^{-3}		Yaws (1999)	?	21
	5.7×10^{-3}		Yaws and Yang (1992)	?	21
	9.9×10^{-4}		Abraham et al. (1990)	?	

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
propyl isopropyl ether	5.0×10^{-3}		Yaws (2003)	X	237
$C_6H_{14}O$	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[627-08-7]	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
JIEJJGMNDWIGBJ-UHFFFAOYSA-N	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	5.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
	6.3×10^{-3}		Modarresi et al. (2007)	Q	67
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
2-ethoxy-2-methylbutane	5.0×10^{-3}	7400	Brockbank (2013)	L	1
$C_7H_{16}O$	4.8×10^{-3}	7600	Haimi et al. (2006)	M	525
(*tert*-amyl ethyl ether)	5.2×10^{-4}		Duchowicz et al. (2020)	V	186
[919-94-8]	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
KFRVYYGHSPLXSZ-UHFFFAOYSA-N	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	2.4×10^{-3}		Hilal et al. (2008)	Q	
	1.1×10^{-2}		Modarresi et al. (2007)	Q	67
tert-butyl isopropyl ether	6.6×10^{-4}		Yaws (1999)	?	21
$C_7H_{16}O$					
[17348-59-3]					
HNFSPSWQNZVCTB-UHFFFAOYSA-N					
dipropylene glycol monomethyl ether	8.6×10^{3}		Bartelt-Hunt et al. (2008)	?	21
$C_7H_{16}O_3$					
[34590-94-8]					
WGYZMNBUZFHYRX-UHFFFAOYSA-N					
dibutyl ether	2.1×10^{-3}	6700	Brockbank (2013)	L	1
$C_4H_9OC_4H_9$	7.2×10^{-3}	10000	Hwang et al. (2010)	M	519, 11
[142-96-1]	2.2×10^{-3}		Li and Carr (1993)	M	
DURPTKYDGMDSBL-UHFFFAOYSA-N	1.3×10^{-3}		Li et al. (1993)	M	
	2.1×10^{-3}		Ioffe et al. (1984)	M	
	2.1×10^{-3}		Mackay et al. (2006c)	V	
	2.1×10^{-3}		Mackay et al. (1993)	V	
	1.6×10^{-3}		Pierotti et al. (1959)	X	414
	1.4×10^{-2}		Keshavarz et al. (2022)	Q	
	7.4×10^{-3}		Duchowicz et al. (2020)	Q	
	1.6×10^{-3}		Li et al. (2014)	Q	241
	2.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-3}		Hilal et al. (2008)	Q	
	6.1×10^{-3}		Modarresi et al. (2007)	Q	67
		6600	Kühne et al. (2005)	Q	
	1.8×10^{-3}		Yaffe et al. (2003)	Q	248, 249

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.9×10^{-3}		Katritzky et al. (1998)	Q	
	6.4×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	2.2×10^{-3}		Russell et al. (1992)	Q	279
	2.5×10^{-3}		Suzuki et al. (1992)	Q	232
	1.6×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		7000	Kühne et al. (2005)	?	
	1.8×10^{-2}		Yaws (1999)	?	21
	1.6×10^{-3}		Abraham et al. (1990)	?	
diisobutyl ether $C_8H_{18}O$ [628-55-7] SZNYYWIUQFZLLT-UHFFFAOYSA-N	3.7×10^{-3}		Hilal et al. (2008)	Q	
di-*sec*-butyl ether $C_8H_{18}O$ [6863-58-7] HHBZZTKMMLDNDN-UHFFFAOYSA-N	1.8×10^{-3}		Yaws (2003)	X	258
	1.8×10^{-3}		Yaws (2003)	X	237
	1.0×10^{-3}		Dupeux et al. (2022)	Q	259
	8.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.7×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.8×10^{-3}		Yaws (1999)	?	21
di-*tert*-butyl ether $C_8H_{18}O$ [6163-66-2] AQEFLFZSWDEAIP-UHFFFAOYSA-N	2.1×10^{-3}		Yaws (2003)	X	237
	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
	3.0×10^{-3}		Yaws (1999)	?	21
2-methoxy-2,4,4-trimethylpentane $C_9H_{20}O$ (methyl *tert*-octyl ether) [62108-41-2] IKZVAPMTXDXWMX-UHFFFAOYSA-N	1.9×10^{-3}		Ebert et al. (2023)	?	526
2-methoxy-2-methylheptane $C_9H_{20}O$ [76589-16-7] KJRACWZCOVHBQU-UHFFFAOYSA-N	1.9×10^{-3}	8100	Haimi et al. (2006)	M	527
2-ethoxy-2,4,4-trimethylpentane $C_{10}H_{22}O$ (ethyl tert-octyl ether) [187103-12-4] JGPJRBWLBUGAQN-UHFFFAOYSA-N	7.7×10^{-4}	6900	Haimi et al. (2006)	M	528
1,1'-oxybispentane $C_{10}H_{22}O$ (dipentyl ether) [693-65-2] AOPDRZXCEAKHHW-UHFFFAOYSA-N	3.5×10^{-4}		Yaws (2003)	X	258
	3.5×10^{-4}		Yaws (2003)	X	237
	4.5×10^{-4}		Dupeux et al. (2022)	Q	259
	4.3×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.3×10^{-4}		Gharagheizi et al. (2010)	Q	246
	2.7×10^{-3}		Hilal et al. (2008)	Q	
	1.0×10^{-3}		Yaws (1999)	?	21
			Brockbank (2013)	W	529

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1'-oxybis(3-methylbutane)	6.8×10^{-3}		Duchowicz et al. (2020)	V	186
$C_{10}H_{22}O$	6.6×10^{-3}		HSDB (2015)	V	
(diisopentyl ether)	1.1×10^{-3}		Duchowicz et al. (2020)	Q	
[544-01-4]	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
AQZGPSLYZOOYQP-UHFFFAOYSA-N	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.3×10^{-3}		Hilal et al. (2008)	Q	
	4.8×10^{-3}		Modarresi et al. (2007)	Q	67
1,1'-oxybishexane	2.9×10^{-4}		Yaws (2003)	X	237
$C_{12}H_{26}O$	5.6×10^{-3}		Gharagheizi et al. (2012)	Q	
(dihexyl ether)	1.7×10^{-4}		Gharagheizi et al. (2010)	Q	246
[112-58-3]	1.8×10^{-3}		Hilal et al. (2008)	Q	
BPIUIOXAFBGMNB-UHFFFAOYSA-N	3.0×10^{-3}		Yaws (1999)	?	21
			Brockbank (2013)	W	530
1-ethoxy-3,7-dimethyloctane	6.7×10^{-4}		Zhang et al. (2010)	Q	287, 288
$C_{12}H_{26}O$	5.3×10^{-3}		Zhang et al. (2010)	Q	287, 289
[22810-10-2]	1.3×10^{-3}		Zhang et al. (2010)	Q	287, 290
HCHHIPCZJSRFRT-UHFFFAOYSA-N	2.5×10^{-4}		Zhang et al. (2010)	Q	287, 291
diheptyl ether	2.8×10^{-5}		Yaws (2003)	X	237
$C_{14}H_{30}O$	8.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
[629-64-1]					
UJEGHEMJVNQWOJ-UHFFFAOYSA-N					
dioctyl ether	1.3×10^{-4}		Yaws (2003)	X	237
$C_{16}H_{34}O$	6.7×10^{-5}		Gharagheizi et al. (2010)	Q	246
[629-82-3]	8.2×10^{-2}		Yaws (1999)	?	21
NKJOXAZJBOMXID-UHFFFAOYSA-N					
methoxycyclohexane	3.1×10^{-2}		Hilal et al. (2008)	Q	
$C_7H_{14}O$					
[931-56-6]					
GHDIHPNJQVDFBL-UHFFFAOYSA-N					
methyl cedryl ether	2.5×10^{-3}		Zhang et al. (2010)	Q	287, 288
$C_{16}H_{28}O$	2.4×10^{-3}		Zhang et al. (2010)	Q	287, 289
[19870-74-7]	7.7×10^{-3}		Zhang et al. (2010)	Q	287, 290
HRGPYCVTDOECMG-WALBABNVSA-N	1.2×10^{-3}		Zhang et al. (2010)	Q	287, 291
dimethoxymethane	6.1×10^{-2}	4700	Brockbank (2013)	L	1
$CH_3OCH_2OCH_3$	6.3×10^{-2}	4800	Ondo and Dohnal (2007)	M	1
(methylal)	6.1×10^{-2}		HSDB (2015)	V	
[109-87-5]	5.7×10^{-2}		Pierotti et al. (1959)	X	414
NKDDWNXOKDWJAK-UHFFFAOYSA-N	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	4.6×10^{-1}		Duchowicz et al. (2020)	Q	184
	7.1×10^{-2}		Wang et al. (2017)	Q	80, 238
	3.6×10^{-1}		Wang et al. (2017)	Q	80, 239
	6.5×10^{-2}		Wang et al. (2017)	Q	80, 240

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Table A3.9: Ethers (ROR) (. . . continued)

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	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.3×10^{-1}		Hilal et al. (2008)	Q	
	6.9×10^{-2}		Modarresi et al. (2007)	Q	67
	5.7×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	6.9×10^{-2}		Yaws (1999)	?	21, 12
trimethoxymethane $HC(OCH_3)_3$ [149-73-5] PYOKUURKVVELLB-UHFFFAOYSA-N	6.9×10^{-1}		Guthrie (1973)	V	
diethoxymethane	1.5×10^{-1}		Duchowicz et al. (2020)	V	186
$C_5H_{12}O_2$	7.5×10^{-2}		Duchowicz et al. (2020)	Q	
[462-95-3]	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
KLKFAASOGCDTDT-UHFFFAOYSA-N	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	7.2×10^{-2}		Modarresi et al. (2007)	Q	67
1,1-diethoxyethane	1.0×10^{-1}		Duchowicz et al. (2020)	V	186
$(C_2H_5O)_2CHCH_3$	1.0×10^{-1}		HSDB (2015)	V	
(acetal)	1.0×10^{-1}		Hine and Mookerjee (1975)	V	
[105-57-7]	1.2×10^{-1}		Abney (2021)	Q	399
DHKHKXVYLBGOIT-UHFFFAOYSA-N	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
	5.7×10^{-2}		Hilal et al. (2008)	Q	
	6.9×10^{-2}		Modarresi et al. (2007)	Q	67
	1.1×10^{-1}		Yaws (1999)	?	21
1,2-diethoxyethane	1.6×10^{-1}		Duchowicz et al. (2020)	V	186
$C_2H_5OC_2H_4OC_2H_5$	1.6×10^{-1}		HSDB (2015)	V	
[629-14-1]	1.6×10^{-1}		Hine and Mookerjee (1975)	V	
LZDKZFUFMNSQCJ-UHFFFAOYSA-N	1.2×10^{-1}		Howard and Meylan (1997)	X	446
	8.3×10^{-2}		Duchowicz et al. (2020)	Q	
	3.9×10^{-1}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	67
1,1,1-trimethoxyethane $CH_3C(OCH_3)_3$ [1445-45-0] HDPNBNXLBDFELL-UHFFFAOYSA-N	6.4×10^{-1}		Guthrie (1973)	V	
1,2-dimethoxyethane	1.3	7300	Brockbank (2013)	L	1, 531
$C_4H_{10}O_2$	2.1		O'Farrell and Waghorne (2010)	M	
[110-71-4]	1.4	7200	Ondo and Dohnal (2007)	M	1
XTHFKEDIFFGKHM-UHFFFAOYSA-N	1.4	7100	Cabani et al. (1978)	T	
	9.0		HSDB (2015)	Q	99
	5.3×10^{-1}		Hilal et al. (2008)	Q	

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3-oxa-1-hexanol	2.0×10^{1}	8400	Cabani et al. (1978)	T	
$C_5H_{12}O_2$	6.6×10^{2}		HSDB (2015)	Q	99
(2-propoxyethanol)	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
[2807-30-9]	9.9		Raventos-Duran et al. (2010)	Q	244
YEYKMVJDLWJFOA-UHFFFAOYSA-N	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	245
	1.0×10^{1}		Hilal et al. (2008)	Q	
	5.8		Nirmalakhandan et al. (1997)	Q	
3-oxa-1-heptanol	1.3×10^{1}	8300	Brockbank (2013)	L	1
$C_6H_{14}O_2$	3.5	7700	Hiatt (2013)	M	
(2-butoxyethanol; butyl cellosolve)	1.3×10^{1}	8300	Kim et al. (2000)	M	33
[111-76-2]	2.7		Johanson and Dynésius (1988)	M	14
POAOYUHQDCAZBD-UHFFFAOYSA-N	1.6×10^{1}	8900	Cabani et al. (1978)	T	
	1.7×10^{1}		Keshavarz et al. (2022)	Q	
	7.4		Duchowicz et al. (2020)	Q	184
	5.4		Wang et al. (2017)	Q	80, 238
	1.9×10^{1}		Wang et al. (2017)	Q	80, 239
	3.2		Wang et al. (2017)	Q	80, 240
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	271, 243
	7.8		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	7.7		Hilal et al. (2008)	Q	
	1.9×10^{1}		Modarresi et al. (2007)	Q	67
	4.5		Nirmalakhandan et al. (1997)	Q	
	6.2		Duchowicz et al. (2020)	?	185, 21
	2.8×10^{1}		Yaws (1999)	?	21, 12
1-methoxy-2-propanol	4.8		Johanson and Dynésius (1988)	M	14
$C_4H_{10}O_2$	1.1×10^{1}		Hilal et al. (2008)	C	
[107-98-2]	9.2		Keshavarz et al. (2022)	Q	
ARXJGSRGQADJSQ-UHFFFAOYSA-N	6.7		Duchowicz et al. (2020)	Q	299
	8.3		Wang et al. (2017)	Q	80, 238
	4.7×10^{1}		Wang et al. (2017)	Q	80, 239
	4.9		Wang et al. (2017)	Q	80, 240
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{1}		Hilal et al. (2008)	Q	
	2.8×10^{1}		Modarresi et al. (2007)	Q	67
	1.1×10^{1}		Yaffe et al. (2003)	Q	248, 249
	3.5		Katritzky et al. (1998)	Q	
	1.1×10^{1}		Duchowicz et al. (2020)	?	185, 21

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4-methyl-3-oxa-1-pentanol	4.8		Johanson and Dynésius (1988)	M	14
$C_5H_{12}O_2$	1.2×10^{1}		Keshavarz et al. (2022)	Q	
(2-isopropoxyethanol)	2.6		Duchowicz et al. (2020)	Q	184
[109-59-1]	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	271, 243
HCGFUIQPSOCUHI-UHFFFAOYSA-N	7.8		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	245
	7.9		Hilal et al. (2008)	Q	
	2.7×10^{1}		Modarresi et al. (2007)	Q	67
	1.1×10^{1}		Duchowicz et al. (2020)	?	185, 21
1,2-dibutoxyethane	9.9×10^{-1}		HSDB (2015)	V	
$C_{10}H_{22}O_2$	1.4×10^{-1}		Hilal et al. (2008)	Q	
[112-48-1]	1.1×10^{-1}		Modarresi et al. (2007)	Q	67
GDXHBFHOEYVPED-UHFFFAOYSA-N					
3,6-dioxa-1-decanol	1.4×10^{3}		Kim et al. (2000)	M	
$C_8H_{18}O_3$					
(butyl carbitol)					
[112-34-5]					
OAYXUHPQHDHDDZ-UHFFFAOYSA-N					
diethylene glycol dibutyl ether	2.5	13000	Brockbank (2013)	L	1
$C_{12}H_{26}O_3$	3.9		Duchowicz et al. (2020)	V	186
[112-73-2]	6.1		Yaws (2003)	X	237, 12
KZVBBTZJMSWGTK-UHFFFAOYSA-N	1.3		Duchowicz et al. (2020)	Q	
	6.0		Gharagheizi et al. (2010)	Q	246
	3.5		Hilal et al. (2008)	Q	
	1.5		Modarresi et al. (2007)	Q	67
	4.0		Yaws (1999)	?	21, 12
methyl vinyl ether	1.5×10^{-3}		HSDB (2015)	V	
C_3H_6O	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
[107-25-5]	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	244
XJRBAMWJDBPFIM-UHFFFAOYSA-N	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	245
ethyl vinyl ether	1.8×10^{-3}		Duchowicz et al. (2020)	V	186
C_4H_8O	2.3×10^{-2}		Duchowicz et al. (2020)	Q	
[109-92-2]	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
FJKIXWOMBXYWOQ-UHFFFAOYSA-N	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
propyl vinyl ether	3.1×10^{-3}	4800	Hwang et al. (2010)	M	519, 11
$C_5H_{10}O$					
[764-47-6]					
OVGRCEFMXPHEBL-UHFFFAOYSA-N					
allyl glycidyl ether	2.1		Ebert et al. (2023)	?	316
$C_6H_{10}O_2$					
[106-92-3]					
LSWYGACWGAICNM-UHFFFAOYSA-N					

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
butyl vinyl ether	4.6×10^{-3}		Duchowicz et al. (2020)	V	186
$C_6H_{12}O$	4.5×10^{-3}		HSDB (2015)	V	
[111-34-2]	7.3×10^{-4}		Dupeux et al. (2022)	Q	259
UZKWTJUDCOPSNM-UHFFFAOYSA-N	2.5×10^{-2}		Duchowicz et al. (2020)	Q	
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-3}		Modarresi et al. (2007)	Q	67
isobutyl vinyl ether	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
$C_6H_{12}O$	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	244
[109-53-5]	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245
OZCMOJQQLBXBKI-UHFFFAOYSA-N	1.9×10^{-4}		Hilal et al. (2008)	Q	
	2.5×10^{-3}		Modarresi et al. (2007)	Q	67
benzyl methyl ether	1.1×10^{-1}		Duchowicz et al. (2020)	V	186
$C_8H_{10}O$	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
[538-86-3]					
GQKZBCPTCWJTAS-UHFFFAOYSA-N					
benzyl ethyl ether	6.7×10^{-2}		Dupeux et al. (2022)	Q	259
$C_9H_{12}O$					
[539-30-0]					
AXPZDYVDTMMLNB-UHFFFAOYSA-N					
methoxybenzene	2.9×10^{-2}	4200	Brockbank (2013)	L	1
$C_6H_5OCH_3$	2.9×10^{-2}	4200	Brockbank et al. (2013)	M	
(anisole)	2.6×10^{-2}	4800	Dewulf et al. (1999)	M	
[100-66-3]	3.2×10^{-2}		Li and Carr (1993)	M	
RDOXTESZEPMUJZ-UHFFFAOYSA-N	2.0×10^{-2}		Duchowicz et al. (2020)	V	186
	3.1×10^{-2}		Mackay et al. (2006c)	V	
	4.0×10^{-2}		Mackay et al. (1993)	V	
	2.3×10^{-3}		Hine and Mookerjee (1975)	V	
	2.3×10^{-3}		Hine and Weimar (1965)	R	
	2.7×10^{-3}		Yaws (2003)	X	258
	2.7×10^{-3}		Yaws (2003)	X	237
	6.9×10^{-2}		Schüürmann (2000)	C	21
	1.9×10^{-2}		Dupeux et al. (2022)	Q	259
	1.2×10^{-1}		Duchowicz et al. (2020)	Q	
	2.3×10^{-3}		HSDB (2015)	Q	99
	1.9×10^{-2}		Li et al. (2014)	Q	241
	1.3×10^{-1}		Gharagheizi et al. (2010)	Q	246
	9.0×10^{-3}		Hilal et al. (2008)	Q	
	3.3×10^{-2}		Modarresi et al. (2007)	Q	67
		4500	Kühne et al. (2005)	Q	
	8.6×10^{-3}		Yao et al. (2002)	Q	229
	1.2×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	2.3×10^{-3}		Suzuki et al. (1992)	Q	232
		4300	Kühne et al. (2005)	?	

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.7×10^{-3}		Yaws (1999)	?	21
	2.5×10^{-2}		Abraham et al. (1990)	?	
ethoxybenzene	1.7×10^{-2}		Li and Carr (1993)	M	
$C_8H_{10}O$	2.2×10^{-2}		Duchowicz et al. (2020)	V	186
(phenetole)	2.2×10^{-2}		HSDB (2015)	V	
[103-73-1]	2.3×10^{-2}		Mackay et al. (2006c)	V	
DLRJIFUOBPOJNS-UHFFFAOYSA-N	4.4×10^{-2}		Duchowicz et al. (2020)	Q	
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.5×10^{-3}		Hilal et al. (2008)	Q	
	2.9×10^{-2}		Modarresi et al. (2007)	Q	67
	2.6×10^{-1}		Katritzky et al. (1998)	Q	
	1.0×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	1.7×10^{-2}		Abraham et al. (1990)	?	
1,2-dimethoxybenzene		5100	Kühne et al. (2005)	Q	
$C_8H_{10}O_2$		2400	Kühne et al. (2005)	?	
[91-16-7]					
ABDKAPXRBAPSQN-UHFFFAOYSA-N					
2-phenoxyethanol	2.1×10^{2}		Duchowicz et al. (2020)	V	186
$C_8H_{10}O_2$	2.0×10^{2}		HSDB (2015)	V	
[122-99-6]	4.0×10^{1}		Duchowicz et al. (2020)	Q	
QCDWFXQBSFUVSP-UHFFFAOYSA-N	3.4×10^{1}		Hilal et al. (2008)	Q	
	1.4×10^{2}		Modarresi et al. (2007)	Q	67
2-(phenylmethoxy)-ethanol	8.2×10^{1}		Duchowicz et al. (2020)	V	186
$C_9H_{12}O_2$	4.4×10^{1}		Duchowicz et al. (2020)	Q	
[622-08-2]	1.6×10^{3}		Raventos-Duran et al. (2010)	Q	242, 243
CUZKCNWZBXLAJX-UHFFFAOYSA-N	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{3}		Raventos-Duran et al. (2010)	Q	245
	1.5×10^{2}		Hilal et al. (2008)	Q	
	7.0×10^{2}		Modarresi et al. (2007)	Q	67
1,2,3-trimethoxybenzene	3.6		Schüürmann (2000)	V	
$C_9H_{12}O_3$					
[634-36-6]					
CRUILBNAQILVHZ-UHFFFAOYSA-N					
1-methoxy-4-(1-propenyl)-benzene	9.9×10^{-2}	6200	van Roon et al. (2005)	V	
$C_{10}H_{12}O$	1.0×10^{-1}		Yaws (2003)	X	258
(anethole)	3.7×10^{-2}		Dupeux et al. (2022)	Q	259
[104-46-1]	1.4×10^{-1}		HSDB (2015)	Q	99
RUVINXPYWBROJD-UHFFFAOYSA-N	2.0×10^{-2}		Hilal et al. (2008)	Q	
	1.0×10^{-1}		Yaws (1999)	?	21

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Table A3.9: Ethers (ROR) (. . . continued)

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2-methoxy-4-(2-propenyl)-phenol	9.2		McFall et al. (2020)	M	
$C_{10}H_{12}O_2$	5.0		Duchowicz et al. (2020)	V	186
(eugenol)	6.9		Martins et al. (2017)	V	315
[97-53-0]	5.1		HSDB (2015)	V	
RRAFCDWBNXTKKO-UHFFFAOYSA-N	7.2	9700	van Roon et al. (2005)	V	
	3.9		Dupeux et al. (2022)	Q	259
	3.5×10^{-1}		Abney (2021)	Q	399
	2.0×10^{1}		Duchowicz et al. (2020)	Q	
	5.7		McFall et al. (2020)	Q	474
1,2-dimethoxy-4-(2-propenyl)-benzene	1.8		Duchowicz et al. (2020)	V	186
$C_{11}H_{14}O_2$	1.8		HSDB (2015)	V	
[93-15-2]	1.0		Duchowicz et al. (2020)	Q	
ZYEMGPIYFIJGTP-UHFFFAOYSA-N	3.6		Hilal et al. (2008)	Q	
	1.9×10^{-1}		Modarresi et al. (2007)	Q	67
diphenyl ether	1.9×10^{-2}		Brockbank (2013)	L	
$C_{12}H_{10}O$	3.5×10^{-2}		Duchowicz et al. (2020)	V	186
[101-84-8]	3.5×10^{-2}		HSDB (2015)	V	
USIUVYZYUHIAEV-UHFFFAOYSA-N	3.7×10^{-2}		Mackay et al. (2006c)	V	
	1.1×10^{-1}		Kurz and Ballschmiter (1999)	V	
	3.7×10^{-2}		Mackay et al. (1993)	V	
	1.8×10^{-2}		Yaws (2003)	X	237
	2.9×10^{-1}		Duchowicz et al. (2020)	Q	
	1.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
	1.7×10^{-2}		Hilal et al. (2008)	Q	
	1.7×10^{-1}		Modarresi et al. (2007)	Q	67
	1.9×10^{-2}		Yaws (1999)	?	21
(phenoxymethyl)-oxirane	1.2×10^{1}		Duchowicz et al. (2020)	V	186
$C_9H_{10}O_2$	1.2×10^{1}		HSDB (2015)	V	
[122-60-1]	4.8		Duchowicz et al. (2020)	Q	
FQYUMYWMJTYZTK-UHFFFAOYSA-N	6.1×10^{-1}		Hilal et al. (2008)	Q	
	1.9		Modarresi et al. (2007)	Q	67
1-dodecyl-4-phenoxybenzene	3.4×10^{-3}		Zhang et al. (2010)	Q	287, 288
$C_{24}H_{34}O$	1.4×10^{-3}		Zhang et al. (2010)	Q	287, 289
[119345-02-7]	1.7×10^{-2}		Zhang et al. (2010)	Q	287, 290
XSAHYEQPUFJGKW-UHFFFAOYSA-N	7.7×10^{-2}		Zhang et al. (2010)	Q	287, 291
2,2,4-trimethyl-4-(4-(4-(2,4,4-trimethylpentan-2-yl)phenoxy)phenyl)pentane	1.3×10^{-3}		Zhang et al. (2010)	Q	287, 288
$C_{28}H_{42}O$	1.2×10^{-3}		Zhang et al. (2010)	Q	287, 289
[61702-88-3]	5.4×10^{-2}		Zhang et al. (2010)	Q	287, 290
AJDONJVWDSZZQF-UHFFFAOYSA-N	6.9×10^{-3}		Zhang et al. (2010)	Q	287, 291

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Table A3.9: Ethers (ROR) (. . . continued)

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etofenprox $C_{25}H_{28}O_3$ [80844-07-1] YREQHYQNNWYQCJ-UHFFFAOYSA-N	7.4×10^{1}		Maniere et al. (2011)	?	165
di-*tert*-butyl *sec*-butylidene diperoxide	1.2×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{12}H_{26}O_4$	6.1×10^{-5}		Zhang et al. (2010)	Q	287, 289
[2167-23-9]	1.6×10^{-2}		Zhang et al. (2010)	Q	287, 290
HQOVXPHOJANJBR-UHFFFAOYSA-N	1.1		Zhang et al. (2010)	Q	287, 291
peroxide, 1,1-dimethylethyl 1-methyl-1-phenylethyl	1.4×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{13}H_{20}O_2$	4.8×10^{-3}		Zhang et al. (2010)	Q	287, 289
[3457-61-2]	1.6×10^{-2}		Zhang et al. (2010)	Q	287, 290
BIISIZOQPWZPPS-UHFFFAOYSA-N	1.9×10^{-1}		Zhang et al. (2010)	Q	287, 291
di-*tert*-butyl 1,1,4,4-tetramethyltetramethylene diperoxide	3.9×10^{-3}		Zhang et al. (2010)	Q	287, 288
$C_{16}H_{34}O_4$	7.9×10^{-4}		Zhang et al. (2010)	Q	287, 289
[78-63-7]	1.3×10^{-1}		Zhang et al. (2010)	Q	287, 290
DMWVYCCGCQPJEA-UHFFFAOYSA-N	3.4×10^{-1}		Zhang et al. (2010)	Q	287, 291
1,4-bis(1-*tert*-butylperoxy-1-methyl-ethyl)benzene	1.0×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_{20}H_{34}O_4$	1.8×10^{-2}		Zhang et al. (2010)	Q	287, 289
[2781-00-2]	2.9×10^{-1}		Zhang et al. (2010)	Q	287, 290
GWQOYRSARAWVTC-UHFFFAOYSA-N	8.6		Zhang et al. (2010)	Q	287, 291
MCM:CH3OCH2OOH	2.2×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_6O_3$	6.9×10^{1}		Wang et al. (2017)	Q	80, 239
CDXAGPPPWKCPRI-UHFFFAOYSA-N	7.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ETHOXOOH	7.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_4O_3$	1.7×10^{2}		Wang et al. (2017)	Q	80, 239
NOEKFNMWGHEGBN-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DMMAOOH	5.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_8O_4$	3.0×10^{2}		Wang et al. (2017)	Q	80, 239
SHLFZQKLTPTTSZ-UHFFFAOYSA-N	1.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DMMBOOH	5.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_8O_4$	5.6×10^{1}		Wang et al. (2017)	Q	80, 239
HODDSHZVZWXLHR-UHFFFAOYSA-N	2.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:ETOMEOOH	1.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_3H_8O_3$	3.9×10^{1}		Wang et al. (2017)	Q	80, 239
NZBMKAZNWPZJND-UHFFFAOYSA-N	6.9×10^{1}		Wang et al. (2017)	Q	80, 240

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MCM:MEMOXYCO3H	2.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_4$	7.1×10^{1}		Wang et al. (2017)	Q	80, 239
PWWCDEMRYRBWOJ-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DIETETOOH	1.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	1.3×10^{1}		Wang et al. (2017)	Q	80, 239
CXWWPQGYBJCHJL-UHFFFAOYSA-N	4.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ETOC2OOH	1.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	8.1×10^{1}		Wang et al. (2017)	Q	80, 239
NYVGIYPKZJSYSP-UHFFFAOYSA-N	6.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ETOMECO3H	2.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	3.4×10^{1}		Wang et al. (2017)	Q	80, 239
ULYBJOMJQUHMOL-UHFFFAOYSA-N	4.8		Wang et al. (2017)	Q	80, 240
MCM:IPRMETOOH	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	4.5		Wang et al. (2017)	Q	80, 239
PSBSELFEZHDPTA-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:BOXMOOH	1.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	2.0×10^{1}		Wang et al. (2017)	Q	80, 239
DCHWALHTYQHXTG-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:EIPEOOH	8.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	3.0		Wang et al. (2017)	Q	80, 239
ZZXLAMSYBUVKJS-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:IPROC21OOH	1.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	6.6		Wang et al. (2017)	Q	80, 239
VGMUBGNCFVOQDX-UHFFFAOYSA-N	2.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MTBEAOOH	8.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	8.5		Wang et al. (2017)	Q	80, 239
BGZKVDIFKPQYHL-UHFFFAOYSA-N	6.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MTBEBCO3H	1.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	4.7		Wang et al. (2017)	Q	80, 239
NGYXBYFCPPVOQA-UHFFFAOYSA-N	3.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:MTBEBOOH	8.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_3$	2.5×10^{1}		Wang et al. (2017)	Q	80, 239
FPTBRWWJTBOWHN-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:BOXMCO3H	1.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	1.7×10^{1}		Wang et al. (2017)	Q	80, 239
BMXLBBYCODRNIJ-UHFFFAOYSA-N	8.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:DIIPRETOOH	8.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	1.6		Wang et al. (2017)	Q	80, 239
PFVPTWUDXVSVAC-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	80, 240

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MCM:ETBEACO3H	1.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	3.4		Wang et al. (2017)	Q	80, 239
UAVAAIVEDVDYSQ-UHFFFAOYSA-N	3.1×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:ETBEAOOH	8.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	1.7×10^{1}		Wang et al. (2017)	Q	80, 239
ITRUGVUCIYLYDK-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ETBEBOOH	8.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	2.5		Wang et al. (2017)	Q	80, 239
VOZHKKMLSSYDIG-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ETBECCO3H	1.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	8.9		Wang et al. (2017)	Q	80, 239
AELSWALKLVZVPO-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ETBECOOH	8.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	2.0×10^{1}		Wang et al. (2017)	Q	80, 239
WJMPPRSRRBMJID-UHFFFAOYSA-N	5.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:IPROMC2OOH	1.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	2.2×10^{1}		Wang et al. (2017)	Q	80, 239
JCIUPJDJCBRYHD-UHFFFAOYSA-N	2.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:IPROMCCO3H	1.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_4$	7.8		Wang et al. (2017)	Q	80, 239
SFJQIQZNOBLTBZ-UHFFFAOYSA-N	7.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:BCSOZ	9.1		Wang et al. (2017)	Q	80, 238
$C_{15}H_{24}O_3$	2.0×10^{-1}		Wang et al. (2017)	Q	80, 239
DXZCAIRIBLPJLG-UHFFFAOYSA-N	7.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CH3OCH2OH	8.1		Wang et al. (2017)	Q	80, 238
$C_2H_6O_2$	5.4×10^{1}		Wang et al. (2017)	Q	80, 239
VHWYCFISAQVCCP-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DMMAOH	1.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_3H_8O_3$	4.1×10^{2}		Wang et al. (2017)	Q	80, 239
YANOHILBFNXRFM-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DMMBOH	2.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_3H_8O_3$	4.6×10^{1}		Wang et al. (2017)	Q	80, 239
IIGJYLXJNYBXEO-UHFFFAOYSA-N	9.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ETOMEOH	6.8		Wang et al. (2017)	Q	80, 238
$C_3H_8O_2$	3.0×10^{1}		Wang et al. (2017)	Q	80, 239
RRLWYLINGKISHN-UHFFFAOYSA-N	3.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MO2EOLA2OH	9.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_8O_3$	9.6×10^{3}		Wang et al. (2017)	Q	80, 239
CSCSROFYRUZJJH-UHFFFAOYSA-N	4.5×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MO2EOLAOOH	8.1×10^5		Wang et al. (2017)	Q	80, 238
$C_3H_8O_4$	2.8×10^4		Wang et al. (2017)	Q	80, 239
PFSIOEPXGRVTPO-UHFFFAOYSA-N	6.9×10^3		Wang et al. (2017)	Q	80, 240
MCM:MO2EOLB2OH	2.3×10^4		Wang et al. (2017)	Q	80, 238
$C_3H_8O_3$	2.0×10^4		Wang et al. (2017)	Q	80, 239
ONSWVOSXVUHESJ-UHFFFAOYSA-N	4.8×10^4		Wang et al. (2017)	Q	80, 240
MCM:MO2EOLBOOH	6.0×10^5		Wang et al. (2017)	Q	80, 238
$C_3H_8O_4$	1.4×10^5		Wang et al. (2017)	Q	80, 239
VULCDXDIAONDTM-UHFFFAOYSA-N	2.5×10^4		Wang et al. (2017)	Q	80, 240
MCM:DIETETOH	6.0		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_2$	1.7×10^1		Wang et al. (2017)	Q	80, 239
CAFAOQIVXSSFSY-UHFFFAOYSA-N	1.1×10^1		Wang et al. (2017)	Q	80, 240
MCM:EOX2ETA2OH	8.0×10^3		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	6.6×10^3		Wang et al. (2017)	Q	80, 239
WWVBRUMYFUDEJQ-UHFFFAOYSA-N	4.6×10^2		Wang et al. (2017)	Q	80, 240
MCM:EOX2ETB2OH	2.1×10^4		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	8.9×10^3		Wang et al. (2017)	Q	80, 239
RZYMXMZJVMXDRP-UHFFFAOYSA-N	2.1×10^4		Wang et al. (2017)	Q	80, 240
MCM:EOX2OLAOOH	6.3×10^5		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_4$	1.7×10^4		Wang et al. (2017)	Q	80, 239
OSAXOMWTXDBXFG-UHFFFAOYSA-N	4.1×10^3		Wang et al. (2017)	Q	80, 240
MCM:EOX2OLBOOH	6.3×10^5		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_4$	6.2×10^4		Wang et al. (2017)	Q	80, 239
IWDPPKCJRWMAAT-UHFFFAOYSA-N	1.5×10^4		Wang et al. (2017)	Q	80, 240
MCM:H2C3OCOH	2.1×10^4		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	1.0×10^4		Wang et al. (2017)	Q	80, 239
OAPWFUZUONIVKV-UHFFFAOYSA-N	2.2×10^4		Wang et al. (2017)	Q	80, 240
MCM:H2C3OCOOH	6.3×10^5		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_4$	1.3×10^5		Wang et al. (2017)	Q	80, 239
ZZOFHQOVQLUGOX-UHFFFAOYSA-N	1.6×10^4		Wang et al. (2017)	Q	80, 240
MCM:IPRMEETOH	4.2		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_2$	9.3		Wang et al. (2017)	Q	80, 239
BFSUQRCCKXZXEX-UHFFFAOYSA-N	7.4		Wang et al. (2017)	Q	80, 240
MCM:PR2OHMOOOH	7.6×10^5		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_4$	1.1×10^4		Wang et al. (2017)	Q	80, 239
BIISZUJLPYTCKS-UHFFFAOYSA-N	2.7×10^3		Wang et al. (2017)	Q	80, 240
MCM:PROH2MOX	8.9×10^3		Wang et al. (2017)	Q	80, 238
$C_4H_{10}O_3$	7.6×10^3		Wang et al. (2017)	Q	80, 239
OEYNWAWWSZUGDU-UHFFFAOYSA-N	9.3×10^1		Wang et al. (2017)	Q	80, 240

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Table A3.9: Ethers (ROR) (. . . continued)

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MCM:BOXMOH	4.7		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	1.5×10^{1}		Wang et al. (2017)	Q	80, 239
CRHLZRRTZDFDAJ-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:EIPEOH	3.4		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	6.3		Wang et al. (2017)	Q	80, 239
MGMXTRZFWPWZFH-UHFFFAOYSA-N	7.4		Wang et al. (2017)	Q	80, 240
MCM:HIEPOXB	1.5×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_4$	1.8×10^{8}		Wang et al. (2017)	Q	80, 239
YTIKZIBPNMOYQX-UHFFFAOYSA-N	5.6×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:IEACO3H	7.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	3.6×10^{3}		Wang et al. (2017)	Q	80, 239
WBOLSVSGSKMCPN-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:IECCO3H	7.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_5$	2.7×10^{3}		Wang et al. (2017)	Q	80, 239
CEWHGLGNUIHIJU-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:IEPOXA	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	9.3×10^{4}		Wang et al. (2017)	Q	80, 239
CIDUHKBATDRWPE-UHFFFAOYSA-N	4.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:IEPOXC	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	4.7×10^{4}		Wang et al. (2017)	Q	80, 239
REKLCZSNEUFIBP-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:IPROC21OH	5.6		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	1.0×10^{1}		Wang et al. (2017)	Q	80, 239
PWLPTLCMMFJZIU-UHFFFAOYSA-N	9.8		Wang et al. (2017)	Q	80, 240
MCM:MTBEAOH	3.4		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	7.4		Wang et al. (2017)	Q	80, 239
NHNNIMVRQJIZFW-UHFFFAOYSA-N	2.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MTBEBOH	4.8		Wang et al. (2017)	Q	80, 238
$C_5H_{12}O_2$	1.5×10^{1}		Wang et al. (2017)	Q	80, 239
VMPUAIZSESMILD-UHFFFAOYSA-N	3.6		Wang et al. (2017)	Q	80, 240
MCM:BOX2E2OH	5.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	3.6×10^{3}		Wang et al. (2017)	Q	80, 239
WQHNZXURJISVCT-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:BOX2OHAOOH	4.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_4$	3.6×10^{4}		Wang et al. (2017)	Q	80, 239
XRZMTAXNHOGTME-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:BOX2OHBOOH	4.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_4$	8.1×10^{3}		Wang et al. (2017)	Q	80, 239
LCMMTUJPIXBSDS-UHFFFAOYSA-N	2.2×10^{3}		Wang et al. (2017)	Q	80, 240

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MCM:BOXOHETOH	1.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_3$	6.0×10^{3}		Wang et al. (2017)	Q	80, 239
QLKNFVRAYYHHDF-UHFFFAOYSA-N	7.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:DIIPRETOH	3.2		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	3.5		Wang et al. (2017)	Q	80, 239
FRKCZFUUIQCQPC-UHFFFAOYSA-N	4.8		Wang et al. (2017)	Q	80, 240
MCM:ETBEAOH	3.7		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	1.0×10^{1}		Wang et al. (2017)	Q	80, 239
WOSZILCYMCIWFB-UHFFFAOYSA-N	3.0		Wang et al. (2017)	Q	80, 240
MCM:ETBEBOH	3.2		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	4.1		Wang et al. (2017)	Q	80, 239
DUNYNUFVLYAWTI-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ETBECOH	3.7		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	8.5		Wang et al. (2017)	Q	80, 239
BDLXTDLGTWNUFM-UHFFFAOYSA-N	2.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:IPROMC2OH	6.5		Wang et al. (2017)	Q	80, 238
$C_6H_{14}O_2$	1.3×10^{1}		Wang et al. (2017)	Q	80, 239
ZFEKANLLFQEKED-UHFFFAOYSA-N	4.2		Wang et al. (2017)	Q	80, 240
1-butoxy-2-propanol	5.0		Wang et al. (2017)	Q	80, 238
$C_7H_{16}O_2$	1.7×10^{1}		Wang et al. (2017)	Q	80, 239
(MCM:BOX2PROL)	8.7×10^{-1}		Wang et al. (2017)	Q	80, 240
[5131-66-8]					
RWNUSVWFHDHRCJ-UHFFFAOYSA-N					
MCM:BOXOHPROL	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{16}O_3$	7.8×10^{3}		Wang et al. (2017)	Q	80, 239
ITIQJVOJGXCBQB-UHFFFAOYSA-N	6.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:BOXPOLAOOH	3.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{16}O_4$	2.6×10^{4}		Wang et al. (2017)	Q	80, 239
JGCUFCZSCOGTSN-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:BOXPOLBOOH	4.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{16}O_4$	6.0×10^{3}		Wang et al. (2017)	Q	80, 239
AJCGQJRNRRPZGZ-UHFFFAOYSA-N	9.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:BOXPR2OH	5.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{16}O_3$	2.9×10^{3}		Wang et al. (2017)	Q	80, 239
XKPKIGSYCLTAJO-UHFFFAOYSA-N	4.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:BCSOZOH	1.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{26}O_5$	1.1×10^{5}		Wang et al. (2017)	Q	80, 239
JQRHKAPCWHNLMS-UHFFFAOYSA-N	3.4×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:BCSOZOOH	8.5×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{26}O_6$	1.4×10^{5}		Wang et al. (2017)	Q	80, 239
VCKYKGHDZKOMMJ-UHFFFAOYSA-N	5.0×10^{7}		Wang et al. (2017)	Q	80, 240

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MCM:MEMOXYCHO	2.1		Wang et al. (2017)	Q	80, 238
$C_3H_6O_2$	2.0×10^{1}		Wang et al. (2017)	Q	80, 239
YSEFYOVWKJXNCH-UHFFFAOYSA-N	3.0		Wang et al. (2017)	Q	80, 240
MCM:EOX2ETCHO	2.0		Wang et al. (2017)	Q	80, 238
$C_4H_8O_2$	6.9		Wang et al. (2017)	Q	80, 239
IAHZBRPNDIVNNR-UHFFFAOYSA-N	2.3		Wang et al. (2017)	Q	80, 240
MCM:EPXC4DIAL	6.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_3$	7.1×10^{3}		Wang et al. (2017)	Q	80, 239
IRJHVNZVWOCVLV-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	80, 240
MCM:EPXDLCO3H	7.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_5$	9.6×10^{4}		Wang et al. (2017)	Q	80, 239
OKYIQGCZHSMTGV-UHFFFAOYSA-N	7.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:EPXMC4DIAL	3.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_3$	1.2×10^{3}		Wang et al. (2017)	Q	80, 239
SYCYSIWUSJFZTN-UHFFFAOYSA-N	7.4		Wang et al. (2017)	Q	80, 240
MCM:EPXMDLCO3H	3.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_5$	3.1×10^{4}		Wang et al. (2017)	Q	80, 239
LLYFBEXLHOFXFI-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MTBEBCHO	1.1		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_2$	1.5		Wang et al. (2017)	Q	80, 239
HSCUZOQCNBPBST-UHFFFAOYSA-N	5.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:BOX2ECHO	1.2		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	6.5		Wang et al. (2017)	Q	80, 239
RPLPGIHCAYAYKX-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:BZEMUCCO3H	2.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_5$	1.1×10^{5}		Wang et al. (2017)	Q	80, 239
LTCNUSVDDXPSIF-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:BZEPOXMUC	1.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_3$	5.4×10^{3}		Wang et al. (2017)	Q	80, 239
NQHJMOLWTXQPLS-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:EPXM2C4DAL	2.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	3.0×10^{2}		Wang et al. (2017)	Q	80, 239
QTKFOEFUZGORGI-UHFFFAOYSA-N	4.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:EPXM2DCO3H	2.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	6.8×10^{3}		Wang et al. (2017)	Q	80, 239
CFBRPHMFNHCZFV-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ETBEACHO	9.8×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	1.2		Wang et al. (2017)	Q	80, 239
HHIYJPQUMUPZIZ-UHFFFAOYSA-N	4.5×10^{-1}		Wang et al. (2017)	Q	80, 240

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MCM:ETBECCHO	9.8×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	3.5		Wang et al. (2017)	Q	80, 239
SMUYZOMGNHBYHU-UHFFFAOYSA-N	6.8		Wang et al. (2017)	Q	80, 240
MCM:IPROMCCHO	1.6		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_2$	3.3		Wang et al. (2017)	Q	80, 239
AAPDVSFWBQNMLJ-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	80, 240
MCM:EPXMEC4DAL	1.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	2.8×10^{2}		Wang et al. (2017)	Q	80, 239
MOJUYSNCEBTQMW-UHFFFAOYSA-N	2.5		Wang et al. (2017)	Q	80, 240
MCM:EPXMEDCO3H	1.7×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	3.7×10^{3}		Wang et al. (2017)	Q	80, 239
IBELTJZUJIPVRI-UHFFFAOYSA-N	5.6		Wang et al. (2017)	Q	80, 240
MCM:OXYEPOXMUC	5.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_3$	6.8×10^{2}		Wang et al. (2017)	Q	80, 239
QLTFECLMPRWGQQ-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:OXYMUCCO3H	6.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_5$	6.6×10^{3}		Wang et al. (2017)	Q	80, 239
PBSKNYKKTPMDFL-UHFFFAOYSA-N	8.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:OETLMUCO3H	5.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	4.0×10^{3}		Wang et al. (2017)	Q	80, 239
UVJSWMTUJCHEOZ-UHFFFAOYSA-N	5.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:OETLPOXMUC	4.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	4.6×10^{2}		Wang et al. (2017)	Q	80, 239
NORSPZZKBNMHEY-UHFFFAOYSA-N	5.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:IEACHO	7.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	4.2×10^{3}		Wang et al. (2017)	Q	80, 239
SXTKPSXTIDLSQV-UHFFFAOYSA-N	3.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:IECCHO	7.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_8O_3$	1.9×10^{3}		Wang et al. (2017)	Q	80, 239
FUNIHXJAXNKVQS-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:BZEMUCOH	1.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	1.7×10^{9}		Wang et al. (2017)	Q	80, 239
HYRDKGAOZPVDDL-UHFFFAOYSA-N	1.1×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:BZEMUCOOH	7.6×10^{10}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_6$	1.2×10^{9}		Wang et al. (2017)	Q	80, 239
YPGXWAYLBNMEJL-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:OXYMUCOH	3.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	1.3×10^{8}		Wang et al. (2017)	Q	80, 239
SKTLSFGOHJFJLD-UHFFFAOYSA-N	9.3×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:OXYMUCOOH	4.6×10^{11}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_6$	2.9×10^{8}		Wang et al. (2017)	Q	80, 239
ZBCSCRLAPOVYAB-UHFFFAOYSA-N	1.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:OETLMUCOH	2.6×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	7.4×10^{7}		Wang et al. (2017)	Q	80, 239
BKCWOZADWPGCRT-UHFFFAOYSA-N	4.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:OETLMUCOOH	4.2×10^{11}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_6$	1.7×10^{8}		Wang et al. (2017)	Q	80, 239
OMPONQJDZISYFQ-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:PRONEMOOOH	1.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_4$	8.1×10^{2}		Wang et al. (2017)	Q	80, 239
WKDIYCKWLNCFHJ-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PRONEMOX	1.4		Wang et al. (2017)	Q	80, 238
$C_4H_8O_2$	1.4×10^{1}		Wang et al. (2017)	Q	80, 239
CUZLJOLBIRPEFB-UHFFFAOYSA-N	8.1		Wang et al. (2017)	Q	80, 240
MCM:EPXKTMCO3H	2.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	3.2×10^{4}		Wang et al. (2017)	Q	80, 239
ABDSVLWFPNKKBV-UHFFFAOYSA-N	4.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:EPXMKTCO3H	2.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_5$	3.2×10^{4}		Wang et al. (2017)	Q	80, 239
CAGQARJHZCESJI-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:BOXPROBOOH	7.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_4$	2.0×10^{2}		Wang et al. (2017)	Q	80, 239
YHFJWWLEGMYFFZ-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:BOXPRONE	8.1×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_2$	8.0		Wang et al. (2017)	Q	80, 239
UYNCDYOFUJEUQN-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	80, 240
MCM:BOXPROOOH	7.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_4$	6.3×10^{3}		Wang et al. (2017)	Q	80, 239
YUTHBWBUPOPMPG-UHFFFAOYSA-N	2.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:EPXEKTCO3H	2.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	2.4×10^{4}		Wang et al. (2017)	Q	80, 239
PGCJNBUAAIEYIA-UHFFFAOYSA-N	2.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:TLEMUCCO3H	1.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_5$	2.0×10^{5}		Wang et al. (2017)	Q	80, 239
RISGILSSNRWCFR-UHFFFAOYSA-N	5.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:EBZMUCCO3H	1.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_5$	9.6×10^{4}		Wang et al. (2017)	Q	80, 239
GTEVSPXWKYUSQE-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MXYMUCCO3H	7.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_5$	3.6×10^{4}		Wang et al. (2017)	Q	80, 239
ROKAXOITEMHIEK-UHFFFAOYSA-N	3.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:PXYMUCCO3H	7.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_5$	5.5×10^{4}		Wang et al. (2017)	Q	80, 239
AYUPQGRQZSTAMO-UHFFFAOYSA-N	1.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:IPBZMUCO3H	1.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	5.6×10^{4}		Wang et al. (2017)	Q	80, 239
SKJBPGYNTSYQCQ-UHFFFAOYSA-N	9.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:METLMUCO3H	6.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	1.7×10^{4}		Wang et al. (2017)	Q	80, 239
CXRRYJPLLOUVIM-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:PBZMUCCO3H	9.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	5.4×10^{4}		Wang et al. (2017)	Q	80, 239
ZGGPGQBINYKWGU-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:PETLMUCO3H	6.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	2.6×10^{4}		Wang et al. (2017)	Q	80, 239
KWWJCAVGGMMMRV-UHFFFAOYSA-N	7.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:TM123OXMUC	4.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	3.9×10^{3}		Wang et al. (2017)	Q	80, 239
XYHNNFZVTWOCNN-UHFFFAOYSA-N	1.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:TM124MUO3H	4.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	1.2×10^{4}		Wang et al. (2017)	Q	80, 239
FTWAFKXUKWKGAJ-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:TM135MUO3H	5.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	3.4×10^{4}		Wang et al. (2017)	Q	80, 239
JNFPQQOSCDIIIK-UHFFFAOYSA-N	6.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DMEBMUO3H	4.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{14}O_5$	1.7×10^{4}		Wang et al. (2017)	Q	80, 239
JWBQDZWURHDWCA-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DETLMUO3H	3.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{16}O_5$	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
QEEAHFHJZRPBGG-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:BCKSOZ	3.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{22}O_4$	1.4×10^{2}		Wang et al. (2017)	Q	80, 239
JTZKRSQXPBULRM-UHFFFAOYSA-N	1.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:PRONEMOXOH	2.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
RETWRLMOZHRKHX-UHFFFAOYSA-N	6.6		Wang et al. (2017)	Q	80, 240

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
MCM:BOXPRONBOH	1.2×10^{2}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_3$	3.2×10^{2}		Wang et al. (2017)	Q	80, 239
ANPLAICHKIQBPV-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	80, 240
MCM:BOXPRONOH	2.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{14}O_3$	1.0×10^{4}		Wang et al. (2017)	Q	80, 239
NQJNHGUTJISDHM-UHFFFAOYSA-N	9.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:TM123MUCCO	2.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	4.1×10^{7}		Wang et al. (2017)	Q	80, 239
ZVWGUKJQFRZUIG-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:TM123MUCOH	2.6×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	3.7×10^{8}		Wang et al. (2017)	Q	80, 239
JUUFKUYJQYFRGA-UHFFFAOYSA-N	1.1×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:TM123MUOOH	1.7×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_6$	2.7×10^{8}		Wang et al. (2017)	Q	80, 239
LLVDHGQYZCXGKH-UHFFFAOYSA-N	1.9×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:EPXALMKT	2.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	9.8×10^{2}		Wang et al. (2017)	Q	80, 239
QIJMAVIYYVSLPO-UHFFFAOYSA-N	4.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:EPXMALKT	2.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_3$	9.8×10^{2}		Wang et al. (2017)	Q	80, 239
MWBGBWUOLRJCDU-UHFFFAOYSA-N	3.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:EPXEALKT	2.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_3$	1.0×10^{3}		Wang et al. (2017)	Q	80, 239
HQSBJPSKMKUTIT-UHFFFAOYSA-N	9.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:EBZPOXMUC	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_3$	9.1×10^{3}		Wang et al. (2017)	Q	80, 239
UTCVUMOGNJSPDS-UHFFFAOYSA-N	6.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MXYEPOXMUC	6.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_3$	3.5×10^{3}		Wang et al. (2017)	Q	80, 239
VLMKIGFKBHEGBU-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:PXYEPOXMUC	6.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_3$	5.4×10^{3}		Wang et al. (2017)	Q	80, 239
LGKLIBFTBUCZPW-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:IPBZPOXMUC	9.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	6.6×10^{3}		Wang et al. (2017)	Q	80, 239
NUCYHGVQTCVYLO-UHFFFAOYSA-N	4.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:METLPOXMUC	5.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	1.9×10^{3}		Wang et al. (2017)	Q	80, 239
SWHMTTAIKVELRE-UHFFFAOYSA-N	4.8×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A3.9: Ethers (ROR) (. . . continued)

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MCM:PBZPOXMUC	8.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	6.0×10^{3}		Wang et al. (2017)	Q	80, 239
AHKQGNMGHQLOPP-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PETLPOXMUC	5.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	3.0×10^{3}		Wang et al. (2017)	Q	80, 239
UTBNMXYREJYVNQ-UHFFFAOYSA-N	6.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:TM124OXMUC	3.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	1.3×10^{3}		Wang et al. (2017)	Q	80, 239
HFTMUUPKJAPOHL-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:TM135OXMUC	4.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_3$	3.7×10^{3}		Wang et al. (2017)	Q	80, 239
JFCWARPMSNNZLY-UHFFFAOYSA-N	3.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DMEBPOXMUC	3.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{14}O_3$	2.0×10^{3}		Wang et al. (2017)	Q	80, 239
VGOICOHBXPGRQT-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DETLPOXMUC	3.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{16}O_3$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
VPGNNECRJBEQEI-UHFFFAOYSA-N	6.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:BZEMUCCO	1.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_5$	1.1×10^{8}		Wang et al. (2017)	Q	80, 239
KQXCODNTIAPVKL-UHFFFAOYSA-N	3.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:TLEMUCCO	3.7×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_8O_5$	1.7×10^{7}		Wang et al. (2017)	Q	80, 239
AJWOUZMMNQLKHW-UHFFFAOYSA-N	3.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:TLEMUCOH	6.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_5$	1.5×10^{9}		Wang et al. (2017)	Q	80, 239
WPTVRQIFDQMAMS-UHFFFAOYSA-N	5.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:TLEMUCOOH	1.0×10^{12}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_6$	4.8×10^{9}		Wang et al. (2017)	Q	80, 239
DVPKQTIPCHKXBD-UHFFFAOYSA-N	4.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:EBZMUCCO	3.5×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_5$	7.6×10^{6}		Wang et al. (2017)	Q	80, 239
MYHWFJZUBUHIGJ-UHFFFAOYSA-N	2.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:EBZMUCOH	5.6×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	1.0×10^{9}		Wang et al. (2017)	Q	80, 239
VKTUBYIQTACODT-UHFFFAOYSA-N	3.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:EBZMUCOOH	9.1×10^{11}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_6$	3.3×10^{9}		Wang et al. (2017)	Q	80, 239
KWCWGZCSJYJCAS-UHFFFAOYSA-N	8.1×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A3.9: Ethers (ROR) (. . . continued)

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MCM:MXYMUCCO	2.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_5$	3.3×10^{6}		Wang et al. (2017)	Q	80, 239
KJOIECUJZBFUMR-UHFFFAOYSA-N	9.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MXYMUCOH	3.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	3.9×10^{8}		Wang et al. (2017)	Q	80, 239
UZLLCOIUEBQPHF-UHFFFAOYSA-N	4.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:MXYMUCOOH	5.6×10^{11}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_6$	1.2×10^{9}		Wang et al. (2017)	Q	80, 239
ZYWDOJNDZBPDDO-UHFFFAOYSA-N	8.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:OXYMUCCO	1.7×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_5$	1.9×10^{6}		Wang et al. (2017)	Q	80, 239
RJHLIQPRSGXWHC-UHFFFAOYSA-N	2.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PXYMUCCO	2.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_5$	4.9×10^{6}		Wang et al. (2017)	Q	80, 239
UICQALDYFNTPHO-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:PXYMUCOH	3.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_5$	5.1×10^{8}		Wang et al. (2017)	Q	80, 239
MIBKDAKBVPRIGB-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:PXYMUCOOH	5.6×10^{11}		Wang et al. (2017)	Q	80, 238
$C_8H_{12}O_6$	1.6×10^{9}		Wang et al. (2017)	Q	80, 239
GSJPWDRXFYTPMH-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:IPBZMUCCO	3.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	1.3×10^{7}		Wang et al. (2017)	Q	80, 239
XOMPDNKHXMMXOK-UHFFFAOYSA-N	5.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:IPBZMUCOH	5.3×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	6.5×10^{8}		Wang et al. (2017)	Q	80, 239
AKVRVUIGBHJRNQ-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:IPBZMUCOOH	8.5×10^{11}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_6$	2.1×10^{9}		Wang et al. (2017)	Q	80, 239
LSOCHQKLDSXALN-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:METLMUCCO	1.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	3.7×10^{6}		Wang et al. (2017)	Q	80, 239
ZRMCSOCJQIXUEX-UHFFFAOYSA-N	5.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:METLMUCOH	3.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	1.8×10^{8}		Wang et al. (2017)	Q	80, 239
ARJLZFCPXRPKBS-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:METLMUCOOH	5.0×10^{11}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_6$	6.0×10^{8}		Wang et al. (2017)	Q	80, 239
UXABECSPQFCGIJ-UHFFFAOYSA-N	2.3×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:OETLMUCCO	1.6×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	2.0×10^{6}		Wang et al. (2017)	Q	80, 239
JSKKVRLLVVSVCZ-UHFFFAOYSA-N	9.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PBZMUCCO	2.7×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	1.1×10^{7}		Wang et al. (2017)	Q	80, 239
FCRYPGHUONBQCX-UHFFFAOYSA-N	9.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PBZMUCOH	4.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	5.8×10^{8}		Wang et al. (2017)	Q	80, 239
VYXNVIKZUYYSSA-UHFFFAOYSA-N	1.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:PBZMUCOOH	7.3×10^{11}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_6$	2.0×10^{9}		Wang et al. (2017)	Q	80, 239
FCKGMMNUJIAHAV-UHFFFAOYSA-N	5.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:PETLMUCCO	1.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	5.9×10^{6}		Wang et al. (2017)	Q	80, 239
RORTYMWKJCCJQU-UHFFFAOYSA-N	6.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PETLMUCOH	3.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	2.5×10^{8}		Wang et al. (2017)	Q	80, 239
ZLOWXLKYIJYQIH-UHFFFAOYSA-N	8.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:PETLMUCOOH	5.0×10^{11}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_6$	8.1×10^{8}		Wang et al. (2017)	Q	80, 239
RSNULGXAYPPPGL-UHFFFAOYSA-N	3.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:TM124MUCCO	2.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_5$	9.8×10^{6}		Wang et al. (2017)	Q	80, 239
DQECTOJLTKBSTJ-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:TM124MUCOH	2.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	1.0×10^{8}		Wang et al. (2017)	Q	80, 239
KPYCPCVRGFCQPX-UHFFFAOYSA-N	7.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:TM124MUOOH	1.4×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_6$	6.8×10^{7}		Wang et al. (2017)	Q	80, 239
DQFPDDPNMNSRMG-UHFFFAOYSA-N	3.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:TM135MUOH	2.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_5$	2.4×10^{8}		Wang et al. (2017)	Q	80, 239
CZQCDAJVGDGQTR-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:TM135MUOOH	1.4×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{14}O_6$	1.2×10^{8}		Wang et al. (2017)	Q	80, 239
FIFCCDBMOKNVLN-UHFFFAOYSA-N	2.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:DMEBMUOH	1.7×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_5$	1.3×10^{8}		Wang et al. (2017)	Q	80, 239
MURMIEBRJYKLPQ-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DMEBMUOOH	1.2×10^{10}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{16}O_6$	6.2×10^{7}		Wang et al. (2017)	Q	80, 239
QHUZCFCKANZAOE-UHFFFAOYSA-N	3.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DETLMUOH	1.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_5$	8.5×10^{7}		Wang et al. (2017)	Q	80, 239
BLCXZNPOSIAMRZ-UHFFFAOYSA-N	5.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:DETLMUOOH	9.8×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{18}O_6$	4.2×10^{7}		Wang et al. (2017)	Q	80, 239
ZGRWZBBDFVAIEE-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:ETOMECO2H	2.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_8O_3$	3.6×10^{2}		Wang et al. (2017)	Q	80, 239
YZGQDNOIGFBYKF-UHFFFAOYSA-N	7.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MTBEBCO2H	1.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}O_3$	3.9×10^{1}		Wang et al. (2017)	Q	80, 239
BKBZFJRHYSCZQA-UHFFFAOYSA-N	8.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:BOXMCO2H	1.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{12}O_3$	1.2×10^{2}		Wang et al. (2017)	Q	80, 239
AJQOASGWDCBKCJ-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:EPXDLCO2H	9.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_4O_4$	1.5×10^{5}		Wang et al. (2017)	Q	80, 239
BIFCJMYQXQSHFE-UHFFFAOYSA-N	5.4×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:EPXMDLCO2H	5.4×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_6O_4$	5.9×10^{4}		Wang et al. (2017)	Q	80, 239
HNJRQDPCPFMZIJ-UHFFFAOYSA-N	2.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:BZEMUCCO2H	2.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_6O_4$	4.8×10^{5}		Wang et al. (2017)	Q	80, 239
YYDFWEKDUXDLMC-UHFFFAOYSA-N	3.7×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:EPXM2DCO2H	2.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	2.6×10^{4}		Wang et al. (2017)	Q	80, 239
TVFMSHFDVSCCSQ-UHFFFAOYSA-N	6.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:EPXMEDCO2H	2.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	1.5×10^{4}		Wang et al. (2017)	Q	80, 239
CTYOPZSWGBYACX-UHFFFAOYSA-N	5.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:OXYMUCCO2H	7.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_4$	8.1×10^{4}		Wang et al. (2017)	Q	80, 239
CDVXJWVOWNWWPU-UHFFFAOYSA-N	7.1×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:OETLMUCO2H	6.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	5.1×10^{4}		Wang et al. (2017)	Q	80, 239
UVQOKFRFLASUOJ-UHFFFAOYSA-N	3.1×10^{5}		Wang et al. (2017)	Q	80, 240

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:EPXKTMCO2H	3.1×10^5		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	5.3×10^4		Wang et al. (2017)	Q	80, 239
BXVGKWFSHJVVPB-UHFFFAOYSA-N	6.6×10^4		Wang et al. (2017)	Q	80, 240
MCM:EPXMKTCO2H	3.1×10^5		Wang et al. (2017)	Q	80, 238
$C_6H_8O_4$	1.1×10^5		Wang et al. (2017)	Q	80, 239
FTLSPZDBESPPRR-UHFFFAOYSA-N	3.3×10^4		Wang et al. (2017)	Q	80, 240
MCM:EPXEKTCO2H	2.8×10^5		Wang et al. (2017)	Q	80, 238
$C_7H_{10}O_4$	1.8×10^5		Wang et al. (2017)	Q	80, 239
XBMXXNQRKRSRRJ-UHFFFAOYSA-N	5.0×10^5		Wang et al. (2017)	Q	80, 240
MCM:TLEMUCCO2H	1.7×10^6		Wang et al. (2017)	Q	80, 238
$C_7H_8O_4$	8.3×10^5		Wang et al. (2017)	Q	80, 239
YZQFSRDEODCLRC-UHFFFAOYSA-N	1.3×10^7		Wang et al. (2017)	Q	80, 240
MCM:EBZMUCCO2H	1.5×10^6		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_4$	5.0×10^5		Wang et al. (2017)	Q	80, 239
BSMJHSATRRVHTI-UHFFFAOYSA-N	6.8×10^6		Wang et al. (2017)	Q	80, 240
MCM:MXYMUCCO2H	9.1×10^5		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_4$	4.2×10^5		Wang et al. (2017)	Q	80, 239
BMJHPUYAWBLOER-UHFFFAOYSA-N	3.2×10^6		Wang et al. (2017)	Q	80, 240
MCM:PXYMUCCO2H	9.1×10^5		Wang et al. (2017)	Q	80, 238
$C_8H_{10}O_4$	2.9×10^5		Wang et al. (2017)	Q	80, 239
FMBYVAMRNZYNGO-UHFFFAOYSA-N	8.3×10^6		Wang et al. (2017)	Q	80, 240
MCM:IPBZMUCO2H	1.4×10^6		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	3.2×10^5		Wang et al. (2017)	Q	80, 239
LXYULRJMRUJREP-UHFFFAOYSA-N	2.2×10^6		Wang et al. (2017)	Q	80, 240
MCM:METLMUCO2H	8.0×10^5		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	2.1×10^5		Wang et al. (2017)	Q	80, 239
TZAADSLPRMCSBM-UHFFFAOYSA-N	1.0×10^6		Wang et al. (2017)	Q	80, 240
MCM:PBZMUCCO2H	1.2×10^6		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	3.0×10^5		Wang et al. (2017)	Q	80, 239
MSVJIRWCUUEXSY-UHFFFAOYSA-N	2.9×10^6		Wang et al. (2017)	Q	80, 240
MCM:PETLMUCO2H	8.0×10^5		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	1.4×10^5		Wang et al. (2017)	Q	80, 239
YZGPSCFZKHZHEQ-UHFFFAOYSA-N	2.6×10^6		Wang et al. (2017)	Q	80, 240
MCM:TM124MUO2H	4.9×10^5		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	1.4×10^5		Wang et al. (2017)	Q	80, 239
VDBMALGYQLXWML-UHFFFAOYSA-N	4.3×10^6		Wang et al. (2017)	Q	80, 240
MCM:TM135MUO2H	6.2×10^5		Wang et al. (2017)	Q	80, 238
$C_9H_{12}O_4$	3.8×10^5		Wang et al. (2017)	Q	80, 239
RLMHTEATULORAU-UHFFFAOYSA-N	2.1×10^6		Wang et al. (2017)	Q	80, 240

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Table A3.9: Ethers (ROR) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DMEBMUO2H	5.4×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{14}O_4$	2.0×10^{5}		Wang et al. (2017)	Q	80, 239
GTDCDBIZJZUTJP-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:DETLMUO2H	4.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{16}O_4$	1.4×10^{5}		Wang et al. (2017)	Q	80, 239
FTAMRHAZJZCWNK-UHFFFAOYSA-N	5.5×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:DMCOOH	2.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_5$	3.7×10^{3}		Wang et al. (2017)	Q	80, 239
ISFGCMQHKVEPTP-UHFFFAOYSA-N	1.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MMF	1.2		Wang et al. (2017)	Q	80, 238
$C_3H_6O_3$	2.1		Wang et al. (2017)	Q	80, 239
VKWJMTLAAJULGF-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	80, 240
MCM:MMFOOH	9.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_5$	5.6×10^{2}		Wang et al. (2017)	Q	80, 239
AAAZTRZXKHTMLL-UHFFFAOYSA-N	9.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DMCOH	7.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_4$	7.4×10^{2}		Wang et al. (2017)	Q	80, 239
YGODNDLTUXBUQH-UHFFFAOYSA-N	6.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MMFOH	3.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_4$	1.5×10^{2}		Wang et al. (2017)	Q	80, 239
GDDJZBRTXIGGHV-UHFFFAOYSA-N	4.5×10^{1}		Wang et al. (2017)	Q	80, 240
GOLIG1 $C_4H_6O_5$ LEKXYOUPWKVTGM-UHFFFAOYSA-N	1.5×10^{12}	19000	Wieser et al. (2023)	Q	437
GOLIG2 $C_4H_8O_6$ GWSRJJGBNXJVPO-UHFFFAOYSA-N	1.5×10^{15}	24000	Wieser et al. (2023)	Q	437
GOLIG3 $C_4H_{10}O_7$ ADECTKUVLJSMDK-UHFFFAOYSA-N	3.8×10^{18}	29000	Wieser et al. (2023)	Q	437
MGLYFB $C_6H_{10}O_6$ UCPBJDKPOQEXSQ-UHFFFAOYSA-N	7.1×10^{8}	23000	Wieser et al. (2023)	Q	437
MGLYOXDA $C_6H_{10}O_5$ QMSLRDMQAWWKIZ-UHFFFAOYSA-N	2.0×10^{8}	16000	Wieser et al. (2023)	Q	437
MGLYOXDB $C_6H_{12}O_6$ IUHMFBWAUOLAFM-UHFFFAOYSA-N	1.5×10^{13}	22000	Wieser et al. (2023)	Q	437

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A3.10 Heterocycles with oxygen

Table A3.10: Heterocycles with oxygen

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
β-propiolactone $C_3H_4O_2$ [57-57-8] VEZXCJBBBCKRPI-UHFFFAOYSA-N	1.3×10^{1}		Ebert et al. (2023)	?	316
2-methyl-1,3-dioxolane $C_4H_8O_2$ [497-26-7] HTWIZMNMTWYQRN-UHFFFAOYSA-N	7.9×10^{-1}		Ebert et al. (2023)	?	316
DIEPOXO3 $C_5H_8O_3$ QGQUFAZKBSHWQB-UHFFFAOYSA-N	1.3×10^{3}	14000	Wieser et al. (2023)	Q	437
IEPOXO4 $C_5H_8O_3$ DNQIATHBSKHPLN-UHFFFAOYSA-N	2.1×10^{4}	14000	Wieser et al. (2023)	Q	437
2,2-dimethyl-1,3-dioxolane $C_5H_{10}O_2$ [2916-31-6] SIJBDWPVNAYVGY-UHFFFAOYSA-N	4.8×10^{-1}		Ebert et al. (2023)	?	316
METHFDIOL $C_5H_{10}O_3$ UNAIOYXCADSMDR-UHFFFAOYSA-N	9.0×10^{5}	11000	Wieser et al. (2023)	Q	437
3,4-dihydro-2-methoxy-2H-pyran $C_6H_{10}O_2$ [4454-05-1] XCYWUZHUTJDTGS-UHFFFAOYSA-N	9.7×10^{-2}		Ebert et al. (2023)	?	316
maltol $C_6H_6O_3$ [118-71-8] XPCTZQVDEJYUGT-UHFFFAOYSA-N	7.3×10^{2}		Abraham et al. (2019)	Q	
2-methylfuran C_5H_6O [534-22-5] VQKFNUFAXTZWDK-UHFFFAOYSA-N	1.5×10^{-3}	4100	Wieland et al. (2015)	M	532
3-methylfuran C_5H_6O [930-27-8] KJRRQXYWFQKJIP-UHFFFAOYSA-N	3.2×10^{-3}		Wu et al. (2022a)	Q	413

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Table A3.10: Heterocycles with oxygen (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-furanmethanol	1.3×10^{2}		Duchowicz et al. (2020)	V	186
$C_5H_6O_2$	1.2×10^{2}		HSDB (2015)	V	
(furfuryl alcohol)	2.5×10^{1}		Yaws (2003)	X	258
[98-00-0]	2.2×10^{1}		Dupeux et al. (2022)	Q	259
XPFVYQJUAUNWIW-UHFFFAOYSA-N	2.4×10^{1}		Duchowicz et al. (2020)	Q	
	5.3×10^{1}		Gharagheizi et al. (2012)	Q	
	6.2×10^{1}		Raventos-Duran et al. (2010)	Q	271, 243
	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	3.4×10^{1}		Hilal et al. (2008)	Q	
	4.8×10^{1}		Modarresi et al. (2007)	Q	67
	4.8×10^{2}		Katritzky et al. (1998)	Q	
	1.1×10^{2}		Yaws (1999)	?	21, 12
tetrahydropyran-2-methanol	6.5×10^{2}		Duchowicz et al. (2020)	V	186
$C_6H_{12}O_2$	5.2×10^{1}		Duchowicz et al. (2020)	Q	
[100-72-1]	6.2×10^{1}		Raventos-Duran et al. (2010)	Q	271, 243
ROTONRWJLXYJBD-UHFFFAOYSA-N	3.1×10^{2}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{3}		Raventos-Duran et al. (2010)	Q	245
	9.0×10^{1}		Hilal et al. (2008)	Q	
	8.5×10^{1}		Modarresi et al. (2007)	Q	67
oxirane	5.8×10^{-2}	3200	Conway et al. (1983)	M	
C_2H_4O	8.3×10^{-2}		Lide and Frederikse (1995)	V	
(ethylene oxide)	8.6×10^{-2}		Mackay et al. (1993)	V	
[75-21-8]	5.0×10^{-2}		Hwang et al. (1992)	V	
IAYPIBMASNFSPL-UHFFFAOYSA-N	6.0×10^{-2}		Keshavarz et al. (2022)	Q	
	1.4×10^{-1}		Duchowicz et al. (2020)	Q	
	9.3×10^{-3}		Wang et al. (2017)	Q	80, 238
	5.9×10^{-2}		Wang et al. (2017)	Q	80, 239
	6.0×10^{-2}		Wang et al. (2017)	Q	80, 240
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	2.9×10^{-2}		Modarresi et al. (2007)	Q	67
	6.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.0×10^{-2}		Katritzky et al. (1998)	Q	
	6.7×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	4.1×10^{-2}		Yaws (1999)	?	21
1,2-epoxypropane	1.4×10^{-1}		Duchowicz et al. (2020)	V	186
C_3H_6O	1.4×10^{-1}		HSDB (2015)	V	
(1,2-propylene oxide)	1.2×10^{-1}		Mackay et al. (2006c)	V	
[75-56-9]	1.2×10^{-1}		Lide and Frederikse (1995)	V	
GOOHAUXETOMSMM-UHFFFAOYSA-N	1.2×10^{-1}		Mackay et al. (1993)	V	
	1.7×10^{-1}		Yaws (2003)	X	237, 12
	5.2×10^{-2}		Goldstein (1982)	X	446
	5.1×10^{-2}	3500	Goldstein (1982)	X	298
	6.3×10^{-2}		Duchowicz et al. (2020)	Q	
	1.2×10^{-1}		Gharagheizi et al. (2010)	Q	246
	1.7×10^{-2}		Hilal et al. (2008)	Q	

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Table A3.10: Heterocycles with oxygen (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.5×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	1.3×10^{-2}		Katritzky et al. (1998)	Q	
	1.4×10^{-1}		Yaws (1999)	?	21, 12
phenyloxirane	6.2×10^{-1}		HSDB (2015)	V	
C_8H_8O	5.8×10^{-1}		Mackay et al. (2006c)	V	
(styrene oxide)	5.8×10^{-1}		Mackay et al. (1993)	V	
[96-09-3]	6.2×10^{-1}		Meylan and Howard (1991)	V	
AWMVMTVKBNGEAK-UHFFFAOYSA-N	2.5×10^{-1}		Hilal et al. (2008)	Q	
	5.5×10^{-1}		Modarresi et al. (2007)	Q	67
	1.0		Meylan and Howard (1991)	Q	
oxacyclopentadiene	1.8×10^{-3}		HSDB (2015)	V	
C_4H_4O	1.8×10^{-3}		Mackay et al. (2006c)	V	
(furan; furfuran)	1.8×10^{-3}		Mackay et al. (1993)	V	
[110-00-9]	1.8×10^{-3}		Yaws (2003)	X	258
YLQBMQCUIZJEEH-UHFFFAOYSA-N	1.8×10^{-3}		Yaws (2003)	X	237
	2.2×10^{-3}		Dupeux et al. (2022)	Q	259
	4.6×10^{-3}		Hayer et al. (2022)	Q	20
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.3×10^{-3}		Hilal et al. (2008)	Q	
	1.9×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	4.3×10^{-3}		Yao et al. (2002)	Q	229
	1.2×10^{-2}		Katritzky et al. (1998)	Q	
	1.8×10^{-3}		Yaws (1999)	?	21
	1.8×10^{-3}		Yaws and Yang (1992)	?	21
dibenzofuran	7.4×10^{-2}	5800	Brockbank (2013)	L	1
$C_{12}H_8O$	4.6×10^{-2}		Duchowicz et al. (2020)	V	186
(2,2'-biphenylene oxide)	4.7×10^{-2}		HSDB (2015)	V	
[132-64-9]	7.1×10^{-2}		Mackay et al. (2006b)	V	
TXCDCPKCNAJMEE-UHFFFAOYSA-N	7.2×10^{-2}		Govers and Krop (1998)	V	
	9.1×10^{-2}		Mackay et al. (1992b)	X	364
	8.9×10^{-3}		Yaws (2003)	X	237
	2.8×10^{-1}		Duchowicz et al. (2020)	Q	
	9.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
	8.2×10^{-2}		Saçan et al. (2005)	Q	
	4.7×10^{-2}		Govers and Krop (1998)	Q	
2-furancarboxaldehyde	2.6		Duchowicz et al. (2020)	V	186
$C_5H_4O_2$	2.6		HSDB (2015)	V	
(furfural; 2-furanaldehyde)	2.7		Mackay et al. (2006c)	V	
[98-01-1]	2.7		Mackay et al. (1995)	V	
HYBBIBNJHNGZAN-UHFFFAOYSA-N	3.0		Yaws (2003)	X	258
	3.0		Yaws (2003)	X	237
	9.6		Dupeux et al. (2022)	Q	259

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Table A3.10: Heterocycles with oxygen (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.4×10^{-1}		Duchowicz et al. (2020)	Q	
	1.7		Gharagheizi et al. (2012)	Q	
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	6.2		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.0		Gharagheizi et al. (2010)	Q	246
	6.0		Hilal et al. (2008)	Q	
	8.1×10^{-1}		Modarresi et al. (2007)	Q	67
	7.2×10^{-2}		Emel'yanenko et al. (2007)	Q	415
	7.2×10^{-2}		Hertel and Sommer (2006)	Q	415
		6100	Kühne et al. (2005)	Q	
		5900	Kühne et al. (2005)	?	
	3.0		Yaws (1999)	?	21
5-methylfurfural $C_6H_6O_2$ [620-02-0] OUDFNZMQXZILJD-UHFFFAOYSA-N	4.7		Ebert et al. (2023)	?	316
2,2-dimethyloxirane C_4H_8O (isobutylene oxide) [558-30-5] GELKGHVAFRCJNA-UHFFFAOYSA-N	2.9×10^{-2}		Ebert et al. (2023)	?	316
tetrahydrofuran	1.5×10^{-1}	5700	Brockbank (2013)	L	1
C_4H_8O	1.5×10^{-1}	5700	Ondo and Dohnal (2007)	M	1
(THF)	6.4×10^{-1}		Welke et al. (1998)	M	
[109-99-9]	6.0×10^{-1}	4200	Pividal et al. (1992)	M	
WYURNTSHIVDZCO-UHFFFAOYSA-N	2.2×10^{-1}		Signer et al. (1969)	M	
	1.4×10^{-1}	5700	Cabani et al. (1971b)	T	
	6.0×10^{-2}		Yaws (2003)	X	237, 12
	1.1×10^{-1}		Keshavarz et al. (2022)	Q	
	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
	8.5×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	6.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
	1.1×10^{-1}		Hilal et al. (2008)	Q	
	3.5×10^{-2}		Modarresi et al. (2007)	Q	67
		4000	Kühne et al. (2005)	Q	
	1.5×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	1.3×10^{-1}		English and Carroll (2001)	Q	230, 231
	2.4×10^{-2}		Katritzky et al. (1998)	Q	
	1.3×10^{-1}		Suzuki et al. (1992)	Q	232
	1.4×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		3200	Kühne et al. (2005)	?	
	1.9×10^{-1}		Yaws (1999)	?	21, 12

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Table A3.10: Heterocycles with oxygen (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.4×10^{-1}		Abraham et al. (1990)	?	
tetrahydrofuran-d8 C_4D_8O (THF-d8) [1693-74-9] WYURNTSHIVDZCO-SVYQBANQSA-N	2.3×10^{-1}	8000	Hiatt (2013)	M	
2-methyltetrahydrofuran $CH_3C_4H_7O$ [96-47-9] JWUJQDFVADABEY-UHFFFAOYSA-N	1.5×10^{-3}		Mackay et al. (1993)	V	
	1.1×10^{-1}	6200	Cabani et al. (1971b)	T	
	1.5×10^{-1}		Keshavarz et al. (2022)	Q	
	5.3×10^{-2}		Duchowicz et al. (2020)	Q	
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.1×10^{-2}		Hilal et al. (2008)	Q	
	1.7×10^{-2}		Modarresi et al. (2007)	Q	67
		4400	Kühne et al. (2005)	Q	
	1.0×10^{-1}		English and Carroll (2001)	Q	230, 260
	2.4×10^{-2}		Katritzky et al. (1998)	Q	
	9.0×10^{-2}		Suzuki et al. (1992)	Q	232
	1.1×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		5400	Kühne et al. (2005)	?	
2,5-dimethyltetrahydrofuran $(CH_3)_2C_4H_6O$ [1003-38-9] OXMIDRBAFOEOQT-UHFFFAOYSA-N	5.5×10^{-2}	6800	Cabani et al. (1971b)	T	
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.1×10^{-2}		Hilal et al. (2008)	Q	
	2.5×10^{-2}		Modarresi et al. (2007)	Q	67
	7.9×10^{-2}		English and Carroll (2001)	Q	230, 231
tetrahydropyran $C_5H_{10}O$ (THP) [142-68-7] DHXVGJBLRPWPCS-UHFFFAOYSA-N	8.1×10^{-2}	5800	Brockbank (2013)	L	1
	8.3×10^{-2}	5900	Ondo and Dohnal (2007)	M	1
	1.0×10^{-1}		Mackay et al. (2006c)	V	
	1.0×10^{-1}		Mackay et al. (1993)	V	
	7.8×10^{-2}	5900	Cabani et al. (1971b)	T	
	1.5×10^{-1}		Keshavarz et al. (2022)	Q	
	1.4×10^{-1}		Duchowicz et al. (2020)	Q	
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.1×10^{-1}		Hilal et al. (2008)	Q	
	6.9×10^{-2}		Modarresi et al. (2007)	Q	67
	7.9×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.0×10^{-1}		English and Carroll (2001)	Q	230, 274
	2.6×10^{-2}		Katritzky et al. (1998)	Q	
	9.9×10^{-2}		Suzuki et al. (1992)	Q	232
	7.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21

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Table A3.10: Heterocycles with oxygen (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	7.9×10^{-2}		Abraham et al. (1990)	?	
3-methyltetrahydropyran $C_6H_{12}O$ [26093-63-0] UJQZTMFRMLEYQN-UHFFFAOYSA-N		4700 5300	Kühne et al. (2005) Kühne et al. (2005)	Q ?	
3,4-dihydro-2H-pyran C_5H_8O [110-87-2] BUDQDWGNQVEFAC-UHFFFAOYSA-N		3500 3600	Kühne et al. (2005) Kühne et al. (2005)	Q ?	
1,3-dioxolane $C_3H_6O_2$ [646-06-0] WNXJIVFYUVYPPR-UHFFFAOYSA-N	4.3×10^{-1} 4.0×10^{-1} 8.1×10^{-2} 2.1 1.5 2.2×10^{-1} 4.0×10^{-1}	4800 4800	Ondo and Dohnal (2007) Cabani et al. (1971b) Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Duchowicz et al. (2020)	M T Q Q Q Q ?	1 184 67 185, 21
1,3-dioxane $C_4H_8O_2$ [505-22-6] VDFVNEFVBPFDSB-UHFFFAOYSA-N	1.8 2.1		O'Farrell and Waghorne (2010) Hilal et al. (2008)	M Q	
1,4-dioxane $C_4H_8O_2$ (dioxane) [123-91-1] RYHBNJHYFVUHQT-UHFFFAOYSA-N	1.8 2.3 2.0 2.0 1.4 2.1 4.4 1.4 2.2 1.9 1.1 2.0 1.1 1.1×10^{-1} 2.8 7.8×10^{-1} 1.2×10^{1} 1.6 3.3 1.3 1.5 8.2×10^{-1} 2.1 	5800 6600 5800 5100 5800 5200 6100	Brockbank (2013) Hiatt (2013) Ondo and Dohnal (2007) Welke et al. (1998) Kolb et al. (1992) Park et al. (1987) Ioffe et al. (1984) Friant and Suffet (1979) Rohrschneider (1973) Hwang et al. (1992) Amoore and Buttery (1978) Cabani et al. (1971b) Hayer et al. (2022) Keshavarz et al. (2022) Duchowicz et al. (2020) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Kühne et al. (2005) English and Carroll (2001) Russell et al. (1992) Duchowicz et al. (2020) Kühne et al. (2005)	L M M M M M M M M V V T Q Q Q Q Q Q Q Q Q Q Q ?	1 1 277 80 38 20 184 242, 243 244 245 67 230, 231 279 185, 21

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Table A3.10: Heterocycles with oxygen (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.8		Yaws (1999)	?	21
	2.0		Betterton (1992)	?	533
	2.2		Betterton (1992)	?	534
	1.4		Yaws and Yang (1992)	?	21
1,4-dioxane-d8 $C_4D_8O_2$ (dioxane-d8) [17647-74-4] RYHBNJHYFVUHQT-SVYQBANQSA-N	2.8	6800	Hiatt (2013)	M	
trioxane $C_3H_6O_3$ [110-88-3] BGJSXRVXTHVRSN-UHFFFAOYSA-N	9.6×10^{-1}		Yaws (2003)	X	258
	2.7		Dupeux et al. (2022)	Q	259
4-methyl-1,3-dioxolan-2-one $C_4H_6O_3$ (propylene carbonate) [108-32-7] RUOJZAUFBMNUDX-UHFFFAOYSA-N	2.9×10^{2}		Duchowicz et al. (2020)	V	186
	2.9×10^{2}		HSDB (2015)	V	
	1.6×10^{-1}		Duchowicz et al. (2020)	Q	
	1.4×10^{2}		Abraham et al. (1990)	?	
1,3,3-trimethyl-2-oxabicyclo[2.2.2]octane $C_{10}H_{18}O$ (eucalyptol; 1,8-cineole) [470-82-6] WEEGYLXZBRQIMU-UHFFFAOYSA-N	5.9×10^{-2}		Kish et al. (2013)	M	
	1.2×10^{-1}		Amoore and Buttery (1978)	M	
	9.0×10^{-2}		Duchowicz et al. (2020)	V	186
	7.5×10^{-2}		Copolovici and Niinemets (2005)	V	
	7.4×10^{-2}		Niinemets and Reichstein (2002)	V	
	7.8×10^{-2}		Amoore and Buttery (1978)	V	
	5.3×10^{-3}		Duchowicz et al. (2020)	Q	
	2.2×10^{-2}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	67
limonene oxide $C_{10}H_{16}O$ [1195-92-2] CCEFMUBVSUDRLG-UHFFFAOYSA-N	5.6×10^{-2}		Fichan et al. (1999)	M	
	5.5×10^{-2}		Duchowicz et al. (2020)	V	186
	2.7×10^{-2}	4600	van Roon et al. (2005)	V	
	4.8×10^{-2}		Duchowicz et al. (2020)	Q	
dibenzo[b,e][1,4]dioxin $C_{12}H_8O_2$ (dibenzo-p-dioxin) [262-12-4] NFBOHOGPQUYFRF-UHFFFAOYSA-N	8.9×10^{-2}		Duchowicz et al. (2020)	V	186
	9.0×10^{-2}		HSDB (2015)	V	
	8.5×10^{-2}		Mackay et al. (2006b)	V	
	9.5×10^{-3}		Saçan et al. (2005)	V	
	8.5×10^{-2}		Govers and Krop (1998)	V	
	8.1×10^{-2}		Shiu et al. (1988)	V	
	2.0		Duchowicz et al. (2020)	Q	
	2.7×10^{-2}		Saçan et al. (2005)	Q	
	6.3×10^{-2}		Wang and Wong (2002)	Q	535
	9.1×10^{-2}		Govers and Krop (1998)	Q	

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Table A3.10: Heterocycles with oxygen (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
piperonal	1.8×10^{1}		Duchowicz et al. (2020)	V	186
$C_8H_6O_3$	1.8×10^{1}		HSDB (2015)	V	
[120-57-0]	1.6×10^{2}		Duchowicz et al. (2020)	Q	
SATCULPHIDQDRE-UHFFFAOYSA-N	4.1×10^{2}		Hilal et al. (2008)	Q	
	1.1×10^{1}		Modarresi et al. (2007)	Q	67
paraldehyde	5.8×10^{-1}		Duchowicz et al. (2020)	V	186
$C_6H_{12}O_3$	2.5×10^{-1}		HSDB (2015)	V	
[123-63-7]	4.7		Duchowicz et al. (2020)	Q	
SQYNKIJPMDEDEG-UHFFFAOYSA-N	3.6×10^{-1}		Hilal et al. (2008)	Q	
	2.1		Modarresi et al. (2007)	Q	67
	6.4×10^{-1}		Yaws (1999)	?	21, 38
benzofuran	1.9×10^{-2}		HSDB (2015)	Q	99
C_8H_6O	1.9×10^{-2}		Hilal et al. (2008)	Q	
[271-89-6]					
IANQTJSKSUMEQM-UHFFFAOYSA-N					
γ-nonalactone	1.8×10^{-1}		Hertel and Sommer (2006)	Q	415
$C_9H_{16}O_2$					
[104-61-0]					
OALYTRUKMRCXNH-UHFFFAOYSA-N					
xanthene	1.3×10^{-1}		Abraham et al. (2019)	Q	
$C_{13}H_{10}O$					
[92-83-1]					
GJCOSYZMQJWQCA-UHFFFAOYSA-N					
1,5,5,9-tetramethyl-13-oxatricyclo(8.3.0.0(4,9))tridecane	2.0×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{16}H_{28}O$	2.9×10^{-1}		Zhang et al. (2010)	Q	287, 289
(ambroxan)	6.5×10^{-2}		Zhang et al. (2010)	Q	287, 290
[3738-00-9]	1.1×10^{-3}		Zhang et al. (2010)	Q	287, 291
YPZUZOLGGMJZJO-UHFFFAOYSA-N					
1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylcyclopenta[g]-2-benzopyran	7.6×10^{-2}		HSDB (2015)	V	
$C_{18}H_{26}O$	7.5×10^{-2}		Zhang et al. (2010)	Q	287, 288
[1222-05-5]	8.2		Zhang et al. (2010)	Q	287, 289
ONKNPOPIGWHAQC-UHFFFAOYSA-N	8.4×10^{-2}		Zhang et al. (2010)	Q	287, 290
	9.9×10^{-3}		Zhang et al. (2010)	Q	287, 291
cinmethylin	1.3×10^{1}		Ebert et al. (2023)	?	318
$C_{18}H_{26}O_2$					
[87818-31-3]					
QMTNOLKHSWIQBE-FGTMMUONSA-N					

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Table A3.10: Heterocycles with oxygen (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
milbemycin A4 $C_{32}H_{46}O_7$ (milbemectin A4) [51596-11-3] VOZIAWLUULBIPN-LRBNAKOISA-N	7.7×10^6		Ebert et al. (2023)	?	318

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A3.11 Oxidized terpenoids

Table A3.11: Oxidized terpenoids

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(1S-endo)-1,7,7-trimethyl-bicyclo[2.2.1]heptan-2-ol	4.5×10^{-1}		Fichan et al. (1999)	M	
$C_{10}H_{18}O$	7.2×10^{-1}		Duchowicz et al. (2020)	V	186
(1S-endo-(-)-borneol)	4.0×10^{-1}		Duchowicz et al. (2020)	Q	
[464-45-9]					
DTGKSKDOIYIVQL-QXFUBDJGSA-N					
(1R)-1,3,3-trimethylbicyclo[2.2.1]heptan-2-ol	3.6×10^{-1}		Fichan et al. (1999)	M	
$C_{10}H_{18}O$	3.6×10^{-1}		Duchowicz et al. (2020)	V	186
(endo-(+)-fenchyl alcohol)	4.0×10^{-1}		Duchowicz et al. (2020)	Q	
[2217-02-9]					
IAIHUHQCLTYTSF-OYNCUSHFSA-N					
2-(4-methyl-3-cyclohexen-1-yl)-2-propanol	4.4	2200	Copolovici and Niinemets (2005)	M	
$C_{10}H_{18}O$	4.1		Copolovici and Niinemets (2005)	V	
(α-terpineol)	6.0×10^{-1}	4800	van Roon et al. (2005)	V	
[98-55-5]	4.2		Niinemets and Reichstein (2002)	V	
WUOACPNHFRMFPN-UHFFFAOYSA-N	7.4×10^{-1}	5400	Li et al. (1998)	V	
	6.5		Dupeux et al. (2022)	Q	259
	3.6		Hilal et al. (2008)	Q	
	8.2×10^{-1}		Modarresi et al. (2007)	Q	67
1,2-dimethyl-3-(1-methylethenyl)-cyclopentanol	5.3×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{10}H_{18}O$	4.0×10^{-1}	17000	Li et al. (1998)	V	
(plinol)	3.4×10^{-1}		Duchowicz et al. (2020)	Q	
[72402-00-7]	1.2		Hilal et al. (2008)	Q	
ZRVPDCMGGOSDKG-UHFFFAOYSA-N	1.6		Modarresi et al. (2007)	Q	67
1-methyl-4-(1-methylethyl)-7-oxabicyclo[2.2.1]heptane	3.9×10^{-2}		Helburn et al. (2008)	M	
$C_{10}H_{18}O$	7.4×10^{-2}		Copolovici and Niinemets (2005)	V	
(1,4-cineole)	1.4×10^{-1}	4000	van Roon et al. (2005)	V	
[470-67-7]					
RFFOTVCVTJUTAD-UHFFFAOYSA-N					
1,7,7-trimethyl-bicyclo[2.2.1]heptan-2-one	1.2×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{10}H_{16}O$	1.2×10^{-1}		HSDB (2015)	V	
(camphor)	1.1		Copolovici and Niinemets (2005)	V	
[76-22-2]	5.4×10^{-1}	4800	van Roon et al. (2005)	V	
DSSYKIVIOFKYAU-UHFFFAOYSA-N	8.2×10^{-1}		Niinemets and Reichstein (2002)	V	
	2.3×10^{-2}		Duchowicz et al. (2020)	Q	
	3.5×10^{-1}		Modarresi et al. (2007)	Q	67

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Table A3.11: Oxidized terpenoids (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,7,7-trimethyl-3-oxatricyclo[4.1.1.0(2,4)]octane	2.3×10^{-2}		Fichan et al. (1999)	M	
$C_{10}H_{16}O$	2.3×10^{-2}		Duchowicz et al. (2020)	V	186
((-)-α-pinene oxide)	2.4×10^{-2}		Copolovici and Niinemets (2005)	V	
[1686-14-2]	5.4×10^{-2}	4400	van Roon et al. (2005)	V	
NQFUSWIGRKFAHK-UHFFFAOYSA-N	2.2×10^{-2}		Duchowicz et al. (2020)	Q	
5-methyl-2-(1-methylethylidene)-cyclohexanone	2.8×10^{-1}	5300	van Roon et al. (2005)	V	
$C_{10}H_{16}O$	1.7×10^{-1}		HSDB (2015)	Q	99
(pulegone)					
[89-82-7]					
NZGWDASTMWDZIW-UHFFFAOYSA-N					
exo-2-[(1,7,7-trimethylbicyclo[2.2.1]hept-2-yl)-oxy]ethanol	1.0	4100	Li et al. (1998)	V	
$C_{12}H_{22}O_2$					
(arbanol)					
[7070-15-7]					
IWWCSDGEIDYEJV-JBLDHEPKSA-N					
bornyl acetate	3.8×10^{-4}	1700	Copolovici and Niinemets (2015)	M	
$C_{12}H_{20}O_2$					
[5655-61-8]					
KGEKLUUHTZCSIP-SCVCMEIPSA-N					
β-ionone	1.2		Fichan et al. (1999)	M	
$C_{13}H_{20}O$	1.2×10^{-1}		Duchowicz et al. (2020)	V	186
[79-77-6]	1.5×10^{-2}		Abney (2021)	Q	399
PSQYTAPXSHCGMF-BQYQJAHWSA-N	6.6×10^{-3}		Duchowicz et al. (2020)	Q	
nerolidol	3.2×10^{-4}	4300	Copolovici and Niinemets (2015)	M	
$C_{15}H_{26}O$					
[7212-44-4]					
FQTLCLSUCSAZDY-UHFFFAOYSA-N					

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A3.12 Miscellaneous

Table A3.12: Miscellaneous

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
oxoethanoic acid	1.1×10^{2}	4800	Burkholder et al. (2019)	L	460
OHCCOOH	1.1×10^{2}	4800	Burkholder et al. (2015)	L	460
(glyoxylic acid)	1.1×10^{2}	4800	Sander et al. (2011)	L	
[298-12-4]	1.1×10^{2}	4800	Ip et al. (2009)	M	
HHLFWLYXYJOTON-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	80, 238
	1.5×10^{1}		Wang et al. (2017)	Q	80, 239
	6.9×10^{1}		Wang et al. (2017)	Q	80, 240
	3.3×10^{3}		HSDB (2015)	Q	99
	7.8×10^{4}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{8}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{3}		Raventos-Duran et al. (2010)	Q	245
	8.9×10^{1}		Saxena and Hildemann (1996)	E	401
			Warneck (2005)	?	536
hydroxyethanoic acid	2.8×10^{2}	4000	Burkholder et al. (2019)	L	460, 537
$HOCH_2COOH$	2.8×10^{2}	4000	Burkholder et al. (2015)	L	460, 538
(glycolic acid)	2.8×10^{2}	4000	Sander et al. (2011)	L	
[79-14-1]	2.8×10^{2}	4000	Ip et al. (2009)	M	
AEMRFAOFKBGASW-UHFFFAOYSA-N	1.9×10^{3}		Wang et al. (2017)	Q	80, 238
	1.4×10^{5}		Wang et al. (2017)	Q	80, 239
	5.3×10^{4}		Wang et al. (2017)	Q	80, 240
	1.2×10^{3}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{4}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	245
2-hydroxyethanal	3.9×10^{2}	4600	Burkholder et al. (2019)	L	460
$HOCH_2CHO$	3.9×10^{2}	4600	Burkholder et al. (2015)	L	460
(hydroxyacetaldehyde; glycolaldehyde)	4.1×10^{2}	4600	Betterton and Hoffmann (1988)	M	460
[141-46-8]	9.9×10^{2}		Lee and Zhou (1993)	C	87
WGCNASOHLSPBMP-UHFFFAOYSA-N	2.9×10^{2}		Keshavarz et al. (2022)	Q	
	1.8×10^{1}		Duchowicz et al. (2020)	Q	299
	1.3×10^{1}		Wang et al. (2017)	Q	80, 238
	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
	4.2		Wang et al. (2017)	Q	80, 240
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	271, 243
	7.8×10^{3}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	6.5×10^{2}		Hilal et al. (2008)	Q	
	2.4×10^{2}		Modarresi et al. (2007)	Q	67
		7600	Kühne et al. (2005)	Q	
	4.1×10^{2}		Duchowicz et al. (2020)	?	185, 21
		4600	Kühne et al. (2005)	?	

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Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
propanonal	3.5×10^{1}	7500	Burkholder et al. (2019)	L	460
CH_3COCHO	3.5×10^{1}	7500	Burkholder et al. (2015)	L	460
(methylglyoxal; pyruvaldehyde)	3.2×10^{2}		Zhou and Mopper (1990)	M	70
[78-98-8]	3.4×10^{1}	7500	Betterton and Hoffmann (1988)	M	460
AIJULSRZWUXGPQ-UHFFFAOYSA-N	3.7×10^{2}		Lee and Zhou (1993)	C	87
	5.4×10^{1}		Wang et al. (2017)	Q	80, 238
	1.3×10^{1}		Wang et al. (2017)	Q	80, 239
	2.9×10^{-2}		Wang et al. (2017)	Q	80, 240
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	271, 243
	4.9×10^{2}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	1.4×10^{1}		Modarresi et al. (2007)	Q	67
		6200	Kühne et al. (2005)	Q	
	8.2		Katritzky et al. (1998)	Q	
		7600	Kühne et al. (2005)	?	
2-oxopropanoic acid	3.1×10^{3}	5100	Burkholder et al. (2019)	L	
$CH_3COCOOH$	3.1×10^{3}	5100	Burkholder et al. (2015)	L	
(pyruvic acid)	3.1×10^{3}	5100	Sander et al. (2011)	L	
[127-17-3]	3.1×10^{3}	5100	Sander et al. (2006)	L	
LCTONWCANYUPML-UHFFFAOYSA-N	3.0×10^{3}	5300	Staudinger and Roberts (2001)	L	
	3.1×10^{3}	5100	Khan et al. (1995)	M	
	3.1×10^{3}		Khan et al. (1992)	M	
	3.1×10^{3}	5200	Khan and Brimblecombe (1992)	M	
	2.2×10^{4}		Keshavarz et al. (2022)	Q	
	2.3×10^{2}		Duchowicz et al. (2020)	Q	184
	7.8×10^{3}		Wang et al. (2017)	Q	80, 238
	5.0×10^{1}		Wang et al. (2017)	Q	80, 239
	1.9×10^{1}		Wang et al. (2017)	Q	80, 240
	1.6×10^{3}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{6}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{3}		Raventos-Duran et al. (2010)	Q	245
	2.6×10^{3}		Hilal et al. (2008)	Q	
	2.6×10^{3}		Modarresi et al. (2007)	Q	67
		5600	Kühne et al. (2005)	Q	
	3.1×10^{3}		Duchowicz et al. (2020)	?	185, 21
		5300	Kühne et al. (2005)	?	
3-oxopropanoic acid	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$OHCCH_2COOH$	1.2×10^{4}		Wang et al. (2017)	Q	80, 239
[926-61-4]	1.7×10^{4}		Wang et al. (2017)	Q	80, 240
OAKURXIZZOAYBC-UHFFFAOYSA-N	6.9×10^{1}		Saxena and Hildemann (1996)	E	401

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Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
2-hydroxypropanoic acid	1.2×10^{2}		Duchowicz et al. (2020)	V	186
$CH_3CHOHCOOH$	1.2×10^{2}		HSDB (2015)	V	
(lactic acid)	1.1×10^{3}		Duchowicz et al. (2020)	Q	
[50-21-5]	9.9×10^{2}		Raventos-Duran et al. (2010)	Q	242, 243
JVTAAEKCZFNVCJ-UHFFFAOYSA-N	9.9×10^{3}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	6.9×10^{5}		Saxena and Hildemann (1996)	E	401
glycidaldehyde	1.9×10^{1}		HSDB (2015)	Q	99
$C_3H_4O_2$					
[765-34-4]					
IWYRWIUNAVNFPE-UHFFFAOYSA-N					
trimethylene oxide	4.0×10^{-1}		Duchowicz et al. (2020)	V	186
C_3H_6O	3.9×10^{-1}		HSDB (2015)	V	
(1,3-epoxypropane; 1,3-propylene oxide; oxetane)	1.2×10^{-1}		Duchowicz et al. (2020)	Q	
[503-30-0]					
AHHWIHXENZJRFG-UHFFFAOYSA-N					
2,3-dihydroxypropanal	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_3$	2.6×10^{4}		Wang et al. (2017)	Q	80, 239
(glyceraldehyde)	8.1×10^{2}		Wang et al. (2017)	Q	80, 240
[367-47-5]	2.0×10^{8}		Saxena and Hildemann (1996)	E	401
MNQZXJOMYWMBOU-UHFFFAOYSA-N					
dihydroxyacetone	1.8×10^{6}		HSDB (2015)	V	
$C_3H_6O_3$	5.5×10^{3}		Wang et al. (2017)	Q	80, 238
[96-26-4]	3.8×10^{3}		Wang et al. (2017)	Q	80, 239
RXKJFZQQPQGTFL-UHFFFAOYSA-N	5.0×10^{3}		Wang et al. (2017)	Q	80, 240
2-methoxyethanol	4.4	7500	Hiatt (2013)	M	
$C_3H_8O_2$	2.2×10^{-4}	-730	Ashworth et al. (1988)	M	539, 42, 278
(methyl cellosolve)	1.4×10^{1}		Johanson and Dynésius (1988)	M	14
[109-86-4]	3.7×10^{1}	7300	Cabani et al. (1978)	T	
XNWFRZJHXBZDAG-UHFFFAOYSA-N	6.8		Keshavarz et al. (2022)	Q	
	1.4×10^{1}		Duchowicz et al. (2020)	Q	184
	8.9		Wang et al. (2017)	Q	80, 238
	5.4×10^{1}		Wang et al. (2017)	Q	80, 239
	1.3×10^{1}		Wang et al. (2017)	Q	80, 240
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{2}		Raventos-Duran et al. (2010)	Q	245
	2.1×10^{1}		Hilal et al. (2008)	Q	
	4.0×10^{1}		Modarresi et al. (2007)	Q	67
	1.5×10^{1}		Nirmalakhandan et al. (1997)	Q	
	3.0×10^{1}		Duchowicz et al. (2020)	?	185, 21

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Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-oxobutanoic acid	8.3×10^{3}		Wang et al. (2017)	Q	80, 238
$OHC(CH_2)_2COOH$	3.2×10^{5}		Wang et al. (2017)	Q	80, 239
[692-29-5]	2.1×10^{4}		Wang et al. (2017)	Q	80, 240
UIUJIQZEACWQSV-UHFFFAOYSA-N	4.9×10^{1}		Saxena and Hildemann (1996)	E	401
2,3-dihydroxybutanedioic acid	4.9×10^{15}		Burkholder et al. (2019)	L	
$HOOCCHOHCHOHCOOH$	4.9×10^{15}		Burkholder et al. (2015)	L	
(tartaric acid)			Compernolle and Müller (2014a)	V	540
[87-69-4]	1.3×10^{13}		Yaws (2003)	X	237, 12
FEWJPZIEWOKRBE-JCYAYHJZSA-N	5.1×10^{10}		Gharagheizi et al. (2012)	Q	
	1.3×10^{13}		Gharagheizi et al. (2010)	Q	246
	9.9×10^{15}		Saxena and Hildemann (1996)	E	401
3-oxapentane-1,5-diol	3.3×10^{4}		Yaws (2003)	X	258
$HO(CH_2)_2O(CH_2)_2OH$	3.3×10^{4}		Yaws (2003)	X	237
(diethylene glycol)	9.0×10^{3}		Dupeux et al. (2022)	Q	259
[111-46-6]	2.5×10^{3}		Olsen et al. (2016)	Q	425
MTHSVFCYNBDYFN-UHFFFAOYSA-N	1.6×10^{3}		Olsen et al. (2016)	Q	426
	1.7×10^{3}		Olsen et al. (2016)	Q	427
	4.9×10^{3}		HSDB (2015)	Q	99
	7.7×10^{3}		Gharagheizi et al. (2012)	Q	
	3.8×10^{4}		Gharagheizi et al. (2010)	Q	246
	2.4×10^{4}		Hilal et al. (2008)	Q	
	2.2×10^{4}		Yao et al. (2002)	Q	229
	2.0×10^{7}		Saxena and Hildemann (1996)	E	401
	3.3×10^{4}		Yaws (1999)	?	21
hydroxybutanedioic acid	2.7×10^{8}		Compernolle and Müller (2014a)	V	
$HOOCCH_2CHOHCOOH$	1.7×10^{9}		Yaws (2003)	X	237, 372
(malic acid)	1.2×10^{7}		HSDB (2015)	Q	99
[6915-15-7]	5.3×10^{8}		Gharagheizi et al. (2012)	Q	
BJEPYKJPYRNKOW-UHFFFAOYSA-N	1.4×10^{9}		Gharagheizi et al. (2010)	Q	246
	2.0×10^{11}		Saxena and Hildemann (1996)	E	401
2-ethoxyethanol	8.9		Johanson and Dynésius (1988)	M	14
$C_4H_{10}O_2$	3.3×10^{1}		Abraham et al. (1994a)	R	
[110-80-5]	2.8×10^{1}	8000	Cabani et al. (1978)	T	
ZNQVEEAIQZEUHB-UHFFFAOYSA-N	9.2		Keshavarz et al. (2022)	Q	
	5.8		Duchowicz et al. (2020)	Q	299
	7.4		Wang et al. (2017)	Q	80, 238
	3.4×10^{1}		Wang et al. (2017)	Q	80, 239
	9.8		Wang et al. (2017)	Q	80, 240
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{1}		Hilal et al. (2008)	Q	
	3.2×10^{1}		Modarresi et al. (2007)	Q	67
	7.5		Nirmalakhandan et al. (1997)	Q	
	2.1×10^{1}		Duchowicz et al. (2020)	?	185, 21

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Table A3.12: Miscellaneous (. . . continued)

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	1.9×10^{1}		Yaws (1999)	?	21, 12
2-methoxy-1-propanol $C_4H_{10}O_2$ [1589-47-5] YTTFFPATQICAQN-UHFFFAOYSA-N	5.5×10^{2}		HSDB (2015)	Q	99
1,1-dimethoxyethane $C_4H_{10}O_2$ [534-15-6] SPEUIVXLLWOEMJ-UHFFFAOYSA-N	1.5×10^{-1}		HSDB (2015)	Q	99
4-methylene-2-oxetanone $C_4H_4O_2$ (acetyl ketene) [674-82-8] WASQWSOJHCZDFK-UHFFFAOYSA-N	1.6×10^{-2}		HSDB (2015)	Q	99
2(5H)-furanone $C_4H_4O_2$ [497-23-4] VIHAEDVKXSOUAT-UHFFFAOYSA-N	3.5×10^{-1} 3.6×10^{2} 1.4×10^{3} 1.0		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) HSDB (2015)	Q Q Q Q	80, 238 80, 239 80, 240 99
2,2'-bioxirane $C_4H_6O_2$ [1464-53-5] ZFIVKAOQEXOYFY-UHFFFAOYSA-N	2.8×10^{2}		HSDB (2015)	Q	99
γ-butyrolactone $C_4H_6O_2$ [96-48-0] YEJRWHAVMIAJKC-UHFFFAOYSA-N	1.9×10^{2} 1.9×10^{2} 6.5×10^{1} 1.2		Duchowicz et al. (2020) HSDB (2015) Dupeux et al. (2022) Duchowicz et al. (2020)	V V Q Q	186 259
ethyloxirane C_4H_8O (1,2-epoxybutane) [106-88-7] RBACIKXCRWGCBB-UHFFFAOYSA-N	5.5×10^{-2} 5.5×10^{-2} 6.9×10^{-2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
2,3-epoxy-2-methyl-1,4-butanediol $C_5H_{10}O_3$ (IEPOX) FLVAIUDBQNOKHB-UHFFFAOYSA-N	5.0×10^{4} 1.3×10^{5} 3.2×10^{4} 2.7×10^{4} 1.3×10^{6} 1.9×10^{5} 3.0×10^{5}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) Pye et al. (2013) Chan et al. (2010) Eddingsaas et al. (2010) Vasilakos et al. (2021) Woo and McNeill (2015)	Q Q Q Q Q Q E ?	80, 238 80, 239 80, 240 492 541 542 543 466
MEDICO1CO $C_5H_8O_4$ RRXXDUUNVWXRFN-UHFFFAOYSA-N	2.5×10^{7}	12000	Wieser et al. (2023)	Q	437

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MEDICO4CO $C_5H_8O_4$ GXKSWJOBVXKANI-UHFFFAOYSA-N	3.1×10^{6}	12000	Wieser et al. (2023)	Q	437
METRICO $C_5H_{10}O_4$ LCGBCDAYKOJPSO-UHFFFAOYSA-N	7.3×10^{6}	12000	Wieser et al. (2023)	Q	437
2,3-epoxy-6-oxo-heptenal $C_7H_8O_3$ (MCM:TLEPOXMUC) YHZQHUOBDYTWMQ-UHFFFAOYSA-N	1.1×10^{4} 1.4×10^{4} 2.8×10^{3} 2.5×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) McNeill et al. (2012)	Q Q Q Q	80, 238 80, 239 80, 240
3-hydroxy-2-butanone $C_4H_8O_2$ (acetoin) [513-86-0] ROWKJAVDOGWPAT-UHFFFAOYSA-N	3.1 5.7×10^{-1} 7.8 1.1×10^{2} 1.2×10^{1} 9.9×10^{-1}		Wu et al. (2022b) Straver and de Loos (2005) Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) HSDB (2015)	M M Q Q Q Q	544 80, 238 80, 239 80, 240 99
2-(vinyloxy)ethanol $C_4H_8O_2$ (ethylene glycol monovinyl ether) [764-48-7] VUIWJRYTWUGOOF-UHFFFAOYSA-N	3.9×10^{1}		HSDB (2015)	Q	99
2-methyloxetane C_4H_8O [2167-39-7] FZIIBDOXPQOKBP-UHFFFAOYSA-N	1.2×10^{-1}		HSDB (2015)	Q	99
5-oxopentanoic acid $OHC(CH_2)_3COOH$ [5746-02-1] VBKPPDYGFUZOAJ-UHFFFAOYSA-N	3.9×10^{1}		Saxena and Hildemann (1996)	E	401
2-oxopentanedioic acid $HOOC(CH_2)_2COCOOH$ (α-keto glutaric acid) [328-50-7] KPGXRSRHYNQIFN-UHFFFAOYSA-N	9.9×10^{6}		Saxena and Hildemann (1996)	E	401
tetrahydro-2-furanmethanol $C_5H_{10}O_2$ (tetrahydrofurfuryl alcohol) [97-99-4] BSYVTEYKTMYBMK-UHFFFAOYSA-N	4.4×10^{1} 1.7×10^{2} 2.4×10^{3}		Yaws (2003) Dupeux et al. (2022) HSDB (2015)	X Q Q	258 259 99

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xylose $C_5H_{10}O_5$ [58-86-6] PYMYPHUHKUWMLA-VPENINKCSA-N	8.2×10^3		HSDB (2015)	Q	99
2-(2-methoxyethoxy)ethanol $C_5H_{12}O_3$ (diethylene glycol monomethyl ether) [111-77-3] SBASXUCJHJRPEV-UHFFFAOYSA-N	6.2×10^5		HSDB (2015)	Q	99
3,6-dioxaoctane-1,8-diol $HO(CH_2CH_2O)_3H$ (triethylene glycol) [112-27-6] ZIBGPFATKBEMQZ-UHFFFAOYSA-N	1.1×10^4 5.9×10^3 6.7×10^3 3.1×10^5 8.9×10^9		Olsen et al. (2016) Olsen et al. (2016) Olsen et al. (2016) HSDB (2015) Saxena and Hildemann (1996)	Q Q Q Q E	425 426 427 99 401
2-oxepanone $C_6H_{10}O_2$ (caprolactone) [502-44-3] PAPBSGBWRJIAAV-UHFFFAOYSA-N	5.5×10^{-2}		HSDB (2015)	Q	99
glycidyl ether $C_6H_{10}O_3$ (diglycidyl ether) [2238-07-5] GYZLOYUZLJXAJU-UHFFFAOYSA-N	7.6×10^2		HSDB (2015)	Q	99
4-hydroxy-4-methyl-2-pentanone $C_6H_{12}O_2$ (diacetone alcohol) [123-42-2] SWXVUIWOUIDPGS-UHFFFAOYSA-N	3.8×10^1 1.3×10^1 3.1×10^2 7.4×10^{-2} 7.6×10^1 8.0×10^2 6.8×10^1 2.3×10^3		Duchowicz et al. (2020) Yaws (2003) Dupeux et al. (2022) Duchowicz et al. (2020) Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) HSDB (2015)	V X Q Q Q Q Q Q	186 258 259 80, 238 80, 239 80, 240 545
1-propoxy-2-propanol $C_6H_{14}O_2$ [1569-01-3] FENFUOGYJVOCRY-UHFFFAOYSA-N	2.9×10^2		HSDB (2015)	Q	545
2-(2-ethoxyethoxy)ethanol $C_6H_{14}O_3$ (diethylene glycol monoethyl ether) [111-90-0] XXJWXESWEXIICW-UHFFFAOYSA-N	4.4×10^2 4.5×10^2 9.0×10^2 6.4×10^1		Duchowicz et al. (2020) HSDB (2015) Dupeux et al. (2022) Duchowicz et al. (2020)	V V Q Q	186 259

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2,5,8-trioxanonane $C_6H_{14}O_3$ (diglyme) [111-96-6] SBZXBUIDTXKZTM-UHFFFAOYSA-N	1.9×10^{1} 1.9×10^{1} 6.2		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
oxydipropanol $C_6H_{14}O_3$ (dipropylene glycol) [25265-71-8] SZXQTJUDPRGNJN-UHFFFAOYSA-N	1.8×10^{3}		HSDB (2015)	V	
p-benzoquinone $C_6H_4O_2$ (1,4-benzoquinone) [106-51-4] AZQWKYJCGOJGHM-UHFFFAOYSA-N	2.1×10^{-2} 5.1 1.7×10^{4} 2.3×10^{1} 2.1×10^{-2} 7.7		HSDB (2015) Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) Yaffe et al. (2003) Katritzky et al. (1998)	V Q Q Q Q Q	 80, 238 80, 239 80, 240 248, 249
5-hydroxymethylfurfural $C_6H_6O_3$ (5-hydroxymethyl-2-furfuraldehyde) [67-47-0] NOEGNKMFWQHSLB-UHFFFAOYSA-N	1.8×10^{4}		HSDB (2015)	Q	99
5-hydroxy-2-(hydroxymethyl)-4H-pyran-4-one $C_6H_6O_4$ (kojic acid) [501-30-4] BEJNERDRQOWKJM-UHFFFAOYSA-N	4.1×10^{1}		HSDB (2015)	Q	99
2-hydroxy-1,2,3-propanetricarboxylic acid $C_6H_8O_7$ (citric acid) [77-92-9] KRKNYBCHXYNGOX-UHFFFAOYSA-N	3.1×10^{15} 3.1×10^{15} 7.6×10^{12} 4.8×10^{11} 7.9×10^{12} 3.0×10^{16}		Burkholder et al. (2019) Burkholder et al. (2015) Compernolle and Müller (2014a) Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Saxena and Hildemann (1996)	L L V X Q Q E	 546 237, 12 246 401
(butoxymethyl)oxirane $C_7H_{14}O_2$ (n-butyl glycidyl ether) [2426-08-6] YSUQLAYJZDEMOT-UHFFFAOYSA-N	4.0×10^{-1} 3.9×10^{-1} 8.9×10^{-1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186

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1-(1,1-dimethylethoxy)-2-propanol $C_7H_{16}O_2$ (propylene glycol mono-t-butyl ether) [57018-52-7] GQCZPFJGIXHZMB-UHFFFAOYSA-N	2.1		HSDB (2015)	V	
2-[2-(2-methoxyethoxy)ethoxy]ethanol $C_7H_{16}O_4$ (triethylene glycol monomethyl ether) [112-35-6] JLGLQAWTXXGVEM-UHFFFAOYSA-N	2.8×10^{8}		HSDB (2015)	Q	99
2-methyl-*p*-benzoquinone $C_7H_6O_2$ [553-97-9] VTWDKFNVVLAELH-UHFFFAOYSA-N	3.1 6.9×10^{3} 2.1×10^{1} 5.2×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) HSDB (2015)	Q Q Q Q	80, 238 80, 239 80, 240 99
patulin $C_7H_6O_4$ [149-29-1] ZRWPUFFVAOMMNM-UHFFFAOYSA-N	9.0×10^{4}		HSDB (2015)	Q	99
1-hydroxy-3-methoxybenzene $C_7H_8O_2$ (3-methoxyphenol) [150-19-6] ASHGTJPOSUFTGB-UHFFFAOYSA-N	1.7×10^{2} 1.7×10^{2} 4.7×10^{2} 2.0×10^{2} 2.5×10^{2} 3.1×10^{2} 1.3×10^{2} 6.4×10^{1} 5.0×10^{2} 1.7×10^{2}		Abraham et al. (1994a) Keshavarz et al. (2022) Duchowicz et al. (2020) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Nirmalakhandan et al. (1997) Duchowicz et al. (2020)	R Q Q Q Q Q Q Q Q ?	 299 242, 243 244 245 67 185, 21
mequinol $C_7H_8O_2$ (4-methoxyphenol) [150-76-5] NWVVVBRKAWDGAB-UHFFFAOYSA-N	6.9×10^{-1} 1.9×10^{1} 6.9×10^{-1} 2.0		Yaws (2003) HSDB (2015) Gharagheizi et al. (2010) Yaws (1999)	X Q Q ?	237, 14 99 246 21, 14
1-hydroxy-2-methoxybenzene $C_7H_8O_2$ (guaiacol; 2-methoxyphenol) [90-05-1] LHGVFZTZFXWLCP-UHFFFAOYSA-N	8.6 9.0 7.7 9.1 9.6 7.7 4.1×10^{1} 5.0	 7900 7600 	McFall et al. (2020) Wieland et al. (2015) Sagebiel et al. (1992) Sagebiel et al. (1992) Mackay et al. (2006c) Sagebiel et al. (1992) Leuenberger et al. (1985) Abraham et al. (1994a)	M M M M V V V R	 547 416

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	1.1×10^{1}		Keshavarz et al. (2022)	Q	
	5.6×10^{-1}		Abney (2021)	Q	399
	8.7		Duchowicz et al. (2020)	Q	299
	8.2		McFall et al. (2020)	Q	474
	5.2		Hilal et al. (2008)	Q	
	7.7		Modarresi et al. (2007)	Q	67
		6700	Kühne et al. (2005)	Q	
	1.2×10^{1}		English and Carroll (2001)	Q	230, 274
	6.4×10^{1}		Katritzky et al. (1998)	Q	
	5.1×10^{2}		Nirmalakhandan et al. (1997)	Q	
	8.2		Duchowicz et al. (2020)	?	185, 21
		7800	Kühne et al. (2005)	?	
	3.3×10^{-1}		Yaws (1999)	?	21, 14
1,4-dimethoxybenzene $C_8H_{10}O_2$ (hydroquinone dimethyl ether) [150-78-7] OHBQPCCCRFSCAX-UHFFFAOYSA-N	2.8×10^{-3}		HSDB (2015)	Q	99
4-methyl-2-methoxyphenol $C_8H_{10}O_2$ [93-51-6] PETRWTHZSKVLRE-UHFFFAOYSA-N	7.7		Sagebiel et al. (1992)	M	
	7.1	7400	Sagebiel et al. (1992)	M	
	1.0×10^{1}		Sagebiel et al. (1992)	V	
	1.6×10^{1}		Keshavarz et al. (2022)	Q	
	5.2		Duchowicz et al. (2020)	Q	
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	271, 243
	3.1		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{2}		Raventos-Duran et al. (2010)	Q	245
	5.2		Hilal et al. (2008)	Q	
	2.5		Modarresi et al. (2007)	Q	67
		7100	Kühne et al. (2005)	Q	
	7.3		Yaffe et al. (2003)	Q	248, 249
	6.2×10^{1}		Katritzky et al. (1998)	Q	
	7.4		Duchowicz et al. (2020)	?	185, 21
		7900	Kühne et al. (2005)	?	
tyrosol $C_8H_{10}O_2$ (4-hydroxybenzeneethanol) [501-94-0] YCCILVSKPBXVIP-UHFFFAOYSA-N	3.5×10^{5}		McFall et al. (2020)	Q	474
1,3-dimethoxy-2-hydroxybenzene $C_8H_{10}O_3$ (2,6-dimethoxyphenol) [91-10-1] KLIDCXVFHGNTTM-UHFFFAOYSA-N	3.7×10^{1}		Sagebiel et al. (1992)	M	
	5.0×10^{1}	6700	Sagebiel et al. (1992)	M	
	1.2×10^{2}		Sagebiel et al. (1992)	V	
	1.6×10^{1}		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	
	7.8×10^{2}		Raventos-Duran et al. (2010)	Q	271, 243
	4.9×10^{2}		Raventos-Duran et al. (2010)	Q	244

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	4.9×10^{3}		Raventos-Duran et al. (2010)	Q	245
	3.5×10^{2}		Hilal et al. (2008)	Q	
	1.1×10^{2}		Modarresi et al. (2007)	Q	67
		7300	Kühne et al. (2005)	Q	
	4.3×10^{1}		Duchowicz et al. (2020)	?	185, 21
		7600	Kühne et al. (2005)	?	
hexahydro-1,3-isobenzofurandione $C_8H_{10}O_3$ (hexahydrophthalic anhydride) [85-42-7] MUTGBJKUEZFXGO-UHFFFAOYSA-N	4.7×10^{-1}		HSDB (2015)	Q	99
vanillyl alcohol $C_8H_{10}O_3$ [498-00-0] ZENOXNGFMSCLLL-UHFFFAOYSA-N	9.6×10^{4} 2.0×10^{5}		McFall et al. (2020) McFall et al. (2020)	M Q	 474
1-methoxy-4-methylbenzene $C_8H_{10}O$ [104-93-8] CHLICZRVGGXEOD-UHFFFAOYSA-N	2.1×10^{-3}		HSDB (2015)	Q	99
dimethoxane $C_8H_{14}O_4$ [828-00-2] PHMNXPYGVPEQSJ-UHFFFAOYSA-N	8.0×10^{1}		HSDB (2015)	Q	99
RO5R5 $C_8H_{14}O_4$ MESHXYGXEHAFFE-UHFFFAOYSA-N	1.3×10^{5}	17000	Wieser et al. (2023)	Q	437
5-hydroxy-2-octanone $C_8H_{16}O_2$ (C82CO5OH) KZPPEBIAPHLFQD-UHFFFAOYSA-N	1.6×10^{3}	11000	Wieser et al. (2023)	Q	437
metaldehyde $C_8H_{16}O_4$ [108-62-3] GKKDCARASOJPNG-UHFFFAOYSA-N	1.9×10^{-1} 2.9×10^{-1}		HSDB (2015) Maniere et al. (2011)	V ?	 12, 165
diethyl carbitol $C_8H_{18}O_3$ (diethylene glycol diethyl ether) [112-36-7] RRQYJINTUHWNHW-UHFFFAOYSA-N	8.9×10^{1} 9.0×10^{1} 9.6×10^{-1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186

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2-[2-(2-ethoxyethoxy)ethoxy]ethanol $C_8H_{18}O_4$ (triethylene glycol monoethyl ether) [112-50-5] WFSMVVDJSNMRAR-UHFFFAOYSA-N	2.1×10^{8}		HSDB (2015)	Q	99
tetraethylene glycol $C_8H_{18}O_5$ [112-60-7] UWHCKJMYHZGTIT-UHFFFAOYSA-N	1.8×10^{13}		HSDB (2015)	Q	99
vanillin $C_8H_8O_3$ [121-33-5] MWOOGOJBHIARFG-UHFFFAOYSA-N	1.7×10^{3}	6800	Brockbank (2013)	L	1
	4.6×10^{3}		Duchowicz et al. (2020)	V	186
	4.7×10^{3}		HSDB (2015)	V	
	1.3×10^{3}		Yaws (2003)	X	258
	1.3×10^{3}		Yaws (2003)	X	237
	1.8×10^{3}		Dupeux et al. (2022)	Q	259
	1.8×10^{3}		Dupeux et al. (2022)	Q	259
	1.8×10^{3}		Abney (2021)	Q	399
	4.0×10^{3}		Duchowicz et al. (2020)	Q	
	2.8×10^{2}		Gharagheizi et al. (2012)	Q	
	4.9×10^{3}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{2}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{5}		Raventos-Duran et al. (2010)	Q	245
	1.3×10^{3}		Gharagheizi et al. (2010)	Q	246
ethylparaben $C_9H_{10}O_3$ [120-47-8] NUVBSKCKDOMJSU-UHFFFAOYSA-N	2.1×10^{3}		HSDB (2015)	Q	99
ethyl vanillin $C_9H_{10}O_3$ [121-32-4] CBOQJANXLMLOSS-UHFFFAOYSA-N	1.2×10^{4}		HSDB (2015)	V	
1-phenoxypropan-2-ol $C_9H_{12}O_2$ (propylene glycol phenyl ether) [770-35-4] IBLKWZIFZMJLFL-UHFFFAOYSA-N	3.4×10^{2}		HSDB (2015)	V	
triacetin $C_9H_{14}O_6$ [102-76-1] URAYPUMNDPQOKB-UHFFFAOYSA-N	8.0×10^{2}		Duchowicz et al. (2020)	V	186
	8.2×10^{2}		HSDB (2015)	V	
	2.7×10^{2}		Duchowicz et al. (2020)	Q	
	2.0×10^{3}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{2}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{3}		Raventos-Duran et al. (2010)	Q	245

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Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tripropylene glycol $C_9H_{20}O_4$ [24800-44-0] LCZVSXRMYJUNFX-UHFFFAOYSA-N	3.0×10^{9}		HSDB (2015)	Q	99
coumarin $C_9H_6O_2$ [91-64-5] ZYGHJZDHTFUPRJ-UHFFFAOYSA-N	9.9×10^{1} 1.0×10^{2} 1.3×10^{2} 5.1		Duchowicz et al. (2020) HSDB (2015) Dupeux et al. (2022) Duchowicz et al. (2020)	V V Q Q	186 259
4-ethylguaiacol $C_9H_{12}O_2$ (4-ethyl-2-methoxyphenol) [2785-89-9] CHWNEIVBYREQRF-UHFFFAOYSA-N	5.5		McFall et al. (2020)	Q	474
4-methylsyringol $C_9H_{12}O_3$ [6638-05-7] ZFBNNSOJNZBLLS-UHFFFAOYSA-N	3.8×10^{1}		McFall et al. (2020)	Q	474
acetovanillone $C_9H_{10}O_3$ (apocynin) [498-02-2] DFYRUELUNQRZTB-UHFFFAOYSA-N	6.3×10^{3}		McFall et al. (2020)	Q	474
syringaldehyde $C_9H_{10}O_4$ [134-96-3] KCDXJAYRVLXPFO-UHFFFAOYSA-N	3.7×10^{5}		McFall et al. (2020)	Q	474
5-(1-propenyl)-1,3-benzodioxole $C_{10}H_{10}O_2$ (isosafrole) [120-58-1] VHVOLFRBFDOUSH-UHFFFAOYSA-N	2.7×10^{-4}		HSDB (2015)	Q	99
safrole $C_{10}H_{10}O_2$ [94-59-7] ZMQAAUBTXCXRIC-UHFFFAOYSA-N	1.1		HSDB (2015)	Q	99
5-propyl-1,3-benzodioxole $C_{10}H_{12}O_2$ (dihydrosafrole) [94-58-6] MYEIDJPOUKASEC-UHFFFAOYSA-N	8.2×10^{-1}		HSDB (2015)	Q	99

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Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methoxy-4-(1-propenyl)phenol $C_{10}H_{12}O_2$ (isoeugenol) [97-54-1] BJIOGJUNALELMI-UHFFFAOYSA-N	2.7 1.7×10^{1}		HSDB (2015) McFall et al. (2020)	V Q	 474
p-cresyl glycidyl ether $C_{10}H_{12}O_2$ [26447-14-3] CUFXMPWHOWYNSO-UHFFFAOYSA-N	1.3×10^{1}		HSDB (2015)	Q	99
4-(4-hydroxyphenyl)-2-butanone $C_{10}H_{12}O_2$ (raspberry ketone) [5471-51-2] NJGBTKGETPDVIK-UHFFFAOYSA-N	1.8×10^{4}		HSDB (2015)	Q	447
guaifenesin $C_{10}H_{14}O_4$ [93-14-1] HSRJKNPTNIJEKV-UHFFFAOYSA-N	2.2×10^{5}		HSDB (2015)	Q	99
RO5R4O2H $C_{10}H_{18}O_7$ YORZXZYHORHTRW-UHFFFAOYSA-N	3.6×10^{10}	24000	Wieser et al. (2023)	Q	437
levomenthol $C_{10}H_{20}O$ (*L*-menthol) [2216-51-5] NOOLISFMXDJSKH-AEJSXWLSSA-N	6.6×10^{-1}		HSDB (2015)	Q	99
diethylene glycol hexyl ether $C_{10}H_{22}O_3$ [112-59-4] GZMAAYIALGURDQ-UHFFFAOYSA-N	5.7×10^{2} 5.8×10^{2} 1.0×10^{2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
2-[2-(2-butoxyethoxy)ethoxy]ethanol $C_{10}H_{22}O_4$ (triethylene glycol monobutyl ether) [143-22-6] COBPKKZHLDDMTB-UHFFFAOYSA-N	1.0×10^{8}		HSDB (2015)	Q	99
4-propylguaiacol $C_{10}H_{14}O_2$ (2-methoxy-4-propylphenol) [2785-87-7] PXIKRTCSSLJURC-UHFFFAOYSA-N	4.3 4.2		McFall et al. (2020) McFall et al. (2020)	M Q	 474

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Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
vanillyl ethyl ether $C_{10}H_{14}O_3$ (4-(ethoxymethyl)-2-methoxyphenol) [13184-86-6] KOCVACNWDMSLBM-UHFFFAOYSA-N	4.1×10^{2} 4.8×10^{2}		McFall et al. (2020) McFall et al. (2020)	M Q	 474
4-ethylsyringol $C_{10}H_{14}O_3$ [14059-92-8] PJWDIHUFLXQRFF-UHFFFAOYSA-N	3.0×10^{1}		McFall et al. (2020)	Q	474
guaiacylacetone $C_{10}H_{12}O_3$ (1-(4-hydroxy-3-methoxyphenyl)-2-propanone) [2503-46-0] LFVCJQWZGDLHSD-UHFFFAOYSA-N	1.2×10^{4} 1.1×10^{4}		McFall et al. (2020) McFall et al. (2020)	M Q	 474
acetosyringone $C_{10}H_{12}O_4$ [2478-38-8] OJOBTAOGJIWAGB-UHFFFAOYSA-N	5.0×10^{5}		McFall et al. (2020)	Q	474
coniferylaldehyde $C_{10}H_{10}O_3$ [458-36-6] UCZOBXQKIUMJDZ-UHFFFAOYSA-N	4.4×10^{4}		McFall et al. (2020)	Q	474
4-methoxy-6-(2-propenyl)-1,3-benzodioxole $C_{11}H_{12}O_3$ (myristicin) [607-91-0] BNWJOHGLIBDBOB-UHFFFAOYSA-N	1.8×10^{1}		HSDB (2015)	Q	99
butylparaben $C_{11}H_{14}O_3$ [94-26-8] QFOHBWFCKVYLES-UHFFFAOYSA-N	1.2×10^{3}		HSDB (2015)	Q	99
2-*tert*-butyl-4-methoxyphenol $C_{11}H_{16}O_2$ (butylated hydroxyanisole) [25013-16-5] MRBKEAMVRSLQPH-UHFFFAOYSA-N	8.4		HSDB (2015)	Q	99

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Table A3.12: Miscellaneous (. . . continued)

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3-hydroxy-2-naphthalenecarboxylic acid	7.0×10^3		HSDB (2015)	Q	99
$C_{11}H_8O_3$	7.2×10^3		Zhang et al. (2010)	Q	287, 288
[92-70-6]	1.2×10^4		Zhang et al. (2010)	Q	287, 289
ALKYHXVLJMQRLQ-UHFFFAOYSA-N	3.8×10^5		Zhang et al. (2010)	Q	287, 290
	8.2×10^3		Zhang et al. (2010)	Q	287, 291
4-propylsyringol	2.2×10^1		McFall et al. (2020)	Q	474
$C_{11}H_{16}O_3$					
[6766-82-1]					
YHEWWEXPVKCVFY-UHFFFAOYSA-N					
zingerone	1.2×10^4		McFall et al. (2020)	M	
$C_{11}H_{14}O_3$	8.4×10^3		McFall et al. (2020)	Q	474
(vanillylacetone)					
[122-48-5]					
OJYLAHXKWMRDGS-UHFFFAOYSA-N					
allylsyringol	6.3×10^2		McFall et al. (2020)	Q	474
$C_{11}H_{14}O_3$					
[5438-54-0]					
IYIVYBWBUQPWAU-UHFFFAOYSA-N					
4-propenylsyringol	1.1×10^3		McFall et al. (2020)	Q	474
$C_{11}H_{14}O_3$					
[6635-22-9]					
YFHOHYAUMDHSBX-UHFFFAOYSA-N					
propionylsyringol	3.8×10^5		McFall et al. (2020)	Q	474
$C_{11}H_{14}O_4$					
[5650-43-1]					
CXCPJZXJNRBTGF-UHFFFAOYSA-N					
sinapylaldehyde	3.1×10^6		McFall et al. (2020)	Q	474
$C_{11}H_{12}O_4$					
[4206-58-0]					
CDICDSOGTRCHMG-ONEGZZNKSA-N					
arbutin	8.2×10^{13}		HSDB (2015)	Q	99
$C_{12}H_{16}O_7$					
[497-76-7]					
BJRNKVDFDLYUGJ-RMPHRYRLSA-N					
butopyronoxyl	2.1×10^2		HSDB (2015)	Q	99
$C_{12}H_{18}O_4$					
(indalone)					
[532-34-3]					
OKIJSNGRQAOIGZ-UHFFFAOYSA-N					

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diethylene glycol bis(methacrylate) $C_{12}H_{18}O_5$ [2358-84-1] XFCMNSHQOZQILR-UHFFFAOYSA-N	1.2×10^{4}		HSDB (2015)	Q	99
dikegulac $C_{12}H_{18}O_7$ [18467-77-1] FWCBATIDXGJRMF-FLNNQWSLSA-N	5.2×10^{10}		HSDB (2015)	Q	99
propofol $C_{12}H_{18}O$ [2078-54-8] OLBCVFGFOZPWHH-UHFFFAOYSA-N	4.7		HSDB (2015)	Q	99
lactitol $C_{12}H_{24}O_{11}$ [585-86-4] VQHSOMBJVWLPSR-JVCRWLNRSA-N	1.2×10^{16}		HSDB (2015)	Q	99
maltitol $C_{12}H_{24}O_{11}$ [585-88-6] VQHSOMBJVWLPSR-WUJBLJFYSA-N	2.3×10^{15}		HSDB (2015)	Q	99
naphthalic anhydride $C_{12}H_6O_3$ [81-84-5] GRSMWKLPSNHDHA-UHFFFAOYSA-N	1.6×10^{1}		HSDB (2015)	Q	99
methoxsalen $C_{12}H_8O_4$ (8-methoxypsoralen) [298-81-7] QXKHYNVANLEOEG-UHFFFAOYSA-N	2.5×10^{2}		HSDB (2015)	Q	99
syringylacetone $C_{12}H_{16}O_4$ [112468-41-4] NULBEPOZYDYWOV-UHFFFAOYSA-N	1.2×10^{6} 5.7×10^{4}		McFall et al. (2020) McFall et al. (2020)	M Q	 474
butyrylsyringol $C_{12}H_{16}O_4$ [69271-91-6] QFHXMVPZYYMTCS-UHFFFAOYSA-N	2.9×10^{5}		McFall et al. (2020)	Q	474
bisphenol F $C_{13}H_{12}O_2$ [620-92-8] PXKLMJQFEQBVLD-UHFFFAOYSA-N	1.9×10^{6}		HSDB (2015)	Q	447

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ibuprofen	6.6×10^{1}		HSDB (2015)	V	
$C_{13}H_{18}O_2$	2.0×10^{2}		Abraham et al. (2019)	Q	
[15687-27-1]					
HEFNNWSXXWATRW-UHFFFAOYSA-N					
trinexapac-ethyl	5.1		Duchowicz et al. (2020)	V	186
$C_{13}H_{16}O_5$	7.6×10^{5}		Duchowicz et al. (2020)	Q	
[95266-40-3]	1.9×10^{3}		Maniere et al. (2011)	?	165
RVKCCVTVZORVGD-QXMHVHEDSA-N					
benzoyl peroxide	2.8		HSDB (2015)	Q	99
$C_{14}H_{10}O_4$	2.8		Zhang et al. (2010)	Q	287, 288
[94-36-0]	1.1×10^{2}		Zhang et al. (2010)	Q	287, 289
OMPJBNCRMGITSC-UHFFFAOYSA-N	4.1×10^{2}		Zhang et al. (2010)	Q	287, 290
	4.3×10^{3}		Zhang et al. (2010)	Q	287, 291
oxybenzone	6.6×10^{2}		HSDB (2015)	Q	99
$C_{14}H_{12}O_3$					
(2-hydroxy-4-methoxybenzophenone)					
[131-57-7]					
DXGLGDHPHMLXJC-UHFFFAOYSA-N					
resveratrol	7.0×10^{10}		HSDB (2015)	Q	447
$C_{14}H_{12}O_3$					
[501-36-0]					
LUKBXSAWLPMMSZ-OWOJBTEDSA-N					
pindone	1.1×10^{6}		HSDB (2015)	Q	99
$C_{14}H_{14}O_3$					
[83-26-1]					
RZKYEQDPDZUERB-UHFFFAOYSA-N					
1,1'-[oxybis(methylene)]bisbenzene	1.5		Duchowicz et al. (2020)	V	186
$C_{14}H_{14}O$	3.7×10^{-1}		Dupeux et al. (2022)	Q	259
(dibenzyl ether)	3.1×10^{-1}		Duchowicz et al. (2020)	Q	
[103-50-4]	1.2×10^{2}		HSDB (2015)	Q	99
MHDVGSVTJDSBDK-UHFFFAOYSA-N	3.6		Modarresi et al. (2007)	Q	67
butanoic acid, 3,3-bis((1,1-dimethylethyl)dioxy)-, ethyl ester	5.0		Zhang et al. (2010)	Q	287, 288
$C_{14}H_{28}O_6$	7.0×10^{-3}		Zhang et al. (2010)	Q	287, 289
[55794-20-2]	1.3×10^{2}		Zhang et al. (2010)	Q	287, 290
HARQWLDROVMFJE-UHFFFAOYSA-N	2.4×10^{2}		Zhang et al. (2010)	Q	287, 291

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1-hydroxy-9,10-anthracenedione $C_{14}H_8O_3$ (1-hydroxyanthraquinone) [129-43-1] BTLXPCBPYBNQNR-UHFFFAOYSA-N	1.4×10^3 1.4×10^3 3.5×10^3		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
danthron $C_{14}H_8O_4$ (1,8-dihydroxyanthraquinone) [117-10-2] QBPFLULOKWLNNW-UHFFFAOYSA-N	1.8×10^5		HSDB (2015)	Q	99
bisphenol A $C_{15}H_{16}O_2$ [80-05-7] IISBACLAFKSPIT-UHFFFAOYSA-N	2.5×10^5		HSDB (2015)	V	
atractylenolide III $C_{15}H_{20}O_3$ [73030-71-4] FBMORZZOJSDNRQ-GLQYFDAESA-N	1.0×10^3		HSDB (2015)	Q	99
deoxynivalenol $C_{15}H_{20}O_6$ [51481-10-8] LINOMUASTDIRTM-WHNKEALZSA-N	4.9×10^8		HSDB (2015)	Q	447
nivalenol $C_{15}H_{20}O_7$ [23282-20-4] UKOTXHQERFPCBU-UHFFFAOYSA-N	1.4×10^{10}		HSDB (2015)	Q	99
tributyrin $C_{15}H_{26}O_6$ [60-01-5] UYXTWWCETRIEDR-UHFFFAOYSA-N	1.0×10^3		HSDB (2015)	Q	99
diosmetin $C_{16}H_{12}O_6$ [520-34-3] MBNGWHIJMBWFHU-UHFFFAOYSA-N	3.3×10^{12}		HSDB (2015)	Q	447
shikonin $C_{16}H_{16}O_5$ [517-89-5] NEZONWMXZKDMKF-SNVBAGLBSA-N	1.2×10^9		HSDB (2015)	Q	447

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2,2-bis(4-hydroxyphenyl)butane $C_{16}H_{18}O_2$ (bisphenol B) [77-40-7] HTVITOHKHWFJKO-UHFFFAOYSA-N	8.2×10^{5}		HSDB (2015)	Q	447
ethyl 3,3-bis(*tert*-amylperoxy)butyrate	2.9		Zhang et al. (2010)	Q	287, 288
$C_{16}H_{32}O_6$	3.7×10^{-3}		Zhang et al. (2010)	Q	287, 289
[67567-23-1]	3.0×10^{1}		Zhang et al. (2010)	Q	287, 290
NICWAKGKDIAMOD-UHFFFAOYSA-N	1.5×10^{2}		Zhang et al. (2010)	Q	287, 291
aflatoxin B1 $C_{17}H_{12}O_6$ [1162-65-8] OQIQSTLJSLGHID-UHFFFAOYSA-N	7.0×10^{7}		HSDB (2015)	Q	99
aflatoxin G1 $C_{17}H_{12}O_7$ [1165-39-5] XWIYFDMXXLINPU-UHFFFAOYSA-N	2.0×10^{7}		HSDB (2015)	Q	99
aflatoxin B2 $C_{17}H_{14}O_6$ [7220-81-7] WWSYXEZEXMQWHT-UHFFFAOYSA-N	3.3×10^{9}		HSDB (2015)	Q	99
aflatoxin G2 $C_{17}H_{14}O_7$ [7241-98-7] WPCVRWVBBXIRMA-UHFFFAOYSA-N	9.0×10^{8}		HSDB (2015)	Q	99
bisphenol C $C_{17}H_{20}O_2$ [79-97-0] YMTYZTXUZLQUSF-UHFFFAOYSA-N	9.0×10^{5}		HSDB (2015)	Q	447
PR-toxin $C_{17}H_{20}O_6$ [56299-00-4] GSPFUBNBRPVALJ-VIEAGMIOSA-N	1.6×10^{8}		HSDB (2015)	Q	99
fusarenon X $C_{17}H_{22}O_8$ [23255-69-8] XGCUCFKWVIWWNW-UHFFFAOYSA-N	2.1×10^{11}		HSDB (2015)	Q	99
dihydrotanshinone I $C_{18}H_{14}O_3$ [87205-99-0] HARGZZNYNSYSGJ-JTQLQIEISA-N	7.6×10^{4}		HSDB (2015)	Q	99

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diethylstilbestrol $C_{18}H_{20}O_2$ [56-53-1] RGLYKWWBQGJZGM-ISLYRVAYSA-N	1.7×10^{2}		HSDB (2015)	Q	99
laminarin $C_{18}H_{32}O_{16}$ [9008-22-4] DBTMGCOVALSLOR-AWHOAIGYSA-N	$>2.9\times10^{6}$		Maniere et al. (2011)	?	72, 165
estrone $C_{18}H_{22}O_2$ [53-16-7] DNXHEGUUPJUMQT-UHFFFAOYSA-N	2.6×10^{4}		HSDB (2015)	Q	99
estradiol $C_{18}H_{24}O_2$ [50-28-2] VOXZDWNPVJITMN-AWDGRILASA-N	2.7×10^{5}		HSDB (2015)	Q	99
estriol $C_{18}H_{24}O_3$ [50-27-1] PROQIPRRNZUXQM-PVGHXWSTSA-N	7.6×10^{6}		HSDB (2015)	Q	99
nandrolone $C_{18}H_{26}O_2$ [434-22-0] NPAGDVCDWIYMMC-SVXFNXITSA-N	3.7×10^{3}		HSDB (2015)	Q	99
diofenolan $C_{18}H_{20}O_4$ [63837-33-2] ZDOOQPFIGYHZFV-UHFFFAOYSA-N	1.5×10^{2} 1.2×10^{3} 1.5×10^{2}		Duchowicz et al. (2020) Duchowicz et al. (2020) MacBean (2012a)	V Q ?	186
dicumarol $C_{19}H_{12}O_6$ [66-76-2] DOBMPNYZJYQDGZ-UHFFFAOYSA-N	7.0×10^{7}		HSDB (2015)	Q	99
coumatetralyl $C_{19}H_{16}O_3$ [5836-29-3] ULSLJYXHZDTLQK-UHFFFAOYSA-N	1.7×10^{8}		HSDB (2015)	V	
warfarin $C_{19}H_{16}O_4$ [81-81-2] PJVWKTKQMONHTI-UHFFFAOYSA-N	3.7×10^{4} 3.6×10^{2}		HSDB (2015) Mackay et al. (2006d)	V V	

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Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tanshinone II $C_{19}H_{18}O_3$ [568-72-9] HYXITZLLTYIPOF-UHFFFAOYSA-N	2.0×10^{3}		HSDB (2015)	Q	99
gibberellic acid $C_{19}H_{22}O_6$ [77-06-5] IXORZMNAPKEEDV-UHFFFAOYSA-N	6.2×10^{9} 1.3×10^{6}		HSDB (2015) Maniere et al. (2011)	Q ?	99 165
prallethrin $C_{19}H_{24}O_3$ [23031-36-9] SMKRKQBMYOFFMU-UHFFFAOYSA-N	6.2		HSDB (2015)	V	
testolactone $C_{19}H_{24}O_3$ [968-93-4] BPEWUONYVDABNZ-LHXSAFEUSA-N	1.6×10^{2}		HSDB (2015)	Q	99
androstenedione $C_{19}H_{26}O_2$ [63-05-8] AEMFNILZOJDQLW-JRCHKSGSSA-N	2.7×10^{2}		HSDB (2015)	Q	99
diacetoxyscirpenol $C_{19}H_{26}O_7$ [2270-40-8] AUGQEEXBDZWUJY-UHFFFAOYSA-N	1.0×10^{11}		HSDB (2015)	Q	447
testosterone $C_{19}H_{28}O_2$ [58-22-0] MUMGGOZAMZWBJJ-JZJKZLICSA-N	2.8×10^{3}		HSDB (2015)	Q	99
5α-androst-16-en-4-one $C_{19}H_{28}O$ (androstenone) [18339-16-7] HFVMLYAGWXSTQI-QYXZOKGRSA-N	3.4×10^{-2}		Amoore and Buttery (1978)	M	
oxandrolone $C_{19}H_{30}O_3$ [53-39-4] QSLJIVKCVHQPLV-WPMSWULFSA-N	4.3×10^{2}		HSDB (2015)	Q	99
piperonyl butoxide $C_{19}H_{30}O_5$ [51-03-6] FIPWRIJSWJWJAI-UHFFFAOYSA-N	1.1×10^{5}		HSDB (2015)	Q	99

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Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methoprene $C_{19}H_{34}O_3$ [40596-69-8] NFGXHKASABOEEW-LDRANXPESA-N	1.4		HSDB (2015)	V	
fluorescein $C_{20}H_{12}O_5$ [2321-07-5] GNBHRKFJIUUOQI-UHFFFAOYSA-N	1.1×10^{11}		HSDB (2015)	Q	99
phenolphthalein $C_{20}H_{14}O_4$ [77-09-8] KJFMBFZCATUALV-UHFFFAOYSA-N	1.1×10^{10}		HSDB (2015)	Q	99
avobenzone $C_{20}H_{22}O_3$ [70356-09-1] XNEFYCZVKIDDMS-UHFFFAOYSA-N	4.9×10^{4}		HSDB (2015)	Q	447
ethinyl estradiol $C_{20}H_{24}O_2$ [57-63-6] BFPYWIDHMRZLRN-UHFFFAOYSA-N	1.2×10^{6}		HSDB (2015)	Q	99
norethynodrel $C_{20}H_{26}O_2$ [68-23-5] ICTXHFFSOAJUMG-CEVCPLMDSA-N	7.6×10^{3}		HSDB (2015)	Q	99
norethindrone $C_{20}H_{26}O$ [68-22-4] VIKNJXKGJWUCNN-BROHZWGRSA-N	1.7×10^{4}		HSDB (2015)	Q	99
methandrostenolone $C_{20}H_{28}O_2$ [72-63-9] XWALNWXLMVGSFR-NSDIEPNESA-N	4.5×10^{3}		HSDB (2015)	Q	99
cinerin I $C_{20}H_{28}O_3$ [25402-06-6] FMTFEIJHMMQUJI-FPLPWBNLSA-N	1.0×10^{1}		HSDB (2015)	Q	99
17-methyltestosterone $C_{20}H_{30}O_2$ [58-18-4] GCKMFJBGXUYNAG-NSDIEPNESA-N	2.1×10^{3}		HSDB (2015)	Q	99

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Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
drostanolone $C_{20}H_{32}O_2$ (dromostanolone) [58-19-5] IKXILDNPCZPPRV-UHFFFAOYSA-N	1.2×10^{3}		HSDB (2015)	Q	99
curcumin $C_{21}H_{20}O_6$ [458-37-7] VFLDPWHFBUODDF-FCXRPNKRSA-N	1.4×10^{16}		HSDB (2015)	Q	99
bisphenol A diglycidyl ether $C_{21}H_{24}O_4$ [1675-54-3] LCFVJGUPQDGYKZ-UHFFFAOYSA-N	2.2×10^{5}		HSDB (2015)	Q	99
mestranol $C_{21}H_{26}O_2$ [72-33-3] IMSSROKUHAOUJS-ALAWOQLPSA-N	2.2×10^{3}		HSDB (2015)	Q	99
prednisone $C_{21}H_{26}O_5$ [53-03-2] XOFYZVNMUHMLCC-NUBBXXJJSA-N	3.5×10^{4}		HSDB (2015)	Q	99
norgestrel $C_{21}H_{28}O_2$ [6533-00-2] WWYNJERNGUHSAO-ZUHHCLADSA-N	1.3×10^{4}		HSDB (2015)	Q	99
levonorgestrel $C_{21}H_{28}O_2$ [797-63-7] WWYNJERNGUHSAO-XUDSTZEESA-N	1.3×10^{4}		HSDB (2015)	Q	99
pyrethrin I $C_{21}H_{28}O_3$ [121-21-1] ROVGZAWFACYCSP-CMDGGOBGSA-N	1.3×10^{1} 2.2×10^{-1} 8.4×10^{-1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
cinerin II $C_{21}H_{28}O_5$ [121-20-0] SHCRDCOTRILILT-WOBDGSLYSA-N	1.1×10^{4}		HSDB (2015)	Q	99
prednisolone $C_{21}H_{28}O_5$ [50-24-8] OIGNJSKKLXVSLS-UHFFFAOYSA-N	3.7×10^{2}		HSDB (2015)	Q	99

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Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dronabinol $C_{21}H_{30}O_2$ (delta 9-tetrahydrocannabinol) [1972-08-3] CYQFCXCEBYINGO-UHFFFAOYSA-N	4.1×10^{1}		HSDB (2015)	Q	99
progesterone $C_{21}H_{30}O_2$ [57-83-0] RJKFOVLPORLFTN-UHFFFAOYSA-N	1.5×10^{2}		HSDB (2015)	Q	99
hydrocortisone $C_{21}H_{30}O_5$ [50-23-7] JYGXADMDTFJGBT-NDNUHCHRSA-N	1.7×10^{2}		HSDB (2015)	Q	99
calusterone $C_{21}H_{32}O_2$ [17021-26-0] IVFYLRMMHVYGJH-UHFFFAOYSA-N	1.6×10^{3}		HSDB (2015)	Q	99
oxymetholone $C_{21}H_{32}O_3$ [434-07-1] ICMWWNHDUZJFDW-RCXBLOTCSA-N	6.6×10^{3}		HSDB (2015)	Q	99
resmethrin $C_{22}H_{26}O_3$ [10453-86-8] VEMKTZHHVJILDY-UHFFFAOYSA-N	4.7×10^{-2} 7.6×10^{1} 2.2×10^{-1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
pyrethrin II $C_{22}H_{28}O_5$ [121-29-9] VJFUPGQZSXIULQ-VKTMSVCMSA-N	4.5×10^{2} 4.5×10^{2} 3.8×10^{2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
methylprednisolone $C_{22}H_{30}O_5$ [83-43-2] VHRSUDSXCMQTMA-UHFFFAOYSA-N	2.7×10^{2}		HSDB (2015)	Q	99
medroxyprogesterone $C_{22}H_{32}O_3$ [520-85-4] FRQMUZJSZHZSGN-HBNHAYAOSA-N	7.6×10^{2}		HSDB (2015)	Q	99
dimethirimol $C_{23}H_{24}O_5$ [5221-53-4] VNKCZJKGJAEOCW-WXUKJITCSA-N	$>2.3\times10^{10}$		MacBean (2012a)	?	

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Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
rotenone $C_{23}H_{22}O_6$ [83-79-4] JUVIOZPCNVVQFO-UHFFFAOYSA-N	8.8×10^{7}		HSDB (2015)	Q	99
phenothrin $C_{23}H_{26}O_3$ [26002-80-2] SBNFWQZLDJGRLK-UHFFFAOYSA-N	1.5		MacBean (2012b)	X	350
spiromesifen $C_{23}H_{30}O_4$ [283594-90-1] GOLXNESZZPUPJE-UHFFFAOYSA-N	1.8×10^{-2}		HSDB (2015)	V	
digoxigenin $C_{23}H_{34}O_5$ [1672-46-4] SHIBSTMRCDJXLN-KCZCNTNESA-N	4.3×10^{5}		HSDB (2015)	Q	99
annatto $C_{24}H_{28}O_4$ [1393-63-1] ZVKOASAVGLETCT-LRRSNBNMSA-N	1.5×10^{11}		HSDB (2015)	Q	99
acequinocyl $C_{24}H_{32}O_4$ [57960-19-7] QDRXWCAVUNHOGA-UHFFFAOYSA-N	1.0×10^{1} 1.0×10^{1}		HSDB (2015) Maniere et al. (2011)	V ?	 241, 165
T-2 mycotoxin $C_{24}H_{34}O_9$ [21259-20-1] SSHHYBPAMCLKRH-UHFFFAOYSA-N	1.8×10^{12}		HSDB (2015)	Q	99
milk thistle extract $C_{25}H_{22}O_{10}$ [84604-20-6] SEBFKMXJBCUCAI-VGHNRKBZSA-N	6.2×10^{17}		HSDB (2015)	Q	99
simvastatin $C_{25}H_{38}O_5$ [79902-63-9] RYMZZMVNJRMUDD-UHFFFAOYSA-N	3.5×10^{4}		HSDB (2015)	Q	99
calcitriol $C_{27}H_{44}O_3$ (1,25-dihydroxycholecalciferol) [32222-06-3] GMRQFYUYWCNGIN-NKMMMXOESA-N	3.2×10^{1}		HSDB (2015)	Q	99

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Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
paricalcitol $C_{27}H_{44}O_3$ [131918-61-1] BPKAHTKRCLCHEA-UBFJEZKGSA-N	2.6×10^{1}		HSDB (2015)	Q	99
cholecalciferol $C_{27}H_{44}O$ [67-97-0] QYSXJUFSXHHAJI-SMGPGMQOSA-N	4.3×10^{-2}		HSDB (2015)	Q	99
cholesterol $C_{27}H_{46}O$ [57-88-5] HVYWMOMLDIMFJA-VUDDDUNTSA-N	5.8×10^{-2}		HSDB (2015)	Q	99
ergosterol $C_{28}H_{44}O$ [57-87-4] DNVPQKQSNYMLRS-CVGROQQCSA-N	6.2×10^{-2}		HSDB (2015)	Q	99
dihydrotachysterol $C_{28}H_{46}O$ [67-96-9] DTSXXSAWQHPLEF-GFVAUXBKSA-N	2.7×10^{-2}		HSDB (2015)	Q	99
etoposide $C_{29}H_{32}O_{13}$ [33419-42-0] VJJPUSNTGOMMGY-KWGSHVRASA-N	5.8×10^{24}		HSDB (2015)	Q	99
stigmasterol $C_{29}H_{48}O$ [83-48-7] HCXVJBMSMIARIN-BASBAMEESA-N	3.8×10^{-2}		HSDB (2015)	Q	99
pseudohypericin $C_{30}H_{16}O_9$ [55954-61-5] YXBUQQDFTYOHQI-UHFFFAOYSA-N	5.5×10^{23}		HSDB (2015)	Q	99
gossypol $C_{30}H_{30}O_8$ [303-45-7] QBKSWRVVCFFDOT-UHFFFAOYSA-N	4.3×10^{22}		HSDB (2015)	Q	99
maslinic acid $C_{30}H_{48}O_4$ [4373-41-5] MDZKJHQSJHYOHJ-LLICELPBSA-N	2.8×10^{5}		HSDB (2015)	Q	447

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Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
milbemectin $C_{31}H_{44}O_7$ [51596-10-2] ZLBGSRMUSVULIE-GSMJGMFJSA-N	6.5×10^{2} 3.9×10^{2}		Maniere et al. (2011) Maniere et al. (2011)	? ?	241, 165 241, 165
difenacoum $C_{31}H_{24}O_3$ [56073-07-5] FVQITOLOYMWVFU-UHFFFAOYSA-N	7.0×10^{6}		HSDB (2015)	Q	447
nonoxynol 9 $C_{33}H_{60}O_{10}$ [26571-11-9] FBWNMEQMRUMQSO-UHFFFAOYSA-N	1.8×10^{16}		HSDB (2015)	Q	99
azadirachtin $C_{35}H_{44}O_{16}$ [11141-17-6] FTNJWQUOZFUQQJ-GWTPYEAISA-N	3.5×10^{19}		HSDB (2015)	V	
monensin $C_{36}H_{62}O_{11}$ [17090-79-8] GAOZTHIDHYLHMS-LXKLZWMJSA-N	4.9×10^{18}		HSDB (2015)	Q	99
gossyplure $C_{36}H_{64}O_4$ [50933-33-0] BXJHOKLLMOYSRQ-QOXWLJPHSA-N	6.6×10^{-2}		HSDB (2015)	V	
capsanthin $C_{40}H_{56}O_3$ [465-42-9] VYIRVAXUEZSDNC-RDJLEWNRSA-N	3.4×10^{2}		HSDB (2015)	Q	99
heptamaloxyloglucan $C_{40}H_{70}O_{33}$ [870721-81-6] RAUODYOTTYNEJP-RQESCVSBSA-N	4.2×10^{13}		Maniere et al. (2011)	?	12, 165
digitoxin $C_{41}H_{64}O_{13}$ [71-63-6] WDJUZGPOPHTGOT-UCKSZOHFSA-N	7.6×10^{19}		HSDB (2015)	Q	99
digoxin $C_{41}H_{64}O_{14}$ [20830-75-5] LTMHDMANZUZIPE-PUGKRICDSA-N	2.1×10^{21}		HSDB (2015)	Q	99

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Table A3.12: Miscellaneous (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pyrethrum $C_{43}H_{56}O_8$ [8003-34-7] VXSIXFKKSNGRRO-YWUDCVDHSA-N	1.5×10^{1} 1.4×10^{4} 1.3×10^{1}		HSDB (2015) Maniere et al. (2011) Maniere et al. (2011)	Q ? ?	99 165 165
punicalagin $C_{48}H_{28}O_{30}$ [65995-63-3] SKNLUADAGHCXKF-UHFFFAOYSA-N	5.5×10^{10}		HSDB (2015)	Q	99
abamectin $C_{48}H_{72}O_{14}$ [71751-41-2] RRZXIRBKKLTSOM-IGNCFFBFSA-N	7.0×10^{3} $>3.7\times10^{2}$		HSDB (2015) Maniere et al. (2011)	V ?	 12, 165
notoginsenoside R1 $C_{48}H_{84}O_{18}$ [80418-24-2] ZBXDHDDTAIOMHK-UWGJVBKGSA-N	6.6×10^{25}		HSDB (2015)	Q	99
triolein $C_{57}H_{104}O_6$ [122-32-7] PHYFQTYBJUILEZ-IUPFWZBJSA-N	1.0×10^{-2}		HSDB (2015)	Q	447
tristearin $C_{57}H_{110}O_6$ [555-43-1] DCXXMTOCNZCJGO-UHFFFAOYSA-N	7.0×10^{-3}		HSDB (2015)	Q	99

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A4 Organic species with nitrogen (N)

A4.1 Amines (C, H, N)

Table A4.1: Amines (C, H, N)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyanamide CH_2N_2 [420-04-2] XZMCDFZZKTWFGF-UHFFFAOYSA-N	3.7×10^{4}		HSDB (2015)	V	
methylhydrazine CH_6N_2 [60-34-4] HDZGCSFEDULWCS-UHFFFAOYSA-N	3.3		HSDB (2015)	V	
methanamine CH_3NH_2 (methylamine) [74-89-5] BAVYZALUXZFZLV-UHFFFAOYSA-N	8.9×10^{-1}		Burkholder et al. (2019)	L	
	8.9×10^{-1}		Burkholder et al. (2015)	L	
	3.5×10^{-1}	2600	Wilhelm et al. (1977)	L	
	8.9×10^{-1}		Christie and Crisp (1967)	M	
	1.1		Yaws (2003)	X	237
	7.4×10^{-1}		Keshavarz et al. (2022)	Q	
	6.2		Duchowicz et al. (2020)	Q	
	1.1		Gharagheizi et al. (2010)	Q	246
	1.2		Hilal et al. (2008)	Q	
	2.3		Modarresi et al. (2007)	Q	67
		5000	Kühne et al. (2005)	Q	
	9.2×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	1.1		English and Carroll (2001)	Q	230, 231
	6.1×10^{-1}		Katritzky et al. (1998)	Q	
	5.6×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	8.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	8.9×10^{-1}		Mackay et al. (2006d)	?	
		3200	Kühne et al. (2005)	?	
	8.8×10^{-1}		Abraham et al. (1990)	?	
		5400	Abraham (1984)	?	21
	1.4		Bone et al. (1983)	?	65
ethanamine $C_2H_5NH_2$ (ethylamine) [75-04-7] QUSNBJAOOMFDIB-UHFFFAOYSA-N	8.0×10^{-1}		Burkholder et al. (2019)	L	
	8.0×10^{-1}		Burkholder et al. (2015)	L	
	8.4×10^{-1}		Brockbank (2013)	L	
	3.5×10^{-1}	3600	Wilhelm et al. (1977)	L	
	8.0×10^{-1}		Christie and Crisp (1967)	M	
	9.9×10^{-1}		Butler and Ramchandani (1935)	M	
	3.0×10^{-1}		Hwang et al. (1992)	V	
	1.0		Keshavarz et al. (2022)	Q	
	2.2		Duchowicz et al. (2020)	Q	299
	9.7×10^{-1}		Li et al. (2014)	Q	241
	7.9×10^{-1}		Hilal et al. (2008)	Q	
	1.7		Modarresi et al. (2007)	Q	67

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.3×10^{-1}		Yao et al. (2002)	Q	229
	9.5×10^{-1}		English and Carroll (2001)	Q	230, 231
	4.7×10^{-1}		Katritzky et al. (1998)	Q	
	4.6×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	2.4		Russell et al. (1992)	Q	279
	1.3		Suzuki et al. (1992)	Q	232
	8.0×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	9.9×10^{-1}		Mackay et al. (2006d)	?	
	3.8×10^{-1}		Yaws (1999)	?	21, 12
	8.0×10^{-1}		Abraham et al. (1990)	?	
		6500	Abraham (1984)	?	21
1H-1,2,4-triazole $C_2H_3N_3$ [288-88-0] NSPMIYGKQJPBQR-UHFFFAOYSA-N	6.6		HSDB (2015)	Q	99
dicyandiamide $C_2H_4N_4$ (cyanoguanidine) [461-58-5] QGBSISYHAICWAH-UHFFFAOYSA-N	4.3×10^{4}		HSDB (2015)	Q	99
ethylenimine C_2H_5N [151-56-4] NOWKCMXCCJGMRR-UHFFFAOYSA-N	8.2×10^{-1} 8.2×10^{-1} 2.9×10^{1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
1,2-dimethylhydrazine $C_2H_8N_2$ [540-73-8] DIIIISSCIXVANO-UHFFFAOYSA-N	1.8		HSDB (2015)	V	
1,1-dimethylhydrazine $C_2H_8N_2$ [57-14-7] RHUYHJGZWVXEHW-UHFFFAOYSA-N	7.6×10^{-1}		HSDB (2015)	V	
1-propanamine $C_3H_7NH_2$ (propylamine) [107-10-8] WGYKZJWCGVVSQN-UHFFFAOYSA-N	6.6×10^{-1} 6.6×10^{-1} 6.7×10^{-1} 5.6×10^{-1} 5.0×10^{-1} 6.6×10^{-1} 7.8×10^{-1} 6.6×10^{-1} 1.4 2.3 4.8×10^{-1} 2.1	 6400 6700 	Burkholder et al. (2019) Burkholder et al. (2015) Brockbank (2013) Leng et al. (2015a) Altschuh et al. (1999) Christie and Crisp (1967) Butler and Ramchandani (1935) Plyasunov et al. (2001) Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007)	L L L M M M M T Q Q Q Q	 184 67

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.7×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.6×10^{-1}		Yao et al. (2002)	Q	229
	5.2×10^{-1}		Katritzky et al. (1998)	Q	
	3.6×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.6		Russell et al. (1992)	Q	279
	1.0		Suzuki et al. (1992)	Q	232
	6.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	7.8×10^{-1}		Mackay et al. (2006d)	?	
	3.9×10^{-1}		Yaws (1999)	?	21
	6.7×10^{-1}		Abraham et al. (1990)	?	
		6700	Abraham (1984)	?	21
2-propanamine	2.2×10^{-1}		Duchowicz et al. (2020)	V	186
C_3H_9N	2.2×10^{-1}		Hilal et al. (2008)	C	
(isopropylamine)	8.9×10^{-1}		Duchowicz et al. (2020)	Q	
[75-31-0]	2.1×10^{-1}		Hilal et al. (2008)	Q	
JJWLVOIRVHMVIS-UHFFFAOYSA-N	2.4		Modarresi et al. (2007)	Q	67
	2.3×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	1.6×10^{-1}		Yao et al. (2002)	Q	229
	3.1×10^{-1}		Katritzky et al. (1998)	Q	
	1.3×10^{-1}		Yaws (1999)	?	21, 12
propanedinitrile	7.5×10^{1}		Duchowicz et al. (2020)	V	186
$C_3H_2N_2$	2.0×10^{1}		Duchowicz et al. (2020)	Q	
(malononitrile)	7.8×10^{2}		HSDB (2015)	Q	99
[109-77-3]	2.0×10^{1}		Gharagheizi et al. (2012)	Q	
CUONGYYJJVDODC-UHFFFAOYSA-N	6.3×10^{1}		Yaws (1999)	?	21, 12
2-methylaziridine	9.9×10^{-1}		Duchowicz et al. (2020)	V	186
C_3H_7N	1.2×10^{1}		Duchowicz et al. (2020)	Q	
[75-55-8]	1.2		Yaffe et al. (2003)	Q	248, 249
OZDGMOYKSFPLSE-UHFFFAOYSA-N	1.5		Katritzky et al. (1998)	Q	
1,2-diaminopropane	1.4×10^{3}	7400	Nguyen (2013)	M	11
$C_3H_{10}N_2$					
[78-90-0]					
AOHJOMMDDJHIJH-UHFFFAOYSA-N					
1-butanamine	5.6×10^{-1}		Burkholder et al. (2019)	L	
$C_4H_9NH_2$	5.6×10^{-1}		Burkholder et al. (2015)	L	
(butylamine)	5.4×10^{-1}		Brockbank (2013)	L	
[109-73-9]	5.6×10^{-1}		Altschuh et al. (1999)	M	
HQABUPZFAYXKJW-UHFFFAOYSA-N	5.2×10^{-1}		Rytting et al. (1978)	M	
	5.6×10^{-1}		Christie and Crisp (1967)	M	
	6.5×10^{-1}		Butler and Ramchandani (1935)	M	
	2.2×10^{-1}		Hwang et al. (1992)	V	
	4.5×10^{-1}		Amoore and Buttery (1978)	V	
	3.7×10^{-1}		Yaws (2003)	X	258
	3.6×10^{-1}		Yaws (2003)	X	237
	2.1×10^{-1}		Dupeux et al. (2022)	Q	259

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-1}		Keshavarz et al. (2022)	Q	
	2.3		Duchowicz et al. (2020)	Q	299
	6.5×10^{-1}		Li et al. (2014)	Q	241
	4.0×10^{-1}		Gharagheizi et al. (2010)	Q	246
	2.9×10^{-1}		Hilal et al. (2008)	Q	
	1.5		Modarresi et al. (2007)	Q	67
	5.2×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.4×10^{-1}		Yao et al. (2002)	Q	229
	7.3×10^{-1}		English and Carroll (2001)	Q	230, 231
	4.0×10^{-1}		Katritzky et al. (1998)	Q	
	2.8×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.1		Russell et al. (1992)	Q	279
	7.9×10^{-1}		Suzuki et al. (1992)	Q	232
	5.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	6.6×10^{-1}		Mackay et al. (2006d)	?	
	2.2×10^{-1}		Yaws (1999)	?	21
	5.2×10^{-1}		Abraham et al. (1990)	?	
		7100	Abraham (1984)	?	21
2-butanamine	4.0×10^{-1}	7700	Kish et al. (2013)	M	548
$C_4H_{11}N$	6.5×10^{-2}		Duchowicz et al. (2020)	V	186
(*sec*-butylamine)	6.5×10^{-2}		Hilal et al. (2008)	C	
[13952-84-6]	9.1×10^{-1}		Duchowicz et al. (2020)	Q	
BHRZNVHARXXAHW-UHFFFAOYSA-N	1.6×10^{-1}		Hilal et al. (2008)	Q	
	1.7		Modarresi et al. (2007)	Q	67
	2.2×10^{-1}		Katritzky et al. (1998)	Q	
2-methyl-1-propanamine	7.3×10^{-1}		Duchowicz et al. (2020)	V	186
$C_4H_{11}N$	7.2×10^{-1}		Hilal et al. (2008)	C	
(isobutylamine)	9.1×10^{-1}		Duchowicz et al. (2020)	Q	
[78-81-9]	2.4×10^{-1}		Hilal et al. (2008)	Q	
KDSNLYIMUZNERS-UHFFFAOYSA-N	2.0		Modarresi et al. (2007)	Q	67
	5.2×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	1.5×10^{-1}		Yao et al. (2002)	Q	229, 267
	3.9×10^{-1}		Katritzky et al. (1998)	Q	
	4.4×10^{-1}		Yaws (1999)	?	21, 12
2-methyl-2-propanamine	2.8×10^{-1}		Duchowicz et al. (2020)	V	186
$C_4H_{11}N$	2.8×10^{-1}		Hilal et al. (2008)	C	
(*tert*-butylamine)	4.0×10^{-1}		Duchowicz et al. (2020)	Q	
[75-64-9]	5.0×10^{-2}		Hilal et al. (2008)	Q	
YBRBMKDOPFTVDT-UHFFFAOYSA-N	1.0×10^{-1}		Modarresi et al. (2007)	Q	67
	2.9×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.1×10^{-1}		Katritzky et al. (1998)	Q	
dimethylethylamine	1.1×10^{-1}		Yaws (2003)	X	237
$C_4H_{11}N$	9.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[598-56-1]	1.1×10^{-1}		Gharagheizi et al. (2010)	Q	246
DAZXVJBJRMWXJP-UHFFFAOYSA-N					

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-propylguanidine $C_4H_{11}N_3$ [462-25-9] BWMDMTSNSXYYSP-UHFFFAOYSA-N	4.1×10^{4}		Ebert et al. (2023)	?	365
1,2-diethylhydrazine $C_4H_{12}N_2$ [1615-80-1] YCBOYOYVDOUXLH-UHFFFAOYSA-N	8.2×10^{1}		HSDB (2015)	Q	99
N-(2-aminoethyl)-1,2-ethanediamine $C_4H_{13}N_3$ (diethylenetriamine) [111-40-0] RPNUMPOLZDHAAY-UHFFFAOYSA-N	9.9×10^{8}		HSDB (2015)	Q	99
butanedinitrile $C_4H_4N_2$ [110-61-2] IAHFWCOBPZCAEA-UHFFFAOYSA-N	8.7×10^{2} 1.5×10^{3} 1.5×10^{3} 4.0×10^{3} 2.6×10^{1} 3.9×10^{3}	7000	Plyasunov et al. (2006) Duchowicz et al. (2020) HSDB (2015) Yaws (2003) Duchowicz et al. (2020) Ghasragheizi et al. (2010)	L V V X Q Q	 186 237, 12 246
2-methyl-1H-imidazole $C_4H_6N_2$ [693-98-1] LXBGSDVWAMZHDD-UHFFFAOYSA-N	8.1×10^{2} 1.8×10^{3} 1.1×10^{3} 2.2		Du et al. (2017) Du et al. (2017) Du et al. (2017) HSDB (2015)	M Q Q Q	478 549 99
4-methyl-1H-imidazole $C_4H_6N_2$ [822-36-6] XLSZMDLNRCVEIJ-UHFFFAOYSA-N	2.4		HSDB (2015)	Q	99
N-methyl-1,3-propanediamine $C_4H_{12}N_2$ (3-(methylamino)propylamine) [6291-84-5] QHJABUZHRJTCAR-UHFFFAOYSA-N	1.4×10^{3} 2.1×10^{3}	7600 8800	Nguyen (2013) Kim et al. (2008)	M M	11 550
1-pentanamine $C_5H_{11}NH_2$ (1-pentylamine) [110-58-7] DPBLXKKOBLCELK-UHFFFAOYSA-N	4.3×10^{-1} 4.0×10^{-1} 3.1×10^{-1} 4.0×10^{-1} 1.7×10^{-1} 2.4 1.6×10^{-1} 1.2 4.0×10^{-1} 5.6×10^{-1}		Brockbank (2013) Rytting et al. (1978) Amoore and Buttery (1978) Christie and Crisp (1967) Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Yaffe et al. (2003) English and Carroll (2001)	L M M M Q Q Q Q Q Q	 299 67 248, 249 230, 260

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.0×10^{-1}		Katritzky et al. (1998)	Q	
	2.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	7.2×10^{-1}		Russell et al. (1992)	Q	358
	1.5×10^{-1}		Suzuki et al. (1992)	Q	232
	4.1×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	4.0×10^{-1}		Abraham et al. (1990)	?	
		7500	Abraham (1984)	?	21
3-methyl-1-butanamine $C_5H_{13}N$ [107-85-7] BMFVGAAISNGQNM-UHFFFAOYSA-N	3.2×10^{-1}		Yaws (2003)	X	237
	3.1×10^{-1}		Gharagheizi et al. (2010)	Q	246
	2.2×10^{-1}		Hilal et al. (2008)	Q	
1,2-dimethylpropylamine $C_5H_{13}N$ [598-74-3] JOZZAIIGWFLONA-UHFFFAOYSA-N	4.0×10^{-1}		Yaws (2003)	X	237
	3.8×10^{-1}		Gharagheizi et al. (2010)	Q	246
dimethylpropylamine $C_5H_{13}N$ [926-63-6] ZUHZZVMEUAUWHY-UHFFFAOYSA-N	7.9×10^{-2}		Yaws (2003)	X	237
	5.3×10^{-2}		Gharagheizi et al. (2012)	Q	
	9.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
dimethylisopropylamine $C_5H_{13}N$ [996-35-0] VMOWKUTXPNPTEN-UHFFFAOYSA-N	7.9×10^{-2}		Yaws (2003)	X	237
	1.2×10^{-1}		Gharagheizi et al. (2010)	Q	246
ethylpropylamine $C_5H_{13}N$ [20193-20-8] XCVNDBIXFPGMIW-UHFFFAOYSA-N	1.7×10^{-1}		Yaws (2003)	X	237
	1.6×10^{-1}		Gharagheizi et al. (2010)	Q	246
ethylisopropylamine $C_5H_{13}N$ [19961-27-4] RIVIDPPYRINTTH-UHFFFAOYSA-N	1.8×10^{-1}		Yaws (2003)	X	237
	1.8×10^{-1}		Gharagheizi et al. (2010)	Q	246
methyldiethylamine $C_5H_{13}N$ [616-39-7] GNVRJGIVDSQCOP-UHFFFAOYSA-N	7.9×10^{-2}		Yaws (2003)	X	237
	1.1×10^{-1}		Gharagheizi et al. (2010)	Q	246
2-methylpiperazine $C_5H_{12}N_2$ [109-07-9] JOMNTHCQHJPVAZ-UHFFFAOYSA-N	5.0×10^{3}	9200	Nguyen (2013)	M	11

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-hexanamine	3.5×10^{-1}		Brockbank (2013)	L	
$C_6H_{13}NH_2$	3.2×10^{-1}		Rytting et al. (1978)	M	
(hexylamine)	3.7×10^{-1}		Christie and Crisp (1967)	M	
[111-26-2]	1.0×10^{-1}		Yaws (2003)	X	237
BMVXCPBXGZKUPN-UHFFFAOYSA-N	2.3×10^{-1}		Keshavarz et al. (2022)	Q	
	2.4		Duchowicz et al. (2020)	Q	184
	1.4×10^{-1}		Gharagheizi et al. (2010)	Q	246
	3.7×10^{-1}		Hilal et al. (2008)	Q	
	1.0		Modarresi et al. (2007)	Q	67
	3.2×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	9.2×10^{-2}		Yao et al. (2002)	Q	229, 267
	4.3×10^{-1}		English and Carroll (2001)	Q	230, 274
	3.3×10^{-1}		Katritzky et al. (1998)	Q	
	1.8×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	3.4×10^{-1}		Russell et al. (1992)	Q	279
	4.6×10^{-1}		Suzuki et al. (1992)	Q	232
	3.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	1.0×10^{-1}		Yaws (1999)	?	21
	3.2×10^{-1}		Abraham et al. (1990)	?	
		7900	Abraham (1984)	?	21
2-hexanamine	1.9×10^{-1}		Yaws (2003)	X	237
$C_6H_{15}N$	1.5×10^{-1}		Gharagheizi et al. (2010)	Q	246
[5329-79-3]					
WGBBUURBHXLGFM-UHFFFAOYSA-N					
3-hexanamine	1.8×10^{-1}		Yaws (2003)	X	237
$C_6H_{15}N$	1.5×10^{-1}		Gharagheizi et al. (2010)	Q	246
[16751-58-9]					
HQLZFBUAULNEGP-UHFFFAOYSA-N					
1-amino-2-methylpentane	2.0×10^{-1}		Yaws (2003)	X	237
$C_6H_{15}N$	1.8×10^{-1}		Gharagheizi et al. (2010)	Q	246
[13364-16-4]					
WNDXRJBYZOSNQO-UHFFFAOYSA-N					
1-amino-3-methylpentane	2.0×10^{-1}		Yaws (2003)	X	237
$C_6H_{15}N$	1.8×10^{-1}		Gharagheizi et al. (2010)	Q	246
[42245-37-4]					
JLAUIBFZZUVOBB-UHFFFAOYSA-N					
1-amino-4-methylpentane	2.0×10^{-1}		Yaws (2003)	X	237
$C_6H_{15}N$	1.8×10^{-1}		Gharagheizi et al. (2010)	Q	246
[5344-20-7]					
QVIAMKXOQGCYCV-UHFFFAOYSA-N					
2-amino-3-methylpentane	1.7×10^{-1}		Yaws (2003)	X	237
$C_6H_{15}N$	2.1×10^{-1}		Gharagheizi et al. (2010)	Q	246
[35399-81-6]					
ZFAGOADKDXXTSV-UHFFFAOYSA-N					

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-amino-4-methylpentane	2.3×10^{-1}		Yaws (2003)	X	237
$C_6H_{15}N$	2.3×10^{-1}		Keshavarz et al. (2022)	Q	
[108-09-8]	3.6×10^{-1}		Duchowicz et al. (2020)	Q	184
UNBMPKNTYKDYCG-UHFFFAOYSA-N	2.0×10^{-1}		Gharagheizi et al. (2010)	Q	246
	3.2×10^{-1}		Duchowicz et al. (2020)	?	185, 21
3-amino-2-methylpentane	1.7×10^{-1}		Yaws (2003)	X	237
$C_6H_{15}N$	2.1×10^{-1}		Gharagheizi et al. (2010)	Q	246
[54287-41-1]					
JYNQKCFJPQEXSL-UHFFFAOYSA-N					
1-amino-2-ethylbutane	1.8×10^{-1}		Yaws (2003)	X	237
$C_6H_{15}N$	1.8×10^{-1}		Gharagheizi et al. (2010)	Q	246
[617-79-8]					
MGWAGIQQTULHGU-UHFFFAOYSA-N					
1-amino-2,2-dimethylbutane	2.1×10^{-1}		Yaws (2003)	X	237
$C_6H_{15}N$	2.0×10^{-1}		Gharagheizi et al. (2010)	Q	246
[41781-17-3]					
PZVPOYBHOPRJNP-UHFFFAOYSA-N					
1-amino-2,3-dimethylbutane	2.5×10^{-1}		Yaws (2003)	X	237
$C_6H_{15}N$	2.2×10^{-1}		Gharagheizi et al. (2010)	Q	246
[66553-05-7]					
GBMSZXWHMSSBGP-UHFFFAOYSA-N					
1-amino-3,3-dimethylbutane	1.6×10^{-1}		Yaws (2003)	X	237
$C_6H_{15}N$	2.0×10^{-1}		Gharagheizi et al. (2010)	Q	246
[15673-00-4]					
GPWHFPWZAPOYNO-UHFFFAOYSA-N					
2-amino-3,3-dimethylbutane	2.4×10^{-1}		Yaws (2003)	X	237
$C_6H_{15}N$	2.4×10^{-1}		Gharagheizi et al. (2010)	Q	246
[3850-30-4]					
DXSUORGKJZADET-UHFFFAOYSA-N					
dimethylbutylamine	8.9×10^{-2}		Yaws (2003)	X	237
$C_6H_{15}N$	4.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[927-62-8]	6.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
DJEQZVQFEPKLOY-UHFFFAOYSA-N					
dimethyl-*sec*-butylamine	1.0×10^{-1}		Yaws (2003)	X	237
$C_6H_{15}N$	1.2×10^{-1}		Gharagheizi et al. (2012)	Q	
[921-04-0]	8.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
USSPHSVODLAWSA-UHFFFAOYSA-N					
dimethyl-*tert*-butylamine	1.0×10^{-1}		Yaws (2003)	X	237
$C_6H_{15}N$	9.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
[918-02-5]					
OXQMIXBVXHWDPX-UHFFFAOYSA-N					

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethylbutylamine $C_6H_{15}N$ [13360-63-9] QHCCDDQKNUYGNC-UHFFFAOYSA-N	1.3×10^{-1} 1.2×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
ethylisobutylamine $C_6H_{15}N$ [13205-60-2] FNLUJDLKYOWMMF-UHFFFAOYSA-N	1.5×10^{-1} 1.2×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
ethyl-*sec*-butylamine $C_6H_{15}N$ [21035-44-9] KFYKZKISJBGVMR-UHFFFAOYSA-N	1.5×10^{-1} 1.3×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
methyl-1,1-dimethylpropylamine $C_6H_{15}N$ [2978-64-5] BUJFTKPQXSIZFX-UHFFFAOYSA-N	1.1×10^{-1} 1.8×10^{-1} 1.4×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
methyl-1,2-dimethylpropylamine $C_6H_{15}N$ [34317-39-0] LJLWVVCWBURGCC-UHFFFAOYSA-N	1.2×10^{-1} 5.9×10^{-2} 1.4×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
methyl-2,2-dimethylpropylamine $C_6H_{15}N$ [26153-91-3] UQGXHNDRCRTZAC-UHFFFAOYSA-N	1.1×10^{-1} 1.1×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
methyl-1-methylbutylamine $C_6H_{15}N$ [51932-19-5] IPBXLJFBVNLKFE-UHFFFAOYSA-N	1.2×10^{-1} 8.7×10^{-2} 1.2×10^{-1}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
methylethylpropylamine $C_6H_{15}N$ [4458-32-6] SMBYUOXUISCLCF-UHFFFAOYSA-N	1.1×10^{-1} 1.0×10^{-1} 8.2×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
methylethylisopropylamine $C_6H_{15}N$ [39198-07-7] UTLDDSNRFHWERZ-UHFFFAOYSA-N	1.1×10^{-1} 9.8×10^{-2}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
methylpentylamine $C_6H_{15}N$ [25419-06-1] UOIWOHLIGKIYFE-UHFFFAOYSA-N	1.2×10^{-1} 1.1×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
propylisopropylamine $C_6H_{15}N$ [21968-17-2] VLSTXUUYLIALPB-UHFFFAOYSA-N	1.4×10^{-1} 1.3×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
1,6-hexanediamine $C_6H_{16}N_2$ (hexamethylenediamine) [124-09-4] NAQMVNRVTILPCV-UHFFFAOYSA-N	1.0×10^{3} 3.1×10^{3}	5000	Nguyen (2013) HSDB (2015)	M Q	11 99
N,N'-methanetetraylbis-2-propanamine $C_7H_{14}N_2$ (1,3-diisopropylcarbodiimide) [693-13-0] BDNKZNFMNDZQMI-UHFFFAOYSA-N	9.9×10^{-3}		HSDB (2015)	Q	447
4-methyl-2-hexanamine $C_7H_{17}N$ [105-41-9] YAHRDLICUYEDAU-UHFFFAOYSA-N	2.3×10^{-1}		HSDB (2015)	Q	447
1-heptanamine $C_7H_{17}N$ (1-heptylamine) [111-68-2] WJYIASZWHGOTOU-UHFFFAOYSA-N	2.8×10^{-1} 2.4×10^{-1} 8.0×10^{-2} 8.3×10^{-2} 4.5×10^{-1} 9.6×10^{-1} 2.1×10^{-1} 3.3×10^{-1} 1.4×10^{-1} 2.4×10^{-1}		Brockbank (2013) Rytting et al. (1978) Yaws (2003) Gharagheizi et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Yaffe et al. (2003) English and Carroll (2001) Nirmalakhandan et al. (1997) Abraham et al. (1990)	L M X Q Q Q Q Q Q ?	 237 246 67 248, 272 230, 231
diethylisopropylamine $C_7H_{17}N$ [6006-15-1] ULWOJODHECIZAU-UHFFFAOYSA-N	7.7×10^{-2} 8.0×10^{-2}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
diethylpropylamine $C_7H_{17}N$ [4458-31-5] PQZTVWVYCLIIJY-UHFFFAOYSA-N	7.7×10^{-2} 1.5×10^{-1} 7.3×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
dimethyl-1,1-dimethylpropylamine $C_7H_{17}N$ [57757-60-5] CUHMMDPUXJFCNB-UHFFFAOYSA-N	6.3×10^{-2} 6.5×10^{-2}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dimethyl-1,2-dimethylpropylamine	6.9×10^{-2}		Yaws (2003)	X	237
$C_7H_{17}N$	5.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[66225-38-5]	7.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
FWBCYOHCOBOARU-UHFFFAOYSA-N					
dimethyl-2,2-dimethylpropylamine	6.3×10^{-2}		Yaws (2003)	X	237
$C_7H_{17}N$	1.8×10^{-2}		Gharagheizi et al. (2012)	Q	
[10076-31-0]	5.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
FUIRUFXAVIHAQB-UHFFFAOYSA-N					
dimethyl-2-methylbutylamine	7.1×10^{-2}		Yaws (2003)	X	237
$C_7H_{17}N$	2.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[66225-39-6]	6.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
BHMZPPHMQJHCHQ-UHFFFAOYSA-N					
dimethyl-3-methylbutylamine	7.2×10^{-2}		Yaws (2003)	X	237
$C_7H_{17}N$	3.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[2315-43-7]	5.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
KOOQJINBDNZUTB-UHFFFAOYSA-N					
dimethylpentylamine	5.3×10^{-2}		Yaws (2003)	X	237
$C_7H_{17}N$	4.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[26153-88-8]	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
IDFANOPDMXWIOP-UHFFFAOYSA-N					
dimethyl-2-pentylamine	7.7×10^{-2}		Yaws (2003)	X	237
$C_7H_{17}N$	6.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[57303-85-2]	6.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
LSTZYJQJHGEVKH-UHFFFAOYSA-N					
dimethyl-3-pentylamine	7.0×10^{-2}		Yaws (2003)	X	237
$C_7H_{17}N$	5.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[18636-94-7]	6.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
SUEKSPIQGIMSQM-UHFFFAOYSA-N					
ethylpentylamine	8.6×10^{-2}		Yaws (2003)	X	237
$C_7H_{17}N$	5.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[17839-26-8]	9.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
ICVFPLUSMYSIFO-UHFFFAOYSA-N					
methyldiisopropylamine	7.1×10^{-2}		Yaws (2003)	X	237
$C_7H_{17}N$	7.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
[10342-97-9]					
ISRXMEYARGEVIU-UHFFFAOYSA-N					
methyldipropylamine	7.5×10^{-2}		Yaws (2003)	X	237
$C_7H_{17}N$	5.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[3405-42-3]	6.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
UVBMZKBIZUWTLV-UHFFFAOYSA-N					

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Table A4.1: Amines (C, H, N) (. . . continued)

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methylethylbutylamine	7.2×10^{-2}		Yaws (2003)	X	237
$C_7H_{17}N$	8.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[66225-40-9]	6.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
WOLFCKKMHUVEPN-UHFFFAOYSA-N					
methylethylisobutylamine	7.8×10^{-2}		Yaws (2003)	X	237
$C_7H_{17}N$	4.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[60247-14-5]	6.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
QQWXQKMVASVXCI-UHFFFAOYSA-N					
methylethyl-*sec*-butylamine	8.2×10^{-2}		Yaws (2003)	X	237
$C_7H_{17}N$	7.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
[66225-41-0]					
HAFZSBASGRZPLA-UHFFFAOYSA-N					
methylethyl-*tert*-butylamine	7.0×10^{-2}		Yaws (2003)	X	237
$C_7H_{17}N$	7.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
[52841-28-8]					
BWWLCYLGZIWOHK-UHFFFAOYSA-N					
methylhexylamine	8.3×10^{-2}		Yaws (2003)	X	237
$C_7H_{17}N$	3.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[35161-70-7]	8.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
XJINZNWPEQMMBV-UHFFFAOYSA-N					
methylpropylisopropylamine	7.3×10^{-2}		Yaws (2003)	X	237
$C_7H_{17}N$	1.6×10^{-1}		Gharagheizi et al. (2012)	Q	
[66225-42-1]	7.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
OYQDUCLFZSKBCZ-UHFFFAOYSA-N					
1-octanamine	2.2×10^{-1}		Brockbank (2013)	L	
C_8H19N	1.9×10^{-1}		Rytting et al. (1978)	M	
(octylamine)	1.2×10^{-2}		Duchowicz et al. (2020)	V	186
[111-86-4]	2.4		Duchowicz et al. (2020)	Q	
IOQPZZOEVPZRBK-UHFFFAOYSA-N	1.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.3×10^{-1}		Hilal et al. (2008)	Q	
		7400	Kühne et al. (2005)	Q	
	2.1×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.5×10^{-1}		English and Carroll (2001)	Q	230, 231
	1.1×10^{-1}		Nirmalakhandan et al. (1997)	Q	
		6600	Kühne et al. (2005)	?	
	1.2×10^{-2}		Yaws (1999)	?	21
	1.9×10^{-1}		Abraham et al. (1990)	?	
2-ethyl-1-hexanamine	1.0×10^{-1}		Duchowicz et al. (2020)	V	186
$C_8H_{19}N$	9.4×10^{-1}		Duchowicz et al. (2020)	Q	
(2-ethylhexylamine)	3.7×10^{-1}		Hilal et al. (2008)	Q	
[104-75-6]	9.7×10^{-1}		Modarresi et al. (2007)	Q	67
LTHNHFOGQMKPOV-UHFFFAOYSA-N		7400	Kühne et al. (2005)	Q	
		7400	Kühne et al. (2005)	?	

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Table A4.1: Amines (C, H, N) (. . . continued)

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diethylbutylamine	5.2×10^{-2}		Yaws (2003)	X	237
$C_8H_{19}N$	1.2×10^{-1}		Gharagheizi et al. (2012)	Q	
[4444-68-2]	5.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
ORSUTASIQKBEFU-UHFFFAOYSA-N					
dimethylhexylamine	3.4×10^{-2}		Yaws (2003)	X	237
$C_8H_{19}N$	3.1×10^{-2}		Gharagheizi et al. (2012)	Q	
[4385-04-0]	3.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
QMHNQZGXPNCMCO-UHFFFAOYSA-N					
ethylhexylamine	6.2×10^{-2}		Yaws (2003)	X	237
$C_8H_{19}N$	4.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[20352-67-4]	7.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
WSTNFGAKGUERTC-UHFFFAOYSA-N					
methylheptylamine	6.2×10^{-2}		Yaws (2003)	X	237
$C_8H_{19}N$	2.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[36343-05-2]	7.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
LTGYRKOQQQWWAF-UHFFFAOYSA-N					
2,2'-azobis-(2-methylpropanenitrile)	2.4		Duchowicz et al. (2020)	V	186
$C_8H_{12}N_4$	8.0×10^{1}		Duchowicz et al. (2020)	Q	
[78-67-1]					
OZAIFHULBGXAKX-UHFFFAOYSA-N					
diethylpentylamine	4.0×10^{-2}		Yaws (2003)	X	237
$C_9H_{21}N$	8.6×10^{-2}		Gharagheizi et al. (2012)	Q	
[2162-91-6]	4.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
YZULHOOBWDXEOT-UHFFFAOYSA-N					
dimethylheptylamine	2.5×10^{-2}		Yaws (2003)	X	237
$C_9H_{21}N$	2.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[5277-11-2]	3.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
LSICDRUYCNGRIF-UHFFFAOYSA-N					
ethylheptylamine	5.2×10^{-2}		Yaws (2003)	X	237
$C_9H_{21}N$	5.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[66793-76-8]	6.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
IUZZLNVABCISOI-UHFFFAOYSA-N					
methyloctylamine	5.4×10^{-2}		Yaws (2003)	X	237
$C_9H_{21}N$	3.0×10^{-2}		Gharagheizi et al. (2012)	Q	
[2439-54-5]	6.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
SEGJNMCIMOLEDM-UHFFFAOYSA-N					
nonylamine	5.9×10^{-2}		Yaws (2003)	X	237
$C_9H_{21}N$	2.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
[112-20-9]					
FJDUDHYHRVPMJZ-UHFFFAOYSA-N					

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
diethylhexylamine	3.3×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{23}N$	6.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[44979-90-0]	3.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
XHDKYWMKOLURNK-UHFFFAOYSA-N					
dimethyloctylamine	2.0×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{23}N$	4.5×10^{-2}		Gharagheizi et al. (2012)	Q	
[7378-99-6]	2.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
UQKAOOAFEFCDGT-UHFFFAOYSA-N					
dipentylamine	5.3×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{23}N$	4.4×10^{-2}		Gharagheizi et al. (2012)	Q	
[2050-92-2]	6.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
JACMPVXHEARCBO-UHFFFAOYSA-N					
ethyloctylamine	5.2×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{23}N$	6.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[4088-36-2]	6.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
SDQCOADWEMMSGK-UHFFFAOYSA-N					
methylnonylamine	5.6×10^{-2}		Yaws (2003)	X	237
$C_{10}H_{23}N$	2.2×10^{-2}		Gharagheizi et al. (2012)	Q	
[39093-27-1]	6.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
OZIXTIPURXIEMB-UHFFFAOYSA-N					
diethylheptylamine	2.3×10^{-2}		Yaws (2003)	X	237
$C_{11}H_{25}N$	1.1×10^{-1}		Gharagheizi et al. (2012)	Q	
[26981-81-7]	2.7×10^{-2}		Gharagheizi et al. (2010)	Q	246
YUCNJMBRLIZNMO-UHFFFAOYSA-N					
dimethylnonylamine	1.5×10^{-2}		Yaws (2003)	X	237
$C_{11}H_{25}N$	3.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[17373-27-2]	2.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
AMAADDMFZSZCNT-UHFFFAOYSA-N					
diethyloctylamine	2.3×10^{-2}		Yaws (2003)	X	237
$C_{12}H_{27}N$	2.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
[4088-37-3]					
BVUGARXRRGZONH-UHFFFAOYSA-N					
dihexylamine	1.3×10^{-1}		Yaws (2003)	X	237
$C_{12}H_{27}N$	8.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
[143-16-8]					
PXSXRABJBXYMFT-UHFFFAOYSA-N					
dimethyldecylamine	1.6×10^{-2}		Yaws (2003)	X	237
$C_{12}H_{27}N$	4.3×10^{-2}		Gharagheizi et al. (2012)	Q	
[1120-24-7]	2.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
YWWNNLPSZSEZNZ-UHFFFAOYSA-N					

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methylundecylamine $C_{12}H_{27}N$ [66553-53-5] JCJFBKCQLFMABE-UHFFFAOYSA-N	1.3×10^{-1} 8.8×10^{-2}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
diethylnonylamine $C_{13}H_{29}N$ [45124-35-4] IBTOMDSHMLGUHA-UHFFFAOYSA-N	3.1×10^{-2} 1.2×10^{-1} 2.8×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
dimethylundecylamine $C_{13}H_{29}N$ [17373-28-3] MMWFTWUMBYZIRZ-UHFFFAOYSA-N	2.7×10^{-2} 4.6×10^{-2} 2.6×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246
ethylundecylamine $C_{13}H_{29}N$ [59570-04-6] LKVBHKWFYHKTSM-UHFFFAOYSA-N	1.4×10^{-1} 1.2×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
methyldodecylamine $C_{13}H_{29}N$ [7311-30-0] OMEMQVZNTDHENJ-UHFFFAOYSA-N	1.5×10^{-1} 1.4×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
diethyldecylamine $C_{14}H_{31}N$ [6308-94-7] UFFQZCPLBHYOFV-UHFFFAOYSA-N	4.2×10^{-2} 3.5×10^{-2}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
diheptylamine $C_{14}H_{31}N$ [2470-68-0] NJWMENBYMFZACG-UHFFFAOYSA-N	1.7×10^{-1} 2.7×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
ethyldodecylamine $C_{14}H_{31}N$ [35902-57-9] LWIPGCTWFZCIKX-UHFFFAOYSA-N	1.8×10^{-1} 2.3×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
methyltridecylamine $C_{14}H_{31}N$ [45165-81-9] XMRPIOZXPHTSCE-UHFFFAOYSA-N	2.0×10^{-1} 2.8×10^{-1}		Yaws (2003) Gharagheizi et al. (2010)	X Q	237 246
tripentylamine $C_{15}H_{33}N$ [621-77-2] OOHAUGDGCWURIT-UHFFFAOYSA-N	6.7×10^{-2} 3.1×10^{-2} 7.1×10^{-2}		Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010)	X Q Q	237 246

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
1-tridecanamine $C_{13}H_{29}N$ [2869-34-3] ABVVEAHYODGCLZ-UHFFFAOYSA-N	9.0×10^{-2}		Altschuh et al. (1999)	M	
dimethylamine $(CH_3)_2NH$ [124-40-3] ROSDSFDQCJNGOL-UHFFFAOYSA-N	5.5×10^{-1}		Burkholder et al. (2019)	L	
	5.5×10^{-1}		Burkholder et al. (2015)	L	
	6.2×10^{-1}		Brockbank (2013)	L	
	3.0×10^{-1}	4000	Wilhelm et al. (1977)	L	
	5.6×10^{-1}		Christie and Crisp (1967)	M	
	5.8×10^{-1}	6400	Bagno et al. (1991)	T	473
	6.8×10^{-2}		Keshavarz et al. (2022)	Q	
	1.8		Duchowicz et al. (2020)	Q	184
	5.6×10^{-1}		Li et al. (2014)	Q	241
	6.0×10^{-1}		Hilal et al. (2008)	Q	
	8.0×10^{-1}		Modarresi et al. (2007)	Q	67
	6.7×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	4.7×10^{-1}		Katritzky et al. (1998)	Q	
	5.4×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	3.7×10^{-1}		Russell et al. (1992)	Q	279
	8.0×10^{-1}		Suzuki et al. (1992)	Q	403, 232
	5.6×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	5.6×10^{-1}		Mackay et al. (2006d)	?	
	5.7×10^{-1}		Abraham et al. (1990)	?	
diethylamine $(C_2H_5)_2NH$ [109-89-7] HPNMFZURTQLUMO-UHFFFAOYSA-N	3.8×10^{-1}		Burkholder et al. (2019)	L	
	3.8×10^{-1}		Burkholder et al. (2015)	L	
	3.7×10^{-1}		Brockbank (2013)	L	
	3.9×10^{-1}		Christie and Crisp (1967)	M	
	4.1×10^{-1}	7700	Bagno et al. (1991)	T	473
	2.9×10^{-1}		Yaws (2003)	X	258
	1.3	10000	Goldstein (1982)	X	298
	5.2×10^{-2}		Dupeux et al. (2022)	Q	259
	1.2×10^{-1}		Keshavarz et al. (2022)	Q	
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	2.5×10^{-1}		Modarresi et al. (2007)	Q	67
	5.2×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	2.5×10^{-1}		Yao et al. (2002)	Q	229
	3.1×10^{-1}		English and Carroll (2001)	Q	230, 231
	1.5×10^{-1}		Katritzky et al. (1998)	Q	
	1.5×10^{-1}		Russell et al. (1992)	Q	358
	4.7×10^{-1}		Suzuki et al. (1992)	Q	232
	3.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	3.8×10^{-1}		Mackay et al. (2006d)	?	
	1.4×10^{-1}		Yaws (1999)	?	21
	1.5×10^{-1}		Yaws and Yang (1992)	?	21
	3.9×10^{-1}		Abraham et al. (1990)	?	

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dipropylamine	2.0×10^{-1}		Burkholder et al. (2019)	L	
$(C_3H_7)_2NH$	2.0×10^{-1}		Burkholder et al. (2015)	L	
[142-84-7]	2.1×10^{-1}		Brockbank (2013)	L	
WEHWNAOGRSTTBQ-UHFFFAOYSA-N	1.2×10^{-1}	8900	Leng et al. (2015a)	M	
	1.9×10^{-1}		Christie and Crisp (1967)	M	
	2.3×10^{-1}		Keshavarz et al. (2022)	Q	
	2.2×10^{-1}		Duchowicz et al. (2020)	Q	
	7.0×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.1×10^{-1}		Hilal et al. (2008)	Q	
	2.7×10^{-1}		Modarresi et al. (2007)	Q	67
		6900	Kühne et al. (2005)	Q	
	2.1×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	9.6×10^{-2}		Yao et al. (2002)	Q	229
	1.9×10^{-1}		English and Carroll (2001)	Q	230, 260
	1.1×10^{-1}		Katritzky et al. (1998)	Q	
	2.3×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	2.8×10^{-1}		Suzuki et al. (1992)	Q	232
	1.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		8100	Kühne et al. (2005)	?	
	1.1×10^{-1}		Yaws (1999)	?	21, 551
	1.9×10^{-1}		Abraham et al. (1990)	?	
			Betterton (1992)	W	552
N-methylpropanamine	1.9×10^{-1}		Hilal et al. (2008)	Q	
$C_4H_{11}N$					
[627-35-0]					
GVWISOJSERXQBM-UHFFFAOYSA-N					
N-methyl-2-propanamine	1.6×10^{-1}		Gharagheizi et al. (2012)	Q	
$C_4H_{11}N$	1.4×10^{-1}		Hilal et al. (2008)	Q	
[4747-21-1]					
XHFGWHUWQXTGAT-UHFFFAOYSA-N					
N-(1-methylethyl)-2-propanamine	1.0×10^{-1}		Duchowicz et al. (2020)	V	186
$C_6H_{15}N$	1.3×10^{-1}		Yaws (2003)	X	237
(diisopropylamine)	3.3×10^{-2}		Duchowicz et al. (2020)	Q	
[108-18-9]	1.4×10^{-1}		Gharagheizi et al. (2010)	Q	246
UAOMVDZJSHZZME-UHFFFAOYSA-N	6.2×10^{-2}		Hilal et al. (2008)	Q	
	4.1×10^{-1}		Modarresi et al. (2007)	Q	67
		6900	Kühne et al. (2005)	Q	
	9.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	9.5×10^{-2}		English and Carroll (2001)	Q	230, 274
	6.7×10^{-2}		Katritzky et al. (1998)	Q	
	1.8×10^{-1}		Nirmalakhandan et al. (1997)	Q	
		8600	Kühne et al. (2005)	?	
	9.2×10^{-2}		Abraham et al. (1990)	?	

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
N,N-dipropyl-1-propanamine	2.6×10^{-2}		Duchowicz et al. (2020)	V	186
$C_9H_{21}N$	2.6×10^{-2}		HSDB (2015)	V	
(tripropylamine)	2.6×10^{-2}		Yaws (2003)	X	237
[102-69-2]	2.6×10^{-2}		Hilal et al. (2008)	C	
YFTHZRPMJXBUME-UHFFFAOYSA-N	5.1×10^{-2}		Duchowicz et al. (2020)	Q	
	3.6×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.4×10^{-2}		Gharagheizi et al. (2010)	Q	246
	6.7×10^{-2}		Hilal et al. (2008)	Q	
	1.3×10^{-2}		Modarresi et al. (2007)	Q	67
	2.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.1×10^{-2}		Yao et al. (2002)	Q	229
	4.2×10^{-2}		Katritzky et al. (1998)	Q	
	2.6×10^{-2}		Yaws (1999)	?	21
N-methyl-1-butanamine	1.3×10^{-1}		Yaws (2003)	X	237
$C_5H_{13}N$	5.7×10^{-2}		Gharagheizi et al. (2012)	Q	
(N-methylbutylamine)	1.4×10^{-1}		Gharagheizi et al. (2010)	Q	246
[110-68-9]	1.1×10^{-1}		Hilal et al. (2008)	Q	
QCOGKXLOEWLIDC-UHFFFAOYSA-N		6600	Kühne et al. (2005)	Q	
		5000	Kühne et al. (2005)	?	
dibutylamine	1.3×10^{-1}		Brockbank (2013)	L	
$(C_4H_9)_2NH$	1.0		Altschuh et al. (1999)	M	
[111-92-2]	1.1×10^{-1}		Christie and Crisp (1967)	M	
JQVDAXLFBXTEQA-UHFFFAOYSA-N	1.2×10^{-1}		Mackay et al. (2006d)	V	
	1.2×10^{-1}		Mackay et al. (1995)	V	
	7.0×10^{-2}		Yaws (2003)	X	237
	4.1×10^{-1}		Keshavarz et al. (2022)	Q	
	2.2×10^{-1}		Duchowicz et al. (2020)	Q	299
	4.5×10^{-2}		Gharagheizi et al. (2012)	Q	
	7.6×10^{-2}		Gharagheizi et al. (2010)	Q	246
	2.4×10^{-1}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Modarresi et al. (2007)	Q	67
		7600	Kühne et al. (2005)	Q	
	9.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	6.2×10^{-2}		Yao et al. (2002)	Q	229
	1.2×10^{-1}		English and Carroll (2001)	Q	230, 231
	8.8×10^{-2}		Katritzky et al. (1998)	Q	
	1.4×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.6×10^{-1}		Suzuki et al. (1992)	Q	232
	1.1×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		7400	Kühne et al. (2005)	?	
	7.0×10^{-2}		Yaws (1999)	?	21
	9.7×10^{-2}		Abraham et al. (1990)	?	

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
diisobutylamine	1.8×10^{-2}		Duchowicz et al. (2020)	V	186
$C_8H_{19}N$	4.3×10^{-2}		Yaws (2003)	X	237
[110-96-3]	3.4×10^{-2}		Duchowicz et al. (2020)	Q	
NJBCRXCAPCODGX-UHFFFAOYSA-N	6.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
	1.5×10^{-1}		Modarresi et al. (2007)	Q	67
		7600	Kühne et al. (2005)	Q	
	1.8×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.5×10^{-2}		Katritzky et al. (1998)	Q	
		7300	Kühne et al. (2005)	?	
bis-(1-methylpropyl)-amine		7600	Kühne et al. (2005)	Q	
$C_8H_{19}N$		7000	Kühne et al. (2005)	?	
(di-*sec*-butylamine)					
[626-23-3]					
OBYVIBDTOCAXSN-UHFFFAOYSA-N					
tetraethylenepentamine	3.3×10^{14}		HSDB (2015)	Q	99
$C_8H_{23}N_5$					
[112-57-2]					
FAGUFWYHJQFNRV-UHFFFAOYSA-N					
N,N-di-2-propenyl-2-propen-1-amine	3.9×10^{-2}	7500	Brockbank (2013)	L	1
$C_9H_{15}N$	3.8×10^{-2}		Duchowicz et al. (2020)	V	186
(triallylamine)	3.8×10^{-2}		HSDB (2015)	V	
[102-70-5]	2.2		Duchowicz et al. (2020)	Q	
VPYJNCGUESNPMV-UHFFFAOYSA-N					
trimethylamine	9.9×10^{-2}		Burkholder et al. (2019)	L	
$(CH_3)_3N$	9.9×10^{-2}		Burkholder et al. (2015)	L	
[75-50-3]	8.4×10^{-2}	6300	Leng et al. (2015a)	M	
GETQZCLCWQTVFV-UHFFFAOYSA-N	9.4×10^{-1}	4200	Tsuji et al. (1990)	M	62
	7.6×10^{-2}		Amoore and Buttery (1978)	M	
	9.5×10^{-2}		Christie and Crisp (1967)	M	
	9.8×10^{-2}		Amoore and Buttery (1978)	V	
	1.0×10^{-1}		Hayer et al. (2022)	Q	20
	9.2×10^{-2}		Keshavarz et al. (2022)	Q	
	1.3		Duchowicz et al. (2020)	Q	
	3.7×10^{-2}		Hilal et al. (2008)	Q	
	3.3×10^{-2}		Modarresi et al. (2007)	Q	67
	9.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	8.4×10^{-2}		English and Carroll (2001)	Q	230, 231
	1.6×10^{-1}		Katritzky et al. (1998)	Q	
	4.7×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	6.4×10^{-2}		Russell et al. (1992)	Q	279
	1.2×10^{-1}		Suzuki et al. (1992)	Q	232
	9.5×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	1.5×10^{-1}		Mackay et al. (2006d)	?	
	9.0×10^{-2}		Abraham et al. (1990)	?	

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
triethylamine	6.6×10^{-2}		Burkholder et al. (2019)	L	
$(C_2H_5)_3N$	6.6×10^{-2}		Burkholder et al. (2015)	L	
[121-44-8]	9.3×10^{-2}		Brockbank (2013)	L	
ZMANZCXQSJIPKH-UHFFFAOYSA-N	5.0×10^{-2}	8300	Leng et al. (2015b)	M	
	6.6×10^{-2}		Christie and Crisp (1967)	M	
	7.1×10^{-2}		Mackay et al. (2006d)	V	
	7.1×10^{-2}		Mackay et al. (1995)	V	
	8.6×10^{-2}		Yaws (2003)	X	258
	8.5×10^{-2}		Yaws (2003)	X	237
	5.0×10^{-3}		Dupeux et al. (2022)	Q	259
	9.2×10^{-3}		Hayer et al. (2022)	Q	20
	2.3×10^{-1}		Keshavarz et al. (2022)	Q	
	5.1×10^{-2}		Duchowicz et al. (2020)	Q	299
	6.7×10^{-2}		Li et al. (2014)	Q	241
	9.5×10^{-2}		Gharagheizi et al. (2010)	Q	246
	8.6×10^{-2}		Hilal et al. (2008)	Q	
	2.3×10^{-2}		Modarresi et al. (2007)	Q	67
		6700	Kühne et al. (2005)	Q	
	2.1×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	7.8×10^{-2}		Yao et al. (2002)	Q	229
	1.3×10^{-1}		English and Carroll (2001)	Q	230, 231
	8.8×10^{-2}		Katritzky et al. (1998)	Q	
	3.3×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	3.1×10^{-2}		Russell et al. (1992)	Q	279
	6.1×10^{-2}		Suzuki et al. (1992)	Q	232
	6.6×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		9000	Kühne et al. (2005)	?	
	8.5×10^{-2}		Yaws (1999)	?	21
	9.2×10^{-2}		Abraham et al. (1990)	?	
tributylamine	3.7×10^{-1}	8700	Brockbank (2013)	L	1
$C_{12}H_{27}N$	4.0×10^{-1}		Altschuh et al. (1999)	M	
[102-82-9]	6.2×10^{-2}		Duchowicz et al. (2020)	V	186
IMFACGCPASFAPR-UHFFFAOYSA-N	4.0×10^{-5}		Mackay et al. (2006d)	V	
	4.0×10^{-5}		Mackay et al. (1995)	V	
	4.9×10^{-2}		Yaws (2003)	X	237
	5.2×10^{-2}		Duchowicz et al. (2020)	Q	
	2.9×10^{-2}		Gharagheizi et al. (2010)	Q	246
		8700	Kühne et al. (2005)	Q	
		7500	Kühne et al. (2005)	?	
	6.1×10^{-2}		Yaws (1999)	?	21
N,N-dimethyl-1-dodecanamine	>4.0		Altschuh et al. (1999)	M	
$C_{14}H_{31}N$	4.6×10^{-2}		Yaws (2003)	X	237
[112-18-5]	2.0×10^{-3}		HSDB (2015)	Q	99
YWFWDNVOPHGWMX-UHFFFAOYSA-N	4.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.5×10^{-2}		Gharagheizi et al. (2010)	Q	246

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Table A4.1: Amines (C, H, N) (. . . continued)

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ethylenediamine	1.8×10^{3}	6700	Nguyen (2013)	M	11
$H_2NCH_2CH_2NH_2$	5.8×10^{3}		Westheimer and Ingraham (1956)	M	
[107-15-3]	1.5×10^{2}	9200	Cabani et al. (1978)	T	
PIICEJLVQHRZGT-UHFFFAOYSA-N	6.7×10^{3}		Keshavarz et al. (2022)	Q	
	2.2×10^{3}		Duchowicz et al. (2020)	Q	
	5.6×10^{3}		Hilal et al. (2008)	Q	
	1.4×10^{4}		Modarresi et al. (2007)	Q	67
	6.2×10^{2}		Yao et al. (2002)	Q	229
	5.7×10^{3}		Duchowicz et al. (2020)	?	185, 21
	2.3×10^{2}		Yaws (1999)	?	21, 12
2-propen-1-amine	1.0	5400	Leng et al. (2015a)	M	
C_3H_7N	5.4×10^{-1}		Duchowicz et al. (2020)	V	186
(allylamine)	5.4×10^{-1}		HSDB (2015)	V	
[107-11-9]	5.4×10^{-1}		Hilal et al. (2008)	C	
VVJKKWFAADXIJK-UHFFFAOYSA-N	7.7		Duchowicz et al. (2020)	Q	
	2.4		Hilal et al. (2008)	Q	
	4.4		Modarresi et al. (2007)	Q	67
di-2-propenylamine	3.3×10^{-1}		Duchowicz et al. (2020)	V	186
$C_6H_{11}N$	3.3×10^{-1}		HSDB (2015)	V	
(diallylamine)	2.6		Duchowicz et al. (2020)	Q	
[124-02-7]		7200	Kühne et al. (2005)	Q	
DYUWTXWIYMHBQS-UHFFFAOYSA-N		8000	Kühne et al. (2005)	?	
hexamethyleneimine	1.6	8200	Cabani et al. (1971a)	T	
$(CH_2)_6NH$	1.0		Keshavarz et al. (2022)	Q	
[111-49-9]	1.3×10^{1}		Duchowicz et al. (2020)	Q	184
ZSIQJIWKELUFRJ-UHFFFAOYSA-N	6.4		Hilal et al. (2008)	Q	
	3.5×10^{-1}		Modarresi et al. (2007)	Q	67
	1.2		Suzuki et al. (1992)	Q	232
	4.3×10^{-1}		Meylan and Howard (1991)	Q	
	1.6		Duchowicz et al. (2020)	?	185, 21
cyclohexanamine	2.2	7500	Brockbank (2013)	L	1
$C_6H_{13}N$	2.4		Altschuh et al. (1999)	M	
(cyclohexylamine)	2.2	7800	Bernauer et al. (2006)	V	1
[108-91-8]	9.4×10^{-1}		Amoore and Buttery (1978)	V	
PAFZNILMFXTMIY-UHFFFAOYSA-N	3.3		Keshavarz et al. (2022)	Q	
	7.3		Duchowicz et al. (2020)	Q	299
	6.7×10^{-1}		Hilal et al. (2008)	Q	
	4.2		Modarresi et al. (2007)	Q	67
	9.5×10^{-1}		English and Carroll (2001)	Q	230, 231
	1.2		Nirmalakhandan et al. (1997)	Q	
	2.4		Duchowicz et al. (2020)	?	185, 21
	9.5×10^{-1}		Abraham et al. (1990)	?	

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methylcyclohexylamine $C_7H_{15}N$ [6850-35-7] JYDYHSHPBDZRPU-UHFFFAOYSA-N	1.1		Hilal et al. (2008)	Q	
N-ethylcyclohexanamine $C_8H_{17}N$ (N-ethylcyclohexylamine) [5459-93-8] AGVKXDPPPSLISR-UHFFFAOYSA-N		7200 6500	Kühne et al. (2005) Kühne et al. (2005)	Q ?	
N,N-dimethylcyclohexylamine $C_8H_{17}N$ [98-94-2] SVYKKECYCPFKGB-UHFFFAOYSA-N	4.2×10^{-1} 4.1×10^{-1} 1.4 5.1×10^{-1} 8.5×10^{-2} 4.2×10^{-1} 	 7000 8500	Altschuh et al. (1999) Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Kühne et al. (2005) Duchowicz et al. (2020) Kühne et al. (2005)	M Q Q Q Q Q ? ?	 299 67 185, 21
hexamethylenetetramine $C_6H_{12}N_4$ [100-97-0] VKYKSIONXSXAKP-UHFFFAOYSA-N	6.2×10^{3} 6.1×10^{-5} 5.8×10^{5} 9.2×10^{2} 5.4×10^{7} 1.3×10^{4} 5.8×10^{3}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Hilal et al. (2008) Modarresi et al. (2007)	V Q Q Q Q Q Q	 287, 288 287, 289 287, 290 287, 291 67
1-decanamine $C_{10}H_{23}N$ [2016-57-1] MHZGKXUYDGKKIU-UHFFFAOYSA-N	2.6×10^{-1} 1.5×10^{-1} 2.4		Duchowicz et al. (2020) Yaws et al. (2001) Duchowicz et al. (2020)	V X Q	186 350
N-cyclohexylcyclohexanamine $C_{12}H_{23}N$ (dicyclohexylamine) [101-83-7] XBPCUCUWBYBCDP-UHFFFAOYSA-N	1.8×10^{-1}		HSDB (2015)	Q	99
1-dodecanamine $C_{12}H_{27}N$ [124-22-1] JRBPAEWTRLWTQC-UHFFFAOYSA-N	3.7×10^{-2}		HSDB (2015)	Q	99
1-octadecanamine $C_{18}H_{39}N$ [124-30-1] REYJJPSVUYRZGE-UHFFFAOYSA-N	1.0×10^{-2}		HSDB (2015)	Q	99

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N,N-dioctyl-1-octanamine $C_{24}H_{51}N$ (tri-N-octylamine) [1116-76-3] XTAZYLNFDRKIHJ-UHFFFAOYSA-N	7.0×10^{-4}		HSDB (2015)	Q	99
aminobenzene	4.9	6800	Brockbank (2013)	L	1
C_6H_7N	4.4		Chao et al. (2017)	M	
(aniline)	5.2		Altschuh et al. (1999)	M	
[62-53-3]	1.2		Heal et al. (1995)	M	373
PAYRUJLWNCNPSJ-UHFFFAOYSA-N	5.0		Jayasinghe et al. (1992)	M	
	1.1		Dallos et al. (1983)	M	553
	4.4		Chao et al. (2017)	V	
	4.6	6500	Bernauer et al. (2006)	V	1
	6.0		Mackay et al. (2006d)	V	
	6.0		Schüürmann (2000)	V	
	7.1×10^{-5}		Lide and Frederikse (1995)	V	
	6.0		Mackay et al. (1995)	V	
	5.5		Hwang et al. (1992)	V	
	3.4		Yoshida et al. (1983)	V	
	5.8		Yaws (2003)	X	258
	7.1×10^{-5}		Howard (1989)	X	364
	5.7		Yaws (2003)	X	237
	8.2×10^{-2}		Howard (1989)	X	412
	2.4		Dupeux et al. (2022)	Q	259
	3.3		Keshavarz et al. (2022)	Q	
	5.1		Duchowicz et al. (2020)	Q	299
	1.8×10^{1}		Gharagheizi et al. (2012)	Q	
	5.5		Gharagheizi et al. (2010)	Q	246
	5.1		Hilal et al. (2008)	Q	
	4.2		Modarresi et al. (2007)	Q	67
		6200	Kühne et al. (2005)	Q	
	4.8		Yaffe et al. (2003)	Q	248, 249
	2.4		Yao et al. (2002)	Q	229
	3.0		Katritzky et al. (1998)	Q	
	4.9		Duchowicz et al. (2020)	?	185, 21
	8.2×10^{-2}		Mackay et al. (2006d)	?	
		7100	Kühne et al. (2005)	?	
	5.8		Yaws (1999)	?	21
	4.3		Abraham et al. (1990)	?	
benzylamine	7.1×10^{-1}		Yao et al. (2002)	Q	229
C_7H_9N	3.4×10^{-1}		Yaws (1999)	?	21
[100-46-9]					
WGQKYBSKWIADBV-UHFFFAOYSA-N					

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methylbenzenamine	4.8	7100	Brockbank (2013)	L	1
C_7H_9N	3.0		Chao et al. (2017)	M	
(2-methylaniline; *o*-toluidine)	5.0		Altschuh et al. (1999)	M	
[95-53-4]	4.0		Chao et al. (2017)	V	
RNVCVTLRINQCPJ-UHFFFAOYSA-N	1.1×10^{1}		Mackay et al. (2006d)	V	
	4.1		Schüürmann (2000)	V	
	1.1×10^{1}		Mackay et al. (1995)	V	
	1.1×10^{1}		Mackay et al. (1995)	V	
	3.4		Yoshida et al. (1983)	V	
	4.6		Abraham et al. (1994a)	R	
	4.1		Yaws (2003)	X	237
	3.0×10^{-1}		Keshavarz et al. (2022)	Q	
	2.7		Duchowicz et al. (2020)	Q	299
	3.3		Gharagheizi et al. (2012)	Q	
	4.4		Gharagheizi et al. (2010)	Q	246
	3.1		Hilal et al. (2008)	Q	
	1.0		Modarresi et al. (2007)	Q	67
	1.6		Yao et al. (2002)	Q	229
	4.0		English and Carroll (2001)	Q	230, 231
	4.4		Katritzky et al. (1998)	Q	
	2.0		Nirmalakhandan et al. (1997)	Q	
	5.0		Duchowicz et al. (2020)	?	185, 21
	4.1		Yaws (1999)	?	21
3-methylbenzenamine	5.6	7200	Brockbank (2013)	L	1
C_7H_9N	3.2		Chao et al. (2017)	M	
(3-methylaniline; *m*-toluidine)	5.9		Altschuh et al. (1999)	M	
[108-44-1]	3.9		Chao et al. (2017)	V	
JJYPMNFTHPTTDI-UHFFFAOYSA-N	3.9		Mackay et al. (2006d)	V	
	3.9		Mackay et al. (1995)	V	
	5.1		Yaws (2003)	X	237, 12
	4.5		Keshavarz et al. (2022)	Q	
	2.7		Duchowicz et al. (2020)	Q	299
	4.7		Gharagheizi et al. (2012)	Q	
	4.4		Gharagheizi et al. (2010)	Q	246
	4.8		Hilal et al. (2008)	Q	
	3.9		Modarresi et al. (2007)	Q	67
	1.5		Yao et al. (2002)	Q	229
	6.4		Katritzky et al. (1998)	Q	
	5.9		Duchowicz et al. (2020)	?	185, 21
	3.5		Yaws (1999)	?	21, 12

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methylbenzenamine	2.9	4400	Brockbank (2013)	L	1
C_7H_9N	4.4		Chao et al. (2017)	M	
(4-methylaniline; *p*-toluidine)	1.3×10^{1}		Altschuh et al. (1999)	M	
[106-49-0]	4.4		Jayasinghe et al. (1992)	M	
RZXMPPFPUUCRFN-UHFFFAOYSA-N	1.5		Mackay et al. (2006d)	V	
	1.5		Mackay et al. (1995)	V	
	1.6		Yoshida et al. (1983)	V	
	5.0		Abraham et al. (1994a)	R	
	4.5		Keshavarz et al. (2022)	Q	
	2.7		Duchowicz et al. (2020)	Q	
	3.9		Gharagheizi et al. (2012)	Q	
	5.3		Hilal et al. (2008)	Q	
	5.0		Modarresi et al. (2007)	Q	67
	4.0		English and Carroll (2001)	Q	230, 231
	6.1		Katritzky et al. (1998)	Q	
	2.0		Nirmalakhandan et al. (1997)	Q	
	4.9		Duchowicz et al. (2020)	?	185, 21
2-ethylaniline	2.6	7300	Brockbank (2013)	L	1, 554
$C_8H_{11}N$	2.7		HSDB (2015)	Q	99
(*o*-ethylaniline)		7200	Kühne et al. (2005)	Q	
[578-54-1]		7500	Kühne et al. (2005)	?	
MLPVBIWIRCKMJV-UHFFFAOYSA-N					
4-ethylaniline	3.1		Mackay et al. (2006d)	V	
$C_8H_{11}N$	3.1		Mackay et al. (1995)	V	
(*p*-ethylaniline)		6900	Kühne et al. (2005)	Q	
[589-16-2]		8100	Kühne et al. (2005)	?	
HRXZRAXKKNUKRF-UHFFFAOYSA-N					
2,4-dimethylbenzenamine	2.8	7700	Brockbank (2013)	L	1
$C_8H_{11}N$	2.4		Mackay et al. (2006d)	V	
(2,4-dimethylaniline; 2,4-xylidine)	1.4×10^{-1}		Schüürmann (2000)	V	
[95-68-1]	2.4		Mackay et al. (1995)	V	
CZZZABOKJQXEBO-UHFFFAOYSA-N	3.9		HSDB (2015)	Q	99
		7200	Kühne et al. (2005)	Q	
		7400	Kühne et al. (2005)	?	
3,4-dimethylbenzenamine	5.3		Jayasinghe et al. (1992)	M	
$C_8H_{11}N$	6.0		Keshavarz et al. (2022)	Q	
(3,4-dimethylaniline; 3,4-xylidine)	1.4		Duchowicz et al. (2020)	Q	
[95-64-7]	6.7		Hilal et al. (2008)	Q	
DOLQYFPDPKPQSS-UHFFFAOYSA-N	1.6		Modarresi et al. (2007)	Q	67
	9.0		Katritzky et al. (1998)	Q	
	5.3		Duchowicz et al. (2020)	?	185, 21

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
2,5-dimethylbenzenamine	2.3		Duchowicz et al. (2020)	V	186
$C_8H_{11}N$	1.4		Duchowicz et al. (2020)	Q	
(2,5-dimethylaniline; 2,5-xylidine)	3.9		HSDB (2015)	Q	99
[95-78-3]	7.7×10^{-1}		Modarresi et al. (2007)	Q	67
VOWZNBNDMFLQGM-UHFFFAOYSA-N		7200	Kühne et al. (2005)	Q	
		7700	Kühne et al. (2005)	?	
2,6-dimethylbenzenamine	3.9		Duchowicz et al. (2020)	V	186
$C_8H_{11}N$	3.9		HSDB (2015)	V	
(2,6-dimethylaniline; 2,6-xylidine)	5.8×10^{-2}		Mackay et al. (2006d)	V	
[87-62-7]	5.8×10^{-2}		Mackay et al. (1995)	V	
UFFBMTHBGFGIHF-UHFFFAOYSA-N	2.7		Abraham et al. (1994a)	R	
	2.9×10^{-1}		Duchowicz et al. (2020)	Q	
	3.3		Hilal et al. (2008)	Q	
	1.7×10^{1}		Modarresi et al. (2007)	Q	67
		7500	Kühne et al. (2005)	Q	
	2.1		English and Carroll (2001)	Q	230, 231
	4.2		Katritzky et al. (1998)	Q	
	1.4		Nirmalakhandan et al. (1997)	Q	
		7600	Kühne et al. (2005)	?	
2,4,5-trimethylbenzenamine	3.9		Jayasinghe et al. (1992)	M	
$C_9H_{13}N$	5.5×10^{-1}		Keshavarz et al. (2022)	Q	
(2,4,5-trimethylaniline)	7.3×10^{-1}		Duchowicz et al. (2020)	Q	184
[137-17-7]	6.0		Hilal et al. (2008)	Q	
BMIPMKQAAJKBKP-UHFFFAOYSA-N	3.5×10^{-1}		Modarresi et al. (2007)	Q	67
	4.0		Duchowicz et al. (2020)	?	185, 21
2-(1-methylethyl)-benzenamine		7500	Kühne et al. (2005)	Q	
$C_9H_{13}N$		6400	Kühne et al. (2005)	?	
(2-isopropylaniline)					
[643-28-7]					
YKOLZVXSPGIIBJ-UHFFFAOYSA-N					
2,6-diethylbenzenamine	8.8		Duchowicz et al. (2020)	V	186
$C_{10}H_{15}N$	9.0		HSDB (2015)	V	
(2,6-diethylaniline)	3.0×10^{-1}		Duchowicz et al. (2020)	Q	
[579-66-8]	9.0×10^{-1}		Hilal et al. (2008)	Q	
FOYHNROGBXVLLX-UHFFFAOYSA-N	6.8		Modarresi et al. (2007)	Q	67
	8.8		Yaffe et al. (2003)	Q	248, 249
	5.0		Katritzky et al. (1998)	Q	
	8.8		Yaws (1999)	?	21, 402
1,2-benzenediamine	1.4×10^{3}		Duchowicz et al. (2020)	V	186
$C_6H_8N_2$	1.4×10^{3}		HSDB (2015)	V	
(*o*-phenylenediamine)	7.6×10^{1}		Schüürmann (2000)	V	
[95-54-5]	1.0×10^{2}		Yaws (2003)	X	237, 555
GEYOCULIXLDCMW-UHFFFAOYSA-N	2.9×10^{3}		Duchowicz et al. (2020)	Q	
	1.2×10^{2}		Gharagheizi et al. (2012)	Q	
	1.0×10^{2}		Gharagheizi et al. (2010)	Q	246

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	1.2×10^{3}		Hilal et al. (2008)	Q	
1,3-benzenediamine	7.9×10^{3}		Duchowicz et al. (2020)	V	186
$C_6H_8N_2$	7.6×10^{3}		HSDB (2015)	V	
(m-phenylenediamine)	1.3×10^{4}		Schüürmann (2000)	V	
[108-45-2]	6.9×10^{3}		Yaws (2003)	X	237
WZCQRUWWHSTZEM-UHFFFAOYSA-N	2.8×10^{3}		Duchowicz et al. (2020)	Q	
	2.8×10^{2}		Gharagheizi et al. (2012)	Q	
	2.2×10^{3}		Gharagheizi et al. (2010)	Q	246
	1.1×10^{5}		Hilal et al. (2008)	Q	
	3.7×10^{4}		Modarresi et al. (2007)	Q	67
1,4-benzenediamine	7.1×10^{2}		Yaws (2003)	X	237, 79
$C_6H_8N_2$	1.5×10^{4}		HSDB (2015)	Q	99
(p-phenylenediamine)	1.7×10^{2}		Gharagheizi et al. (2012)	Q	
[106-50-3]	2.2×10^{3}		Gharagheizi et al. (2010)	Q	246
CBCKQZAAMUWICA-UHFFFAOYSA-N					
2-methyl-1,3-benzenediamine	1.3×10^{4}		HSDB (2015)	Q	99
$C_7H_{10}N_2$					
[823-40-5]					
RLYCRLGLCUXUPO-UHFFFAOYSA-N					
2-methyl-1,4-benzenediamine	1.3×10^{4}		HSDB (2015)	Q	99
$C_7H_{10}N_2$					
[95-70-5]					
OBCSAIDCZQSFQH-UHFFFAOYSA-N					
3-methyl-1,2-benzenediamine	1.0×10^{4}		HSDB (2015)	Q	99
$C_7H_{10}N_2$					
(2,3-diaminotoluene)					
[2687-25-4]					
AXNUJYHFQHQZBE-UHFFFAOYSA-N					
4-methyl-1,3-benzenediamine	1.0×10^{4}		HSDB (2015)	Q	99
$C_7H_{10}N_2$					
(toluene-2,4-diamine)					
[95-80-7]					
VOZKAJLKRJDJLL-UHFFFAOYSA-N					
3,5-diaminotoluene	1.3×10^{4}		HSDB (2015)	Q	545
$C_7H_{10}N_2$					
[108-71-4]					
LVNDUJYMLJDECN-UHFFFAOYSA-N					
phenylhydrazine	2.2×10^{3}		Duchowicz et al. (2020)	V	186
$C_6H_8N_2$	3.4×10^{2}		HSDB (2015)	V	
[100-63-0]	9.6		Duchowicz et al. (2020)	Q	
HKOOXMFOFWEVGF-UHFFFAOYSA-N	6.9×10^{2}		Hilal et al. (2008)	Q	
	8.3×10^{3}		Modarresi et al. (2007)	Q	67

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(methylamino)-benzene	8.7×10^{-1}		HSDB (2015)	V	
C_7H_9N	8.7×10^{-1}		Schüürmann (2000)	V	
(N-methylaniline)	1.1		Abraham et al. (1994a)	R	
[100-61-8]	3.0×10^{-1}		Keshavarz et al. (2022)	Q	
AFBPFSWMIHJQDM-UHFFFAOYSA-N	3.7		Duchowicz et al. (2020)	Q	299
	1.5		Hilal et al. (2008)	Q	
	5.7×10^{-1}		Modarresi et al. (2007)	Q	67
	6.1×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	2.0		Yao et al. (2002)	Q	229
	7.3×10^{-1}		English and Carroll (2001)	Q	230, 231
	4.5		Katritzky et al. (1998)	Q	
	2.7		Nirmalakhandan et al. (1997)	Q	
	1.1		Duchowicz et al. (2020)	?	185, 21
	8.7×10^{-1}		Yaws (1999)	?	21
(ethylamino)-benzene	8.1×10^{-1}	7900	Brockbank (2013)	L	1, 556
$C_8H_{11}N$	1.0		Altschuh et al. (1999)	M	
(N-ethylaniline)	4.1×10^{-1}		Keshavarz et al. (2022)	Q	
[103-69-5]	1.3		Duchowicz et al. (2020)	Q	184
OJGMBLNIHDZDGS-UHFFFAOYSA-N	6.2×10^{-1}		HSDB (2015)	Q	99
	7.0×10^{-1}		Hilal et al. (2008)	Q	
	9.5×10^{-1}		Modarresi et al. (2007)	Q	67
		7100	Kühne et al. (2005)	Q	
	6.1×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	3.1		Katritzky et al. (1998)	Q	
	1.0		Duchowicz et al. (2020)	?	185, 21
		7600	Kühne et al. (2005)	?	
(dimethylamino)-benzene	1.7×10^{-1}		HSDB (2015)	V	
$C_8H_{11}N$	8.5×10^{-2}		Mackay et al. (2006d)	V	
(N,N-dimethylaniline)	8.5×10^{-2}		Mackay et al. (1995)	V	
[121-69-7]	1.3×10^{-1}		Meylan and Howard (1991)	V	
JLTDJTHDQAWBAV-UHFFFAOYSA-N	1.6×10^{-1}		Yoshida et al. (1983)	V	
	9.9×10^{-2}		Hilal et al. (2008)	Q	
	1.0×10^{-1}		Modarresi et al. (2007)	Q	67
		6900	Kühne et al. (2005)	Q	
	1.4×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.5		Katritzky et al. (1998)	Q	
	2.4		Nirmalakhandan et al. (1997)	Q	
	1.1		Meylan and Howard (1991)	Q	
		6300	Kühne et al. (2005)	?	
	9.7×10^{-2}		Yaws (1999)	?	21
	1.4×10^{-1}		Abraham et al. (1990)	?	

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benzeneethanamine $C_8H_{11}N$ (2-phenylethylamine) [64-04-0] BHHGXPLMPWCGHP-UHFFFAOYSA-N	1.2×10^1		HSDB (2015)	Q	99
2,3-dimethylbenzenamine $C_8H_{11}N$ (2,3-xylidine) [87-59-2] VVAKEQGKZNKUSU-UHFFFAOYSA-N	3.9		HSDB (2015)	Q	99
3,5-dimethylbenzenamine $C_8H_{11}N$ [108-69-0] MKARNSWMMBGSHX-UHFFFAOYSA-N	3.9		HSDB (2015)	Q	99
dimethylaniline $C_8H_{11}N$ (xylidine) [1300-73-8] CDULGHZNHURECF-UHFFFAOYSA-N	3.9		HSDB (2015)	Q	99
phenelzine $C_8H_{12}N_2$ [51-71-8] RMUCZJUITONUFY-UHFFFAOYSA-N	2.9×10^3		HSDB (2015)	Q	99
N,N-dimethyl-1,4-benzenediamine $C_8H_{12}N_2$ [99-98-9] BZORFPDSXLZWJF-UHFFFAOYSA-N	3.3×10^2		HSDB (2015)	Q	99
2,4,6-trimethylbenzenamine $C_9H_{13}N$ (2,4,6-trimethylaniline) [88-05-1] KWVPRPSXBZNOHS-UHFFFAOYSA-N	3.7		HSDB (2015)	Q	99
N-ethyl-3-methylbenzenamine $C_9H_{13}N$ [102-27-2] GUYMMHOQXYZMJQ-UHFFFAOYSA-N	1.6		HSDB (2015)	Q	99
N-(1-methylethyl)benzenamine $C_9H_{13}N$ [768-52-5] FRCFWPVMFJMNDP-UHFFFAOYSA-N	1.3		HSDB (2015)	Q	99

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
2-ethyl-6-methylbenzenamine	3.2		Zhang et al. (2010)	Q	287, 288
$C_9H_{13}N$	2.1		Zhang et al. (2010)	Q	287, 289
[24549-06-2]	1.0		Zhang et al. (2010)	Q	287, 290
JJVKJJNCIILLRP-UHFFFAOYSA-N	8.4×10^{-1}		Zhang et al. (2010)	Q	287, 291
N,N-dimethylbenzylamine		7700	Kühne et al. (2005)	Q	
$C_9H_{13}N$		7700	Kühne et al. (2005)	?	
[103-83-3]					
XXBDWLFCJWSEKW-UHFFFAOYSA-N					
N,N,4-trimethylbenzenamine	2.0×10^{-1}		Duchowicz et al. (2020)	V	186
$C_9H_{13}N$	1.1×10^{-1}		Duchowicz et al. (2020)	Q	
[99-97-8]	1.4×10^{-1}		Hilal et al. (2008)	Q	
GYVGXEWAOAAJEU-UHFFFAOYSA-N	4.0×10^{-2}		Modarresi et al. (2007)	Q	67
N,N'-di-*tert*-butylethylenediamine	3.6×10^{2}		Zhang et al. (2010)	Q	287, 288
$C_{10}H_{24}N_2$	2.3		Zhang et al. (2010)	Q	287, 289
[4062-60-6]	9.9×10^{-1}		Zhang et al. (2010)	Q	287, 290
KGHYGBGIWLNFAV-UHFFFAOYSA-N	1.2×10^{1}		Zhang et al. (2010)	Q	287, 291
(diethylamino)-benzene	6.7×10^{-2}	6700	Brockbank (2013)	L	1
$C_{10}H_{15}N$	5.1×10^{-2}		Duchowicz et al. (2020)	V	186
(N,N-diethylaniline)	5.2×10^{-2}		HSDB (2015)	V	
[91-66-7]	4.6×10^{-1}		Mackay et al. (2006d)	V	
GGSUCNLOZRCGPQ-UHFFFAOYSA-N	4.6×10^{-1}		Mackay et al. (1995)	V	
	2.4×10^{-2}		Duchowicz et al. (2020)	Q	
	9.9×10^{-2}		Hilal et al. (2008)	Q	
	6.0×10^{-2}		Modarresi et al. (2007)	Q	67
		7600	Kühne et al. (2005)	Q	
	2.4		Katritzky et al. (1998)	Q	
		5800	Kühne et al. (2005)	?	
	5.2		Yaws (1999)	?	21, 557
1-naphthylamine	1.6×10^{2}		Altschuh et al. (1999)	M	
$C_{10}H_9N$	2.1×10^{1}		HSDB (2015)	V	
[134-32-7]	8.8×10^{1}		Abraham et al. (1994a)	R	
RUFPHBVGCFYCNW-UHFFFAOYSA-N	6.2×10^{2}		Keshavarz et al. (2022)	Q	
	2.0×10^{1}		Duchowicz et al. (2020)	Q	184
	3.0×10^{1}		Hilal et al. (2008)	Q	
	8.3×10^{1}		Modarresi et al. (2007)	Q	67
	1.2×10^{2}		English and Carroll (2001)	Q	230, 231
	4.6×10^{2}		Nirmalakhandan et al. (1997)	Q	
	8.9×10^{1}		Duchowicz et al. (2020)	?	185, 21

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-naphthylamine	1.2×10^2		Abraham et al. (1994a)	R	
$C_{10}H_9N$	1.2×10^2		Keshavarz et al. (2022)	Q	
[91-59-8]	2.0×10^1		Duchowicz et al. (2020)	Q	299
JBIJLHTVPXGSAM-UHFFFAOYSA-N	8.0×10^1		Hilal et al. (2008)	Q	
	1.0×10^2		Modarresi et al. (2007)	Q	67
	1.2×10^2		English and Carroll (2001)	Q	230, 274
	4.5×10^2		Nirmalakhandan et al. (1997)	Q	
	1.2×10^2		Duchowicz et al. (2020)	?	185, 21
	1.2×10^2		HSDB (2015)	?	419
1,5-naphthalenediamine	1.5×10^5		HSDB (2015)	Q	99
$C_{10}H_{10}N_2$					
[2243-62-1]					
KQSABULTKYLFEV-UHFFFAOYSA-N					
phentermine	7.0		HSDB (2015)	Q	99
$C_{10}H_{15}N$					
[122-09-8]					
DHHVAGZRUROJKS-UHFFFAOYSA-N					
N,N-diethyl-1,4-benzenediamine	1.9×10^2		HSDB (2015)	Q	99
$C_{10}H_{16}N_2$					
[93-05-0]					
QNGVNLMMEQUVQK-UHFFFAOYSA-N					
3,5-diethyltoluene-2,6-diamine	6.2×10^3		Zhang et al. (2010)	Q	287, 288
$C_{11}H_{18}N_2$	6.9×10^3		Zhang et al. (2010)	Q	287, 289
[2095-01-4]	6.1×10^1		Zhang et al. (2010)	Q	287, 290
RQEOBXYYEPMCPJ-UHFFFAOYSA-N	2.1×10^2		Zhang et al. (2010)	Q	287, 291
2,4-diethyl-6-methylbenzene-1,3-diamine	6.2×10^3		Zhang et al. (2010)	Q	287, 288
$C_{11}H_{18}N_2$	7.0×10^3		Zhang et al. (2010)	Q	287, 289
[2095-02-5]	6.2×10^1		Zhang et al. (2010)	Q	287, 290
PISLZQACAJMAIO-UHFFFAOYSA-N	2.1×10^2		Zhang et al. (2010)	Q	287, 291
diphenylamine	3.7		Duchowicz et al. (2020)	V	186
$C_{12}H_{11}N$	3.7		HSDB (2015)	V	
[122-39-4]	2.9×10^1		Mackay et al. (2006d)	V	
DMBHHRLKUKUOEG-UHFFFAOYSA-N	2.9×10^1		Mackay et al. (1995)	V	
	3.5		Meylan and Howard (1991)	V	
	1.5		Yaws (2003)	X	237, 12
	3.5		Howard et al. (1991)	X	412
	4.1×10^1		Duchowicz et al. (2020)	Q	
	1.5		Gharagheizi et al. (2010)	Q	246
	3.0		Hilal et al. (2008)	Q	
	9.4		Meylan and Howard (1991)	Q	

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benzidine	2.2×10^{6}		Mackay et al. (2006d)	V	
$C_{12}H_{12}N_2$	2.6×10^{5}		Lide and Frederikse (1995)	V	
[92-87-5]	2.2×10^{6}		Mackay et al. (1995)	V	
HFACYLZERDEVSX-UHFFFAOYSA-N	2.5×10^{1}		Mackay et al. (1995)	C	
	1.9×10^{5}		HSDB (2015)	Q	99
1,1-diphenylhydrazine	2.4×10^{2}		HSDB (2015)	Q	99
$C_{12}H_{12}N_2$					
[530-50-7]					
YHYKLKNNBYLTQY-UHFFFAOYSA-N					
1,2-diphenylhydrazine	2.1×10^{1}		Duchowicz et al. (2020)	V	186
$C_{12}H_{12}N_2$	2.1×10^{1}		HSDB (2015)	V	
(N,N'-bianiline)			Mackay et al. (2006d)	V	558
[122-66-7]	2.9×10^{3}		Mackay et al. (1995)	V	
YBQZXXMEJHZYMB-UHFFFAOYSA-N	2.3×10^{2}		Duchowicz et al. (2020)	Q	
4-(phenylazo)-benzenamine	1.1×10^{5}		HSDB (2015)	Q	99
$C_{12}H_{11}N_3$	9.3×10^{2}		Gharagheizi et al. (2012)	Q	
(4-aminoazobenzene)	1.9×10^{3}		Zhang et al. (2010)	Q	287, 288
[60-09-3]	3.2×10^{3}		Zhang et al. (2010)	Q	287, 289
QPQKUYVSJWQSDY-UHFFFAOYSA-N	7.3×10^{5}		Zhang et al. (2010)	Q	287, 290
	3.4×10^{2}		Zhang et al. (2010)	Q	287, 291
azobenzene	7.3×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{12}H_{10}N_2$	7.0×10^{-1}		HSDB (2015)	V	
[103-33-3]	2.6		Duchowicz et al. (2020)	Q	
DMLAVOWQYNRWNQ-UHFFFAOYSA-N					
2-aminobiphenyl	6.6×10^{1}		HSDB (2015)	Q	99
$C_{12}H_{11}N$					
[90-41-5]					
TWBPWBPGNQWFSJ-UHFFFAOYSA-N					
4-aminobiphenyl	6.6×10^{1}		HSDB (2015)	Q	99
$C_{12}H_{11}N$					
[92-67-1]					
DMVOXQPQNTYEKQ-UHFFFAOYSA-N					
N-phenyl-1,4-benzenediamine	1.5×10^{3}		Yaws (2003)	X	237
$C_{12}H_{12}N_2$	2.7×10^{4}		HSDB (2015)	Q	99
(p-aminodiphenylamine)	5.9×10^{2}		Gharagheizi et al. (2012)	Q	
[101-54-2]	3.6×10^{3}		Gharagheizi et al. (2010)	Q	246
ATGUVEKSASEFFO-UHFFFAOYSA-N					
2-fluorenamine	2.7×10^{2}		HSDB (2015)	Q	545
$C_{13}H_{11}N$					
[153-78-6]					
CFRFHWQYWJMEJN-UHFFFAOYSA-N					

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,4'-methylenebisbenzenamine $C_{13}H_{14}N_2$ [101-77-9] YBRVSVVVWCFQMG-UHFFFAOYSA-N	1.9×10^{5}		HSDB (2015)	V	
2-anthracenamine $C_{14}H_{11}N$ [613-13-8] YCSBALJAGZKWFF-UHFFFAOYSA-N	3.3×10^{1}		HSDB (2015)	Q	545
3,3'-dimethylbenzidine $C_{14}H_{16}N_2$ [119-93-7] NUIURNJTPRWVAP-UHFFFAOYSA-N	1.6×10^{5}		HSDB (2015)	Q	447
N,N-dimethyl-4-(phenylazo)-benzenamine	1.4×10^{3}		HSDB (2015)	V	
$C_{14}H_{15}N_3$	4.2×10^{1}		Zhang et al. (2010)	Q	287, 288
[60-11-7]	4.1×10^{1}		Zhang et al. (2010)	Q	287, 289
JCYPECIVGRXBMO-UHFFFAOYSA-N	8.2×10^{1}		Zhang et al. (2010)	Q	287, 290
	1.0×10^{1}		Zhang et al. (2010)	Q	287, 291
o-aminoazotoluene	3.1×10^{2}		Duchowicz et al. (2020)	V	186
$C_{14}H_{15}N_3$	3.8×10^{2}		Duchowicz et al. (2020)	Q	
[97-56-3] PFRYFZZSECNQOL-UHFFFAOYSA-N					
N-ethyl-N-phenylbenzenemethanamine	1.1		Zhang et al. (2010)	Q	287, 288
$C_{15}H_{17}N$	1.1		Zhang et al. (2010)	Q	287, 289
[92-59-1]	4.6×10^{-1}		Zhang et al. (2010)	Q	287, 290
HSZCJVZRHXPCIA-UHFFFAOYSA-N	6.7		Zhang et al. (2010)	Q	287, 291
N-(1-methylethyl)-N'-phenyl-1,4-benzenediamine $C_{15}H_{18}N_2$ (4-(iso-propylamino)diphenylamine) [101-72-4] OUBMGJOQLXMSNT-UHFFFAOYSA-N	7.0×10^{3}		HSDB (2015)	Q	99
4,4'-methylene-bis-(N-methylaniline) $C_{15}H_{18}N_2$ [1807-55-2] ZMVMYBGDGJLCHV-UHFFFAOYSA-N	3.4×10^{4}		HSDB (2015)	Q	99
C.I. Food Yellow 10 $C_{16}H_{13}N_3$ [85-84-7] KLCDQSGLLRINHY-UHFFFAOYSA-N	1.9×10^{4}		HSDB (2015)	Q	99

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3',5,5'-tetramethylbenzidine $C_{16}H_{20}N_2$ [54827-17-7] UAIUNKRWKOVEES-UHFFFAOYSA-N	1.3×10^5		HSDB (2015)	Q	99
N-phenyl-1-naphthalenamine $C_{16}H_{13}N$ [90-30-2] XQVWYOYUZDUNRW-UHFFFAOYSA-N	7.0×10^1 9.7×10^1 4.6×10^1 1.2×10^1 2.8×10^2		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	V Q Q Q Q	 287, 288 287, 289 287, 290 287, 291
yellow OB $C_{17}H_{15}N_3$ [131-79-3] BWLVSYUUKOQICP-FMQUCBEESA-N	1.8×10^4		HSDB (2015)	Q	99
auramine $C_{17}H_{21}N_3$ [492-80-8] JPIYZTWMUGTEHX-UHFFFAOYSA-N	1.2×10^2		HSDB (2015)	V	
benzphetamine $C_{17}H_{21}N$ [156-08-1] YXKTVDFXDRQTKV-UHFFFAOYSA-N	2.3×10^1		HSDB (2015)	Q	99
4,4'-methylenebis(N,N-dimethylbenzenamine) $C_{17}H_{22}N_2$ (bis(p-dimethylamino)phenylmethane) [101-61-1] JNRLEMMIVRBKJE-UHFFFAOYSA-N	8.2×10^1		HSDB (2015)	Q	99
phencyclidine $C_{17}H_{25}N$ [77-10-1] JTJMJGYZQZDUJJ-UHFFFAOYSA-N	1.8		HSDB (2015)	Q	99
N,N'-diphenyl-1,4-benzenediamine $C_{18}H_{16}N_2$ [74-31-7] UTGQNNCQYDRXCH-UHFFFAOYSA-N	4.7×10^4		HSDB (2015)	Q	99
N-(1,3-dimethylbutyl)-N'-phenyl-1,4-phenylenediamine $C_{18}H_{24}N_2$ [793-24-8] ZZMVLMVFYMGSMY-UHFFFAOYSA-N	2.9×10^3 3.9×10^2 3.9×10^1 2.3×10^3		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291

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Table A4.1: Amines (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
amitraz	1.0		MacBean (2012b)	X	350
$C_{19}H_{23}N_3$	1.3		Keshavarz et al. (2022)	Q	
[33089-61-1]	1.4×10^{2}		Duchowicz et al. (2020)	Q	
QXAITBQSYVNQDR-UHFFFAOYSA-N	2.1×10^{1}		Modarresi et al. (2007)	Q	67
	1.0		Duchowicz et al. (2020)	?	185, 21
N,N'-bis(1-ethyl-3-methylpentyl)-1,4-benzenediamine	5.8×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_{22}H_{40}N_2$	5.8		Zhang et al. (2010)	Q	287, 289
[139-60-6]	1.8		Zhang et al. (2010)	Q	287, 290
JUHXTONDLXIGGK-UHFFFAOYSA-N	1.9×10^{1}		Zhang et al. (2010)	Q	287, 291
p,*p*'-benzylidenebis(N,N-dimethylaniline) $C_{23}H_{26}N_2$ (leucomalachite green) [129-73-7] WZKXBGJNNCGHIC-UHFFFAOYSA-N	1.0×10^{3}		HSDB (2015)	Q	99
N-phenyl-N-(2,4,4-trimethyl-2-pentanyl)-1-naphthalenamine	6.4×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_{24}H_{29}N$	9.7×10^{-1}		Zhang et al. (2010)	Q	287, 289
[51772-35-1]	9.0×10^{-1}		Zhang et al. (2010)	Q	287, 290
SNWVRVDHQRBBFG-UHFFFAOYSA-N	1.1×10^{1}		Zhang et al. (2010)	Q	287, 291
tris(2-ethylhexyl)amine	7.0×10^{-4}		Zhang et al. (2010)	Q	287, 288
$C_{24}H_{51}N$	1.2×10^{-2}		Zhang et al. (2010)	Q	287, 289
[1860-26-0]	6.1×10^{-6}		Zhang et al. (2010)	Q	287, 290
BZUDVELGTZDOIG-UHFFFAOYSA-N	3.7×10^{-4}		Zhang et al. (2010)	Q	287, 291
4,4',4"-methylidyne-tris(N,N-dimethylbenzenamine)	6.4×10^{4}		Zhang et al. (2010)	Q	287, 288
$C_{25}H_{31}N_3$	3.1×10^{4}		Zhang et al. (2010)	Q	287, 289
(Leucocrystal violet)	3.5×10^{2}		Zhang et al. (2010)	Q	287, 290
[603-48-5]	1.1×10^{6}		Zhang et al. (2010)	Q	287, 291
OAZWDJGLIYNYMU-UHFFFAOYSA-N					
N-phenylbenzenamide	8.2×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{30}H_{47}N$	4.7×10^{-1}		Zhang et al. (2010)	Q	287, 289
[68608-79-7]	1.5×10^{-1}		Zhang et al. (2010)	Q	287, 290
FSPSHPMYFQHGQD-UHFFFAOYSA-N	2.9×10^{-1}		Zhang et al. (2010)	Q	287, 291
4,4',4"-methanetriyltris(N,N-diethylaniline)	9.0×10^{4}		Zhang et al. (2010)	Q	287, 288
$C_{31}H_{43}N_3$	7.0×10^{5}		Zhang et al. (2010)	Q	287, 289
[68814-02-8]	1.7×10^{3}		Zhang et al. (2010)	Q	287, 290
HOGMPEULJBVHLZ-UHFFFAOYSA-N	1.5×10^{6}		Zhang et al. (2010)	Q	287, 291

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A4.2 Heterocycles with nitrogen (C, H, N)

Table A4.2: Heterocycles with nitrogen (C, H, N)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
amitrole	4.5×10^{7}		Duchowicz et al. (2020)	V	186
$C_2H_4N_4$	4.5×10^{7}		HSDB (2015)	V	
[61-82-5]	6.1×10^{9}		Mackay et al. (2006d)	V	
KLSJWNVTNUYHDU-UHFFFAOYSA-N	1.5×10^{3}		Duchowicz et al. (2020)	Q	
azetidine	4.8		Ebert et al. (2023)	?	365
C_3H_7N					
[503-29-7]					
HONIICLYMWZJFZ-UHFFFAOYSA-N					
imidazole	3.3×10^{3}		Du et al. (2017)	M	478
$C_3H_4N_2$	2.1×10^{3}		Du et al. (2017)	Q	549
[288-32-4]	3.1×10^{3}		Du et al. (2017)	Q	
RAXXELZNTBOGNW-UHFFFAOYSA-N					
1,3,5-triazine-2,4,6-triamine	5.5×10^{8}		HSDB (2015)	V	
$C_3H_6N_6$	5.2×10^{7}		Zhang et al. (2010)	Q	287, 288
[108-78-1]	6.7×10^{8}		Zhang et al. (2010)	Q	287, 289
JDSHMPZPIAZGSV-UHFFFAOYSA-N	5.8×10^{9}		Zhang et al. (2010)	Q	287, 290
	8.4×10^{8}		Zhang et al. (2010)	Q	287, 291
pyrrolidine	4.2		Amoore and Buttery (1978)	V	
C_4H_8NH	4.2	7600	Cabani et al. (1971a)	T	
[123-75-1]	1.8		Keshavarz et al. (2022)	Q	
RWRDLPDLKQPQOW-UHFFFAOYSA-N	1.3×10^{1}		Duchowicz et al. (2020)	Q	299
	6.0		Hilal et al. (2008)	Q	
	5.3×10^{-1}		Modarresi et al. (2007)	Q	67
	4.1		Yaffe et al. (2003)	Q	248, 249
	8.4×10^{-1}		Katritzky et al. (1998)	Q	
	2.0		Suzuki et al. (1992)	Q	232
	4.1		Duchowicz et al. (2020)	?	185, 21
1-pyrroline	1.6		Amoore and Buttery (1978)	M	
C_4H_7N					
[5724-81-2]					
ZVJHJDDKYZXRJI-UHFFFAOYSA-N					
3-pyrroline	4.9		Amoore and Buttery (1978)	V	
C_4H_7N					
[109-96-6]					
JVQIKJMSUIMUDI-UHFFFAOYSA-N					
1,4-diazacyclohexane	4.5×10^{3}	7400	Nguyen (2013)	M	11
$C_4H_{10}N_2$	1.0×10^{2}	11000	Cabani et al. (1975a)	T	
(piperazine)					
[110-85-0]					
GLUUGHFHXGJENI-UHFFFAOYSA-N					

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Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pyrrole	5.5×10^{-1}		Hawthorne et al. (1985)	M	
C_4H_5N	6.1×10^{-1}		Mackay et al. (2006d)	V	
(1H-pyrrole)	6.1×10^{-1}		Mackay et al. (1995)	V	
[109-97-7]	1.8		Keshavarz et al. (2022)	Q	
KAESVJOAVNADME-UHFFFAOYSA-N	4.1		Duchowicz et al. (2020)	Q	184
	7.2×10^{-1}		Hilal et al. (2008)	Q	
	8.6×10^{-1}		Modarresi et al. (2007)	Q	67
	5.4×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	4.2		Katritzky et al. (1998)	Q	
	5.5×10^{-1}		Duchowicz et al. (2020)	?	185, 21
1-methyl-1H-imidazole	6.9×10^{1}		Du et al. (2017)	M	478
$C_4H_6N_2$	3.4×10^{2}		Du et al. (2017)	Q	549
[616-47-7]	8.9×10^{1}		Du et al. (2017)	Q	
MCTWTZJPVLRJOU-UHFFFAOYSA-N	1.1×10^{2}		Hilal et al. (2008)	Q	
1,3-diazine	1.0×10^{1}		Hilal et al. (2008)	Q	
$C_4H_4N_2$					
[289-95-2]					
CZPWVGJYEJSRLH-UHFFFAOYSA-N					
N-methylpyrrolidine	3.3×10^{-1}	7600	Cabani et al. (1971a)	T	
$C_4H_8NCH_3$	1.7×10^{-1}		Keshavarz et al. (2022)	Q	
[120-94-5]	1.2		Duchowicz et al. (2020)	Q	184
AVFZOVWCLRSYKC-UHFFFAOYSA-N	2.2×10^{-1}		Hilal et al. (2008)	Q	
	5.6×10^{-2}		Modarresi et al. (2007)	Q	67
	3.2×10^{-1}		Suzuki et al. (1992)	Q	232
	3.3×10^{-1}		Duchowicz et al. (2020)	?	185, 21
piperidine	2.8	7900	Bernauer and Dohnal (2009)	M	
$C_5H_{10}NH$	2.0		Amoore and Buttery (1978)	V	
[110-89-4]	2.2	7900	Cabani et al. (1971a)	T	
NQRYJNQNLNOLGT-UHFFFAOYSA-N	2.5		Keshavarz et al. (2022)	Q	
	1.3×10^{1}		Duchowicz et al. (2020)	Q	299
	7.3		Hilal et al. (2008)	Q	
	1.0		Modarresi et al. (2007)	Q	67
	7.2×10^{-1}		Katritzky et al. (1998)	Q	
	6.7×10^{-1}		Russell et al. (1992)	Q	279
	1.5		Suzuki et al. (1992)	Q	232
	2.2		Duchowicz et al. (2020)	?	185, 21
2-ethylimidazole	7.6×10^{2}		Du et al. (2017)	M	478
$C_5H_8N_2$	1.4×10^{4}		Du et al. (2017)	Q	549
[1072-62-4]	8.2×10^{2}		Du et al. (2017)	Q	
PQAMFDRRWURCFQ-UHFFFAOYSA-N					
1,2-dimethylimidazole	4.3×10^{1}		Du et al. (2017)	M	478
$C_5H_8N_2$	2.9×10^{2}		Du et al. (2017)	Q	549
[1739-84-0]	3.3×10^{1}		Du et al. (2017)	Q	
GIWQSPITLQVMSG-UHFFFAOYSA-N					

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Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-methylpiperazine $C_5H_{12}N_2$ (1-methylpiperazine) [109-01-3] PVOAHINGSUIXLS-UHFFFAOYSA-N	1.8×10^{3} 2.0×10^{2}	9900 11000	Nguyen (2013) Cabani et al. (1975a)	M T	11
1-methyl-1H-pyrrole C_5H_7N [96-54-8] OXHNLMTVIGZXSG-UHFFFAOYSA-N	9.0×10^{-3}		Hilal et al. (2008)	Q	
pyridine C_5H_5N [110-86-1] JUJWROOIHBZHMG-UHFFFAOYSA-N	9.1×10^{-1} 1.1 4.6×10^{-2} 9.8×10^{-1} 5.5×10^{-1} 8.2×10^{-1} 1.1 7.1×10^{-1} 1.1 8.4×10^{-1} 2.4×10^{-1} 1.1 7.5×10^{-1} 6.4×10^{-1} 1.2 1.3 1.2 9.0×10^{-2} 1.8 3.3 1.2 9.0×10^{-1} 1.1 1.1 8.9×10^{-1} 1.1 	4700 6000 -2300 5900 6000 5400 	Brockbank (2013) Bernauer and Dohnal (2009) Dewulf et al. (1999) Welke et al. (1998) Chaintreau et al. (1995) Hawthorne et al. (1985) Arnett and Chawla (1979) Amoore and Buttery (1978) Andon et al. (1954) Keshavarz et al. (2022) Duchowicz et al. (2020) Li et al. (2014) Hilal et al. (2008) Modarresi et al. (2007) Kühne et al. (2005) Yaffe et al. (2003) Yao et al. (2002) English and Carroll (2001) Katritzky et al. (1998) Nirmalakhandan et al. (1997) Russell et al. (1992) Suzuki et al. (1992) Duchowicz et al. (2020) Mackay et al. (2006d) Kühne et al. (2005) Yaws (1999) Yaws and Yang (1992) Abraham et al. (1990) Staudinger and Roberts (2001)	L M M M M M M M M Q Q Q Q Q Q Q Q Q Q Q Q ? ? ? ? ? ? W	1 559 336 299 241 67 248, 249 229 230, 231 279 232 185, 21 21 21 560
pyridine-d5 C_5D_5N [7291-22-7] JUJWROOIHBZHMG-RALIUCGRSA-N	4.2	10000	Hiatt (2013)	M	

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Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-aminopyridine $C_5H_6N_2$ [504-24-5] NUKYPUAOHBNCPY-UHFFFAOYSA-N	4.3×10^{4}		HSDB (2015)	V	
2-aminopyridine $C_5H_6N_2$ [504-29-0] ICSNLGPSRYBMBD-UHFFFAOYSA-N	3.9×10^{3}		HSDB (2015)	Q	99
2-methylpyrazine $C_4N_2H_3CH_3$ [109-08-0] CAWHJQAVHZEVTJ-UHFFFAOYSA-N	4.5		Buttery et al. (1971)	M	
	4.9		Keshavarz et al. (2022)	Q	
	6.8×10^{-1}		Duchowicz et al. (2020)	Q	184
	4.8		Hilal et al. (2008)	Q	
	4.9		Modarresi et al. (2007)	Q	67
	1.6×10^{2}		Katritzky et al. (1998)	Q	
	3.1		Nirmalakhandan et al. (1997)	Q	
	1.2		Russell et al. (1992)	Q	279
	4.5		Duchowicz et al. (2020)	?	185, 21
adenine $C_5H_5N_5$ [73-24-5] GFFGJBXGBJISGV-UHFFFAOYSA-N	1.3×10^{9}		Duchowicz et al. (2020)	V	186
	5.3×10^{5}		Duchowicz et al. (2020)	Q	
9-methyladenine $C_6H_7N_5$ [700-00-5] WRXCXOUDSPTXNX-UHFFFAOYSA-N	3.9×10^{6}		Ebert et al. (2023)	?	365
N-methylpiperidine $C_5H_{10}NCH_3$ [626-67-5] PAMIQIKDUOTOBW-UHFFFAOYSA-N	2.4×10^{-1}		Abraham et al. (1994a)	R	
	2.9×10^{-1}	7900	Cabani et al. (1971a)	T	
	2.3×10^{-1}		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	
	4.8×10^{-1}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	67
		6300	Kühne et al. (2005)	Q	
	3.0×10^{-1}		English and Carroll (2001)	Q	230, 231
	2.9×10^{-1}		Katritzky et al. (1998)	Q	
	2.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	9.9×10^{-2}		Russell et al. (1992)	Q	279
	2.5×10^{-1}		Suzuki et al. (1992)	Q	232
	2.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		6600	Kühne et al. (2005)	?	
triethylenediamine $C_6H_{12}N_2$ [280-57-9] IMNIMPAHZVJRPE-UHFFFAOYSA-N	3.1×10^{3}		Du et al. (2017)	M	478
	8.9×10^{2}		Du et al. (2017)	Q	549
	2.2×10^{3}		Du et al. (2017)	Q	

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Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-ethyl-4-methylimidazole	2.8×10^{2}		Du et al. (2017)	M	478
$C_6H_{10}N_2$	1.4×10^{3}		Du et al. (2017)	Q	549
[931-36-2]	3.1×10^{2}		Du et al. (2017)	Q	
ULKLGIFJWFIQFF-UHFFFAOYSA-N					
3-(aminomethyl)pyridine	4.3×10^{2}		Du et al. (2017)	M	478
$C_6H_8N_2$	5.0×10^{2}		Du et al. (2017)	Q	549
[3731-52-0]	3.7×10^{2}		Du et al. (2017)	Q	
HDOUGSFASVGDCS-UHFFFAOYSA-N					
N,N'-dimethylpiperazine	2.0×10^{2}	11000	Nguyen (2013)	M	11
$C_6H_{14}N_2$	1.4×10^{2}	11000	Cabani et al. (1975a)	T	
(1,4-dimethylpiperazine)					
[106-58-1]					
RXYPXQSKLGGKOL-UHFFFAOYSA-N					
cyromazine	1.7×10^{8}		Duchowicz et al. (2020)	V	186
$C_6H_{10}N_6$	1.7×10^{8}		HSDB (2015)	V	
[66215-27-8]	1.3×10^{8}		Duchowicz et al. (2020)	Q	
LVQDKIWDGQRHTE-UHFFFAOYSA-N					
1H-benzotriazole	3.1×10^{1}		HSDB (2015)	V	
$C_6H_5N_3$					
(1,2,3-benzotriazole)					
[95-14-7]					
QRUDEWIWKLJBPS-UHFFFAOYSA-N					
1-piperazineethanamine	1.5×10^{7}		HSDB (2015)	Q	99
$C_6H_{15}N_3$					
(N-(2-aminoethyl)piperazine)					
[140-31-8]					
IMUDHTPIFIBORV-UHFFFAOYSA-N					
2-methylpyridine	9.8×10^{-1}	6300	Brockbank (2013)	L	1
$C_5H_4NCH_3$	9.9×10^{-1}	6400	Andon et al. (1954)	M	336
(2-picoline; α-picoline)	1.1		Keshavarz et al. (2022)	Q	
[109-06-8]	8.0×10^{-2}		Duchowicz et al. (2020)	Q	
BSKHPKMHTQYZBB-UHFFFAOYSA-N	4.1×10^{-1}		Hilal et al. (2008)	Q	
	1.2		Modarresi et al. (2007)	Q	67
		6400	Kühne et al. (2005)	Q	
	1.0		Yaffe et al. (2003)	Q	248, 249
	1.0		Yao et al. (2002)	Q	229
	1.4×10^{2}		English and Carroll (2001)	Q	230, 231
	2.1		Katritzky et al. (1998)	Q	
	1.3		Nirmalakhandan et al. (1997)	Q	
	8.8×10^{-1}		Suzuki et al. (1992)	Q	232
	9.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	9.9×10^{-1}		Mackay et al. (2006d)	?	
		6300	Kühne et al. (2005)	?	
	9.9×10^{-1}		Yaws (1999)	?	21

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Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.4×10^{-1}		Yaws and Yang (1992)	?	21
	9.9×10^{-1}		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	560
3-methylpyridine	1.2	6400	Brockbank (2013)	L	1
$C_5H_4NCH_3$	4.2×10^{-1}		Chaintreau et al. (1995)	M	
(3-picoline; β-picoline)	1.3	6300	Andon et al. (1954)	M	336
[108-99-6]	1.1		Keshavarz et al. (2022)	Q	
ITQTTZVARXURQS-UHFFFAOYSA-N	8.0×10^{-2}		Duchowicz et al. (2020)	Q	299
	8.8×10^{-1}		Hilal et al. (2008)	Q	
	8.5×10^{-1}		Modarresi et al. (2007)	Q	67
		6400	Kühne et al. (2005)	Q	
	1.0		Yaffe et al. (2003)	Q	248, 272
	1.3		Yao et al. (2002)	Q	229, 267
	9.5×10^{-1}		English and Carroll (2001)	Q	230, 231
	2.3		Katritzky et al. (1998)	Q	
	1.3		Nirmalakhandan et al. (1997)	Q	
	8.8×10^{-1}		Suzuki et al. (1992)	Q	232
	1.3		Duchowicz et al. (2020)	?	185, 21
	1.3		Mackay et al. (2006d)	?	
		6300	Kühne et al. (2005)	?	
	1.4		Yaws (1999)	?	21
	5.4×10^{-1}		Yaws and Yang (1992)	?	21
	1.3		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	560
4-methylpyridine	1.6	6500	Brockbank (2013)	L	1
$C_5H_4NCH_3$	1.7	6500	Andon et al. (1954)	M	336
[108-89-4]	1.1		Keshavarz et al. (2022)	Q	
FKNQCJSGGFJEIZ-UHFFFAOYSA-N	8.0×10^{-2}		Duchowicz et al. (2020)	Q	184
	1.6		Li et al. (2014)	Q	241
	9.0×10^{-1}		Hilal et al. (2008)	Q	
	8.6×10^{-1}		Modarresi et al. (2007)	Q	67
		6400	Kühne et al. (2005)	Q	
	1.2		Yaffe et al. (2003)	Q	248, 272
	1.2		Yao et al. (2002)	Q	229
	1.1		English and Carroll (2001)	Q	230, 231
	2.4		Katritzky et al. (1998)	Q	
	1.3		Nirmalakhandan et al. (1997)	Q	
	2.1		Russell et al. (1992)	Q	279
	8.8×10^{-1}		Suzuki et al. (1992)	Q	232
	1.6		Duchowicz et al. (2020)	?	185, 21
	1.7		Mackay et al. (2006d)	?	
		6500	Kühne et al. (2005)	?	
	1.7		Yaws (1999)	?	21, 12
	1.6		Abraham et al. (1990)	?	
	1.4		Arnett and Chawla (1979)	?	559
			Staudinger and Roberts (2001)	W	560

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Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-cyanopyridine	3.6×10^{1}		Abraham et al. (1994a)	R	
$C_6H_4N_2$	1.9×10^{1}		Keshavarz et al. (2022)	Q	
[100-54-9]	5.4		Duchowicz et al. (2020)	Q	
GZPHSAQLYPIAIN-UHFFFAOYSA-N	3.6×10^{1}		HSDB (2015)	Q	99
	1.6×10^{1}		Hilal et al. (2008)	Q	
	1.1×10^{1}		Modarresi et al. (2007)	Q	67
	6.9×10^{1}		English and Carroll (2001)	Q	230, 231
	1.2×10^{2}		Nirmalakhandan et al. (1997)	Q	
	3.6×10^{1}		Duchowicz et al. (2020)	?	185, 21
4-cyanopyridine	1.1×10^{1}		Abraham et al. (1994a)	R	
$C_6H_4N_2$	1.9×10^{1}		Keshavarz et al. (2022)	Q	
[100-48-1]	5.4		Duchowicz et al. (2020)	Q	
GPHQHTOMRSGBNZ-UHFFFAOYSA-N	1.7×10^{1}		Hilal et al. (2008)	Q	
	1.0×10^{1}		Modarresi et al. (2007)	Q	67
	1.2×10^{2}		Nirmalakhandan et al. (1997)	Q	
	1.1×10^{1}		Duchowicz et al. (2020)	?	185, 21
2-ethylpyrazine	4.0		Buttery et al. (1971)	M	
$C_4N_2H_3(C_2H_5)$	6.5		Keshavarz et al. (2022)	Q	
[13925-00-3]	7.3×10^{-1}		Duchowicz et al. (2020)	Q	184
KVFIJIWMDBAGDP-UHFFFAOYSA-N	2.7		Hilal et al. (2008)	Q	
	3.4		Modarresi et al. (2007)	Q	67
	2.7		Nirmalakhandan et al. (1997)	Q	
	4.0		Duchowicz et al. (2020)	?	185, 21
2,5-dimethylpyrazine	7.1		Marin et al. (1999)	M	
$C_6H_8N_2$	5.5		Druaux et al. (1998)	M	
[123-32-0]	5.5		Marin et al. (1999)	V	
LCZUOKDVTBMCMX-UHFFFAOYSA-N	6.4		Marin et al. (1999)	Q	
2,6-dimethylpyrazine	9.8×10^{-1}		Chaintreau et al. (1995)	M	
$C_6H_8N_2$					
(3,5-dimethylpyrazine)					
[108-50-9]					
HJFZAYHYIWGLNL-UHFFFAOYSA-N					
N-ethylpiperidine	3.9×10^{-1}		Hilal et al. (2008)	Q	
$C_7H_{15}N$		6600	Kühne et al. (2005)	Q	
(1-ethylpiperidine)		6600	Kühne et al. (2005)	?	
[766-09-6]					
HTLZVHNRZJPSMI-UHFFFAOYSA-N					
1H-benzimidazole	2.7×10^{1}		HSDB (2015)	Q	99
$C_7H_6N_2$					
[51-17-2]					
HYZJCKYKOHLVJF-UHFFFAOYSA-N					

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Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-ethenylpyridine	7.0×10^{-1}		Duchowicz et al. (2020)	V	186
C_7H_7N	2.8×10^{-1}		Duchowicz et al. (2020)	Q	
(2-vinylpyridine)	2.7		HSDB (2015)	Q	99
[100-69-6]					
KGIGUEBEKRSTEW-UHFFFAOYSA-N					
4-ethenylpyridine	1.2		Duchowicz et al. (2020)	V	186
C_7H_7N	2.8×10^{-1}		Duchowicz et al. (2020)	Q	
(4-vinylpyridine)	3.1		HSDB (2015)	Q	99
[100-43-6]					
KFDVPJUYSDEJTH-UHFFFAOYSA-N					
2-ethylpyridine	6.0×10^{-1}	6700	Andon et al. (1954)	M	336
$C_5H_4NC_2H_5$	1.5		Keshavarz et al. (2022)	Q	
[100-71-0]	8.2×10^{-2}		Duchowicz et al. (2020)	Q	299
NRGGMCIBEHEAIL-UHFFFAOYSA-N	2.9×10^{-1}		Hilal et al. (2008)	Q	
	6.5×10^{-1}		Modarresi et al. (2007)	Q	67
		6700	Kühne et al. (2005)	Q	
	6.1×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.4		Katritzky et al. (1998)	Q	
	1.1		Nirmalakhandan et al. (1997)	Q	
	1.4		Suzuki et al. (1992)	Q	232
	6.0×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		7900	Kühne et al. (2005)	?	
	6.0×10^{-1}		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	560
3-ethylpyridine	9.5×10^{-1}	6400	Andon et al. (1954)	M	336
$C_5H_4NC_2H_5$	1.5		Keshavarz et al. (2022)	Q	
[536-78-7]	8.2×10^{-2}		Duchowicz et al. (2020)	Q	
MFEIKQPHQINPRI-UHFFFAOYSA-N	6.7×10^{-1}		Hilal et al. (2008)	Q	
	6.0×10^{-1}		Modarresi et al. (2007)	Q	67
		6700	Kühne et al. (2005)	Q	
	1.0		English and Carroll (2001)	Q	230, 231
	2.9		Katritzky et al. (1998)	Q	
	1.1		Nirmalakhandan et al. (1997)	Q	
	1.4		Suzuki et al. (1992)	Q	232
	9.5×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		6200	Kühne et al. (2005)	?	
	9.5×10^{-1}		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	560
4-ethylpyridine	1.2	6300	Andon et al. (1954)	M	336
$C_5H_4NC_2H_5$	1.5		Keshavarz et al. (2022)	Q	
[536-75-4]	8.2×10^{-2}		Duchowicz et al. (2020)	Q	299
VJXRKZJMGVSXPX-UHFFFAOYSA-N	1.2		Li et al. (2014)	Q	241
	7.0×10^{-1}		Hilal et al. (2008)	Q	
	5.7×10^{-1}		Modarresi et al. (2007)	Q	67
		6700	Kühne et al. (2005)	Q	

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Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2		Yaffe et al. (2003)	Q	248, 249
	1.0		English and Carroll (2001)	Q	230, 260
	2.9		Katritzky et al. (1998)	Q	
	1.1		Nirmalakhandan et al. (1997)	Q	
	1.4		Suzuki et al. (1992)	Q	232
	1.2		Duchowicz et al. (2020)	?	185, 21
		6300	Kühne et al. (2005)	?	
	1.2		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	560
2,3-dimethylpyridine	1.4	6900	Andon et al. (1954)	M	336
$C_5H_3N(CH_3)_2$	1.5		Keshavarz et al. (2022)	Q	
(2,3-lutidine)	2.7×10^{-2}		Duchowicz et al. (2020)	Q	184
[583-61-9]	6.2×10^{-1}		Hilal et al. (2008)	Q	
HPYNZHMRTTWQTB-UHFFFAOYSA-N	2.1×10^{-1}		Modarresi et al. (2007)	Q	67
		6200	Kühne et al. (2005)	Q	
	1.2		Yaffe et al. (2003)	Q	248, 272
	1.6		English and Carroll (2001)	Q	230, 274
	3.0		Katritzky et al. (1998)	Q	
	9.5×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.3		Suzuki et al. (1992)	Q	232
	1.4		Duchowicz et al. (2020)	?	185, 21
	1.4		Mackay et al. (2006d)	?	
		5800	Kühne et al. (2005)	?	
	1.4		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	560
2,4-dimethylpyridine	9.9×10^{-1}		Hawthorne et al. (1985)	M	
$C_5H_3N(CH_3)_2$	1.5	7100	Andon et al. (1954)	M	336
(2,4-lutidine)	1.5		Keshavarz et al. (2022)	Q	
[108-47-4]	2.7×10^{-2}		Duchowicz et al. (2020)	Q	
JYYNAJVZFGKDEQ-UHFFFAOYSA-N	1.5		Li et al. (2014)	Q	241
	5.1×10^{-1}		Hilal et al. (2008)	Q	
	2.9×10^{-1}		Modarresi et al. (2007)	Q	67
		6700	Kühne et al. (2005)	Q	
	1.5		Yaffe et al. (2003)	Q	248, 272
	1.8		English and Carroll (2001)	Q	230, 231
	3.1		Katritzky et al. (1998)	Q	
	9.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.7		Russell et al. (1992)	Q	279
	1.3		Suzuki et al. (1992)	Q	232
	1.5		Duchowicz et al. (2020)	?	185, 21
	1.5		Mackay et al. (2006d)	?	
		6400	Kühne et al. (2005)	?	
	1.5		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	560

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Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,5-dimethylpyridine	1.1	7000	Andon et al. (1954)	M	336
$C_5H_3N(CH_3)_2$	1.5		Keshavarz et al. (2022)	Q	
(2,5-lutidine)	2.7×10^{-2}		Duchowicz et al. (2020)	Q	299
[589-93-5]	5.7×10^{-1}		Hilal et al. (2008)	Q	
XWKFPIODWVPXLX-UHFFFAOYSA-N	2.1×10^{-1}		Modarresi et al. (2007)	Q	67
		6700	Kühne et al. (2005)	Q	
	1.2		Yaffe et al. (2003)	Q	248, 249
	1.6		English and Carroll (2001)	Q	230, 231
	2.9		Katritzky et al. (1998)	Q	
	9.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.3		Suzuki et al. (1992)	Q	232
	1.2		Meylan and Howard (1991)	Q	
	1.1		Duchowicz et al. (2020)	?	185, 21
		6900	Kühne et al. (2005)	?	
	1.1		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	560
2,6-dimethylpyridine	9.2×10^{-1}	7300	Brockbank (2013)	L	1
$C_5H_3N(CH_3)_2$	6.6×10^{-1}		Hawthorne et al. (1985)	M	
(2,6-lutidine)	9.5×10^{-1}	7300	Andon et al. (1954)	M	336
[108-48-5]	1.5		Keshavarz et al. (2022)	Q	
OISVCGZHLKNMSJ-UHFFFAOYSA-N	2.7×10^{-2}		Duchowicz et al. (2020)	Q	299
	4.5×10^{-1}		Hilal et al. (2008)	Q	
	6.8×10^{-1}		Modarresi et al. (2007)	Q	67
		6700	Kühne et al. (2005)	Q	
	1.6		English and Carroll (2001)	Q	230, 231
	2.4		Katritzky et al. (1998)	Q	
	9.5×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.3		Suzuki et al. (1992)	Q	232
	9.5×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	9.4×10^{-1}		Mackay et al. (2006d)	?	
		6600	Kühne et al. (2005)	?	
	9.5×10^{-1}		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	560
3,4-dimethylpyridine	2.7	6800	Andon et al. (1954)	M	336
$C_5H_3N(CH_3)_2$	1.5		Keshavarz et al. (2022)	Q	
(3,4-lutidine)	2.7×10^{-2}		Duchowicz et al. (2020)	Q	299
[583-58-4]	1.3		Hilal et al. (2008)	Q	
NURQLCJSMXZBPC-UHFFFAOYSA-N	3.8×10^{-1}		Modarresi et al. (2007)	Q	67
		6200	Kühne et al. (2005)	Q	
	2.7		Yaffe et al. (2003)	Q	248, 249
	1.4		English and Carroll (2001)	Q	230, 260
	2.8		Katritzky et al. (1998)	Q	
	9.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.3		Suzuki et al. (1992)	Q	232
	2.7		Duchowicz et al. (2020)	?	185, 21
		6400	Kühne et al. (2005)	?	

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Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.7		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	560
3,5-dimethylpyridine	1.4	6800	Andon et al. (1954)	M	336
$C_5H_3N(CH_3)_2$	1.5		Keshavarz et al. (2022)	Q	
(3,5-lutidine)	2.7×10^{-2}		Duchowicz et al. (2020)	Q	184
[591-22-0]	9.7×10^{-1}		Hilal et al. (2008)	Q	
HWWYDZCSSYKIAD-UHFFFAOYSA-N	5.9×10^{-1}		Modarresi et al. (2007)	Q	67
		6700	Kühne et al. (2005)	Q	
	1.5		Yaffe et al. (2003)	Q	248, 249
	1.2		English and Carroll (2001)	Q	230, 231
	3.3		Katritzky et al. (1998)	Q	
	9.2×10^{-1}		Nirmalakhandan et al. (1997)	Q	
	1.3		Suzuki et al. (1992)	Q	232
	1.4		Duchowicz et al. (2020)	?	185, 21
		6500	Kühne et al. (2005)	?	
	1.4		Abraham et al. (1990)	?	
			Staudinger and Roberts (2001)	W	560
5-ethyl-2-methylpyridine	5.2×10^{-1}		Duchowicz et al. (2020)	V	186
$C_8H_{11}N$	5.2×10^{-1}		HSDB (2015)	V	
[104-90-5]	2.7×10^{-2}		Duchowicz et al. (2020)	Q	
NTSLROIKFLNUIJ-UHFFFAOYSA-N	8.6×10^{-1}		Zhang et al. (2010)	Q	287, 288
	3.8×10^{-1}		Zhang et al. (2010)	Q	287, 289
	7.0×10^{-1}		Zhang et al. (2010)	Q	287, 290
	6.2×10^{-2}		Zhang et al. (2010)	Q	287, 291
	4.4×10^{-1}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Modarresi et al. (2007)	Q	67
2,4,6-trimethylpyridine	1.1		Duchowicz et al. (2020)	V	186
$C_5H_2N(CH_3)_3$	1.1		HSDB (2015)	V	
(2,4,6-collidine)	5.7×10^{-2}		Mackay et al. (2006d)	V	
[108-75-8]	5.7×10^{-2}		Mackay et al. (1995)	V	
BWZVCCNYKMEVEX-UHFFFAOYSA-N	1.1		Hilal et al. (2008)	C	
	8.9×10^{-3}		Duchowicz et al. (2020)	Q	
	5.4×10^{-1}		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	67
		7100	Kühne et al. (2005)	Q	
	2.5		Katritzky et al. (1998)	Q	
		8600	Kühne et al. (2005)	?	
indole	1.9×10^{1}		Duchowicz et al. (2020)	V	186
C_8H_7N	1.9×10^{1}		HSDB (2015)	V	
[120-72-9]	7.1		Mackay et al. (2006d)	V	
SIKJAQJRHWYJAI-UHFFFAOYSA-N	7.1		Mackay et al. (1995)	V	
	1.6×10^{1}		Yaws (2003)	X	258
	1.6×10^{1}		Yaws (2003)	X	237, 12
	1.5×10^{1}		Howard and Meylan (1997)	X	446
	5.3		Dupeux et al. (2022)	Q	259

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Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{1}		Duchowicz et al. (2020)	Q	
	7.0×10^{1}		Gharagheizi et al. (2012)	Q	
	1.7×10^{1}		Gharagheizi et al. (2010)	Q	246
	9.0		Hilal et al. (2008)	Q	
	9.9		Yaws (1999)	?	21, 12
2-ethyl-3,5-dimethylpyrazine $C_8H_{12}N_2$ [13925-07-0] JZBCTZLGKSYRSF-UHFFFAOYSA-N	2.9	8500	Wieland et al. (2015)	M	561
2-isobutylpyrazine $C_4N_2H_3C_4H_9$ [29460-92-2] YAIMUUJMEBJXAA-UHFFFAOYSA-N	2.0		Buttery et al. (1971)	M	
	1.2×10^{1}		Keshavarz et al. (2022)	Q	
	1.4		Nirmalakhandan et al. (1997)	Q	
2-(1-methylpropyl)-pyrazine $C_8H_{12}N_2$ [29460-93-3] NFFQZEXYZVZKNN-UHFFFAOYSA-N	1.6		Hilal et al. (2008)	Q	
	2.2		Modarresi et al. (2007)	Q	67
5-ethenyl-2-methylpyridine C_8H_9N [140-76-1] VJOWMORERYNYON-UHFFFAOYSA-N	2.2		HSDB (2015)	Q	99
4-(1,1-dimethylethyl)-pyridine $C_9H_{13}N$ (4-*tert*-butylpyridine) [3978-81-2] YSHMQTRICHYLGF-UHFFFAOYSA-N	3.9×10^{-1}		Hilal et al. (2008)	Q	
	7.5×10^{-1}		Abraham et al. (1990)	?	
	7.5×10^{-1}	7000	Arnett and Chawla (1979)	?	559
nornicotine $C_9H_{12}N_2$ [494-97-3] MYKUKUCHPMASKF-UHFFFAOYSA-N	7.2×10^{3}		HSDB (2015)	Q	447
2,4-diamino-6-phenyl-1,3,5-triazine $C_9H_9N_5$ [91-76-9] GZVHEAJQGPRDLQ-UHFFFAOYSA-N	2.4×10^{5}		HSDB (2015)	Q	99
N-methylindole C_9H_9N [603-76-9] BLRHMMGNCXNXJL-UHFFFAOYSA-N	8.7		Ebert et al. (2023)	?	365

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Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-methylindole C_9H_9N (skatole) [83-34-1] ZFRKQXVRDFCRJG-UHFFFAOYSA-N	2.9×10^{-5} 4.7	-2500	Wetlaufer et al. (1964) HSDB (2015)	M V	
2,3-diethyl-5-methylpyrazine $C_9H_{14}N_2$ [18138-04-0] PSINWXIDJYEXLO-UHFFFAOYSA-N	8.1×10^{-1}		Roberts and Pollien (1997)	M	
benzo[b]pyridine C_9H_7N (quinoline) [91-22-5] SMWDFEZZVXVKRB-UHFFFAOYSA-N	5.9 5.8 3.8×10^{1} 3.8×10^{1} 6.0 3.9×10^{1} 6.4 3.7×10^{1} 9.3×10^{-1} 5.7×10^{1} 6.4 5.8 6.1 9.0 3.2×10^{-1} 3.4×10^{1} 1.4×10^{1} 6.5	 5400 7300 7300 	Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Mackay et al. (1995) Meylan and Howard (1991) Smith and Bomberger (1980) Abraham et al. (1994a) Goldstein (1982) Duchowicz et al. (2020) Gharagheizi et al. (2012) Hilal et al. (2008) Modarresi et al. (2007) Kühne et al. (2005) Yaffe et al. (2003) English and Carroll (2001) Katritzky et al. (1998) Nirmalakhandan et al. (1997) Meylan and Howard (1991) Kühne et al. (2005) Yaws (1999)	V V V V V V R X Q Q Q Q Q Q Q Q Q ? ?	186 24 298 67 248, 249 230, 231 21, 12
benzo[c]pyridine C_9H_7N (isoquinoline) [119-65-3] AWJUIBRHMBBTKR-UHFFFAOYSA-N	5.2×10^{-2} 5.2×10^{-2} 5.7 5.6 9.2 3.8		Mackay et al. (2006d) Mackay et al. (1995) Yaws (2003) Gharagheizi et al. (2010) Hilal et al. (2008) Yaws (1999)	V V X Q Q ?	 237, 12 246 21, 12
nicotine $C_{10}H_{14}N_2$ [54-11-5] SNICXCGAKADSCV-SNVBAGLBSA-N	3.3×10^{3}		HSDB (2015)	Q	99
2,2'-bipyridine $C_{10}H_8N_2$ [366-18-7] ROFVEXUMMXZLPA-UHFFFAOYSA-N	1.8×10^{4}		HSDB (2015)	Q	545

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Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,4'-bipyridine $C_{10}H_8N_2$ [553-26-4] MWVTWFVJZLCBMC-UHFFFAOYSA-N	3.9×10^{3} 1.7×10^{1}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
2-methylquinoline $C_{10}H_9N$ [91-63-4] SMUQFGGVLNAIOZ-UHFFFAOYSA-N	1.4×10^{1}		Ebert et al. (2023)	?	316
4-methylquinoline $C_{10}H_9N$ [491-35-0] MUDSDYNRBDKLGK-UHFFFAOYSA-N	1.3×10^{1}		HSDB (2015)	Q	99
MEIQX $C_{11}H_{11}N_5$ (2-amino-3,8-dimethylimidazo[4,5-f]quinoxaline) [77500-04-0] DVCCCQNKIYNAKB-UHFFFAOYSA-N	6.2×10^{7}		HSDB (2015)	Q	99
3-(phenylazo)-2,6-pyridinediamine $C_{11}H_{11}N_5$ (phenazopyridine) [94-78-0] QPFYXYFORQJZEC-UHFFFAOYSA-N	3.0×10^{9}		HSDB (2015)	Q	99
2-amino-9H-pyrido[2,3-b]indole $C_{11}H_9N_3$ [26148-68-5] FJTNLJLPLJDTRM-UHFFFAOYSA-N	2.5×10^{8}		HSDB (2015)	Q	99
carbazole $C_{12}H_9N$ [86-74-8] UJOBWOGCFQCDNV-UHFFFAOYSA-N	9.4×10^{1} 9.3×10^{1} 6.6×10^{-2} 6.6×10^{-2} 6.3×10^{-2} 2.0×10^{1} 6.3×10^{1} 1.1×10^{2} 8.5×10^{1}	4300 4300	Brockbank (2013) Odabasi et al. (2006) Mackay et al. (2006d) Mackay et al. (1995) Smith and Bomberger (1980) Keshavarz et al. (2022) Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	L M V V V Q Q Q ?	1 24 99 185, 21
o-phenanthroline $C_{12}H_8N_2$ [66-71-7] DGEZNRSVGBDHLK-UHFFFAOYSA-N	1.1×10^{5} 9.9×10^{3} 1.2×10^{5} 4.4×10^{2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291

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Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benzyladenine $C_{12}H_{11}N_5$ [1214-39-7] NWBJYWHLCVSVIJ-UHFFFAOYSA-N	1.1×10^{8} 1.1×10^{-1}		HSDB (2015) Maniere et al. (2011)	V ?	 241, 165
diquat $C_{12}H_{12}N_2$ [2764-72-9] SYJFEGQWDCRVNX-UHFFFAOYSA-N	2.8×10^{5}		Ebert et al. (2023)	?	318
MEIQ $C_{12}H_{12}N_4$ (2-amino-3,4-dimethylimidazo[4,5-f]quinoxaline) [77094-11-2] GMGWMIJIGUYNAY-UHFFFAOYSA-N	2.5×10^{7}		HSDB (2015)	Q	99
pyrimethanil $C_{12}H_{13}N_3$ [53112-28-0] ZLIBICFPKPWGIZ-UHFFFAOYSA-N	3.4×10^{2} 2.8×10^{2} 2.8×10^{2} 9.2×10^{2} 3.9 2.8×10^{2}	15000	Feigenbrugel and Le Calvé (2021) Duchowicz et al. (2020) Matthews (1998) Duchowicz et al. (2020) HSDB (2015) Maniere et al. (2011)	M V X Q Q ?	 186 562, 12 99 241, 165
paraquat $C_{12}H_{14}N_2$ [4685-14-7] INFDPOAKFNIJBF-UHFFFAOYSA-N	$>2.4\times10^{8}$		HSDB (2015)	V	
N,N-dimethyltryptamine $C_{12}H_{16}N_2$ [61-50-7] DMULVCHRPCFFGV-UHFFFAOYSA-N	1.5×10^{4}		HSDB (2015)	Q	99
benzo[*f*]quinoline $C_{13}H_9N$ [85-02-9] HCAUQPZEWLULFJ-UHFFFAOYSA-N	5.7×10^{1} 1.0×10^{2} 1.0×10^{2} 3.6		Duchowicz et al. (2020) Mackay et al. (2006d) Mackay et al. (1995) Smith and Bomberger (1980) Duchowicz et al. (2020)	V V V V Q	186 558 24
2,6-bis-(1,1-dimethylethyl)-pyridine $C_{13}H_{21}N$ (2,6-di-*tert*-butylpyridine) [585-48-8] UWKQJZCTQGMHKD-UHFFFAOYSA-N	8.0×10^{-4} 2.8×10^{-1}	6900	Arnett and Chawla (1979) Arnett and Chawla (1979)	M V	559 563

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Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
PHIP $C_{13}H_{12}N_4$ (2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine) [105650-23-5] UQVKZNNCIHJZLS-UHFFFAOYSA-N	3.5×10^{7}		HSDB (2015)	Q	99
N,N'-diphenylguanidine $C_{13}H_{13}N_3$ [102-06-7] OWRCNXZUPFZXOS-UHFFFAOYSA-N	1.4×10^{6}		HSDB (2015)	Q	99
acridine $C_{13}H_9N$ [260-94-6] DZBUGLKDJFMEHC-UHFFFAOYSA-N	3.3×10^{1} 3.3×10^{1} 2.5×10^{1}		Mackay et al. (2006d) Mackay et al. (1995) HSDB (2015)	V V Q	 99
phenanthridine $C_{13}H_9N$ [229-87-8] RDOWQLZANAYVLL-UHFFFAOYSA-N	6.0×10^{2} 3.6		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
mepanipyrim $C_{14}H_{13}N_3$ [110235-47-7] CIFWZNRJIBNXRE-UHFFFAOYSA-N	6.0×10^{2}		Maniere et al. (2011)	?	241, 165
cyprodinil $C_{14}H_{15}N_3$ [121552-61-2] HAORKNGNJCEJBX-UHFFFAOYSA-N	1.2×10^{2} 1.2×10^{2} 2.9×10^{3}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
imiquimod $C_{14}H_{16}N_4$ [99011-02-6] DOUYETYNHWVLEO-UHFFFAOYSA-N	1.2×10^{7}		HSDB (2015)	Q	99
ametoctradin $C_{15}H_{25}N_5$ [865318-97-4] GGKQIOFASHYUJZ-UHFFFAOYSA-N	2.4×10^{6}		Maniere et al. (2011)	?	12, 165
ferimzone $C_{15}H_{18}N_4$ [89269-64-7] GOWLARCWZRESHU-UHFFFAOYSA-N	1.6×10^{5} 2.4×10^{2}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
benz[c]acridine $C_{17}H_{11}N$ [225-51-4] OAPPEBNXKAKQGS-UHFFFAOYSA-N	3.7×10^{2}		HSDB (2015)	Q	447

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Table A4.2: Heterocycles with nitrogen (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
6-pentyl-1,2,3,4,7,8,9,10-octahydrophenanthridine	4.5×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_{18}H_{27}N$	2.0×10^{1}		Zhang et al. (2010)	Q	287, 289
[10594-03-3]	6.2		Zhang et al. (2010)	Q	287, 290
FNUATPIDZQSFPD-UHFFFAOYSA-N	2.2×10^{-2}		Zhang et al. (2010)	Q	287, 291
2-diphenylmethylpiperidine $C_{18}H_{21}N$ (desoxypipradrol) [519-74-4] RWTNXJXZVGHMGI-UHFFFAOYSA-N	6.6×10^{1}		HSDB (2015)	Q	99
fenpropidin	7.1×10^{2}	6200	Feigenbrugel and Le Calvé (2021)	M	33
$C_{19}H_{31}N$	1.1×10^{2}		Duchowicz et al. (2020)	V	186
[67306-00-7]	9.9×10^{-2}		Matthews (1998)	X	562, 12
MGNFYQILYYYUBS-UHFFFAOYSA-N	9.5×10^{-2}		Duchowicz et al. (2020)	Q	
	9.3×10^{-2}		Maniere et al. (2011)	?	165
N,N-bis(2-ethylhexyl)-1H-1,2,4-triazole-1-methanamine $C_{19}H_{38}N_4$ [91273-04-0] AVBBHCMDRGQBNW-UHFFFAOYSA-N	2.9×10^{1}		Ebert et al. (2023)	?	365
7H-dibenzo[c,g]carbazole	2.1×10^{3}		Smith and Bomberger (1980)	V	24
$C_{20}H_{13}N$	4.0×10^{3}		HSDB (2015)	Q	99
[194-59-2] STJXCDGCXVZHDU-UHFFFAOYSA-N					
porphyrin $C_{20}H_{14}N_4$ (porphin) [101-60-0] RKCAIXNGYQCCAL-YYOYBPFYSA-N	3.9×10^{5}		Abraham et al. (2019)	Q	
dibenz[a,j]acridine $C_{21}H_{13}N$ [224-42-0] ANUCHZVCBDOPOX-UHFFFAOYSA-N	5.2×10^{3}		HSDB (2015)	Q	99
dibenz[a,h]acridine $C_{21}H_{13}N$ [226-36-8] JNCSIWAONQTVCF-UHFFFAOYSA-N	5.2×10^{3}		HSDB (2015)	Q	99
1,3,5-tricyclohexylhexahydro-1,3,5-triazine	1.7×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{21}H_{39}N_3$	4.0×10^{5}		Zhang et al. (2010)	Q	287, 289
[6281-14-7]	1.2×10^{5}		Zhang et al. (2010)	Q	287, 290
ZLLRUEJANKJPQE-UHFFFAOYSA-N	1.5×10^{4}		Zhang et al. (2010)	Q	287, 291

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A4.3 Nitriles (C, H, N)

Table A4.3: Nitriles (C, H, N)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyano radical CN [2074-87-5] JEVCWSUVFOYBFI-UHFFFAOYSA-N	7.8×10^{-4}	1400	Berdnikov and Bazhin (1970)	T	47
hydrogen cyanide HCN (hydrocyanic acid) [74-90-8] LELOWRISYMNNSU-UHFFFAOYSA-N	8.9×10^{-2}	8200	Burkholder et al. (2019)	L	
	8.9×10^{-2}	8200	Burkholder et al. (2015)	L	
	1.7×10^{-1}	4400	Yoo et al. (1986)	L	1
	1.1×10^{-1}	5000	Edwards et al. (1978)	L	1
	8.9×10^{-2}	8200	Ma et al. (2010a)	M	
	7.5×10^{-2}		Riveros et al. (1998)	M	12
	1.2×10^{-1}		Fredenhagen and Wellmann (1932b)	M	
	9.2×10^{-2}		Hine and Weimar (1965)	R	
	9.9×10^{-2}	4200	Edwards et al. (1975)	T	1
	7.6×10^{-2}	2900	Kotlik and Lebedeva (1974)	X	564
	7.4×10^{-2}		Gaffney and Senum (1984)	X	389, 491
	5.0×10^{-2}		Keshavarz et al. (2022)	Q	
	4.2×10^{-2}		Duchowicz et al. (2020)	Q	184
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Modarresi et al. (2007)	Q	67
	4.7		Katritzky et al. (1998)	Q	
	7.4×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	1.1×10^{-1}		Yaws (1999)	?	21
ethanenitrile CH_3CN (acetonitrile) [75-05-8] WEVYAHXRMPXWCK-UHFFFAOYSA-N	5.2×10^{-1}	4000	Burkholder et al. (2019)	L	
	5.2×10^{-1}	4000	Burkholder et al. (2015)	L	
	4.9×10^{-1}	4300	Brockbank (2013)	L	1
	5.2×10^{-1}	4000	Sander et al. (2011)	L	
	5.2×10^{-1}	4000	Sander et al. (2006)	L	
	3.8×10^{-1}	4200	Plyasunov et al. (2006)	L	
	5.0×10^{-1}	4100	Fogg and Sangster (2003)	L	
	5.1×10^{-1}	4000	Staudinger and Roberts (2001)	L	
	4.7×10^{-1}	3500	Arijs and Brasseur (1986)	L	
	6.0×10^{-1}	6300	Hiatt (2013)	M	
	5.2×10^{-1}	4000	Ji and Evans (2007)	M	
	4.9×10^{-1}		Bebahani et al. (2002)	M	
	3.2×10^{-1}	3300	Hovorka et al. (2002)	M	11
	3.4×10^{-1}		Welke et al. (1998)	M	
	5.3×10^{-1}	4100	Benkelberg et al. (1995)	M	
	4.6×10^{-1}		Li and Carr (1993)	M	
	8.2×10^{-2}		Yu (1992)	M	12
	4.8×10^{-1}	3900	Snider and Dawson (1985)	M	
	5.3×10^{-1}	4100	Hamm et al. (1984)	M	
	3.7×10^{-2}		Abraham and Acree (2007)	V	
	5.0×10^{-1}		Hwang et al. (1992)	V	
	2.9×10^{-1}		Hine and Weimar (1965)	R	

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Table A4.3: Nitriles (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.9×10^{-1}		Gaffney and Senum (1984)	X	389
	4.7×10^{-1}		Hayer et al. (2022)	Q	20
	3.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	
	2.9×10^{-1}		Li et al. (2014)	Q	241
	7.7×10^{-1}		Hilal et al. (2008)	Q	
	3.7×10^{-1}		Modarresi et al. (2007)	Q	67
		4200	Kühne et al. (2005)	Q	
	2.9×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.9×10^{-1}		English and Carroll (2001)	Q	230, 231
	4.4		Katritzky et al. (1998)	Q	
	2.9×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	3.1×10^{-1}		Suzuki et al. (1992)	Q	232
	2.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	3.6×10^{-1}		Mackay et al. (2006d)	?	
		4300	Kühne et al. (2005)	?	
	4.9×10^{-1}		Yaws (1999)	?	21
	4.9×10^{-1}		Yaws and Yang (1992)	?	21
	2.9×10^{-1}		Abraham et al. (1990)	?	
propanenitrile	3.4×10^{-1}	4500	Brockbank (2013)	L	1
C_2H_5CN	2.4×10^{-1}	4800	Plyasunov et al. (2006)	L	
(propionitrile)	4.3×10^{-1}	6200	Hiatt (2013)	M	
[107-12-0]	3.3×10^{-1}	4600	Ji and Evans (2007)	M	
FVSKHRXBFJPNKK-UHFFFAOYSA-N	1.8×10^{-1}		Hovorka et al. (2002)	M	38
	2.5×10^{-1}		Li and Carr (1993)	M	
	1.9×10^{-1}		Hawthorne et al. (1985)	M	
	2.6×10^{-1}		Butler and Ramchandani (1935)	M	
	3.1×10^{-1}		Mackay et al. (2006d)	V	
	3.1×10^{-1}		Mackay et al. (1995)	V	
	1.7×10^{-1}		Howard (1990)	X	412
	3.5×10^{-1}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	
	5.0×10^{-1}		Hilal et al. (2008)	Q	
	2.6×10^{-1}		Modarresi et al. (2007)	Q	67
	2.9×10^{-1}		English and Carroll (2001)	Q	230, 231
	5.6×10^{-1}		Russell et al. (1992)	Q	279
	2.4×10^{-1}		Suzuki et al. (1992)	Q	232
	2.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	2.6×10^{-1}		Mackay et al. (2006d)	?	
	2.9×10^{-1}		Yaws (1999)	?	21
	2.7×10^{-1}		Abraham et al. (1990)	?	

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Table A4.3: Nitriles (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
butanenitrile	1.8×10^{-1}	5100	Brockbank (2013)	L	1
C_3H_7CN	1.8×10^{-1}	5100	Plyasunov et al. (2006)	L	
(butyronitrile)	2.7×10^{-1}	5100	Ji and Evans (2007)	M	
[109-74-0]	1.3×10^{-1}		Ramachandran et al. (1996)	M	
KVNRLNFWIYMESJ-UHFFFAOYSA-N	1.9×10^{-1}		Li and Carr (1993)	M	
	1.4×10^{-1}		Hawthorne et al. (1985)	M	
	1.9×10^{-1}		Butler and Ramchandani (1935)	M	
	1.8×10^{-1}		Yaws (2003)	X	258
	1.8×10^{-1}		Yaws (2003)	X	237
	3.7×10^{-1}		Dupeux et al. (2022)	Q	259
	1.2×10^{-1}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.8×10^{-1}		Gharagheizi et al. (2010)	Q	246
	3.5×10^{-1}		Hilal et al. (2008)	Q	
	1.5×10^{-1}		Modarresi et al. (2007)	Q	67
		4900	Kühne et al. (2005)	Q	
	1.5×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	5.7×10^{-2}		English and Carroll (2001)	Q	230, 274
	1.9×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	5.4×10^{-1}		Russell et al. (1992)	Q	279
	1.9×10^{-1}		Suzuki et al. (1992)	Q	232
	1.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	1.9×10^{-1}		Mackay et al. (2006d)	?	
		4700	Kühne et al. (2005)	?	
	1.8×10^{-1}		Yaws (1999)	?	21
	1.9×10^{-1}		Abraham et al. (1990)	?	
2-methylpropanenitrile	1.1×10^{-1}	5200	Brockbank (2013)	L	1
C_4H_7N	1.0×10^{-1}	4800	Plyasunov et al. (2006)	L	
(isobutyronitrile)	9.4×10^{-2}		Li and Carr (1993)	M	
[78-82-0]	1.8×10^{-1}		HSDB (2015)	Q	99
LRDFRRGEGBBSRN-UHFFFAOYSA-N	1.9×10^{-1}		Hilal et al. (2008)	Q	
		4900	Kühne et al. (2005)	Q	
		5100	Kühne et al. (2005)	?	
pentanenitrile	1.6×10^{-1}	6100	Brockbank (2013)	L	1
C_4H_9CN	1.4×10^{-1}	5500	Plyasunov et al. (2006)	L	
(butyl cyanide; valeronitrile)	1.4×10^{-1}		Li and Carr (1993)	M	
[110-59-8]	1.6×10^{-1}		Amoore and Buttery (1978)	V	
RFFFKMOABOFIDF-UHFFFAOYSA-N	2.7×10^{-1}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	67
	1.5×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	4.1×10^{-2}		English and Carroll (2001)	Q	230, 231
	1.5×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	1.5×10^{-1}		Abraham et al. (1990)	?	

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Table A4.3: Nitriles (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexanenitrile $C_6H_{11}N$ [628-73-9] AILKHAQXUAOOFU-UHFFFAOYSA-N	1.2×10^{-1} 2.3×10^{-1}		Plyasunov et al. (2006) Hilal et al. (2008)	L Q	
heptanenitrile $C_7H_{13}N$ [629-08-3] SDAXRHHPNYTELL-UHFFFAOYSA-N	1.6×10^{-1}		Hilal et al. (2008)	Q	
octanenitrile $C_8H_{15}N$ [124-12-9] YSIMAPNUZAVQER-UHFFFAOYSA-N	5.7×10^{-2} 1.3×10^{-1}		Plyasunov et al. (2006) Hilal et al. (2008)	L Q	
nonanenitrile $C_9H_{17}N$ [2243-27-8] PLZZPPHAMDJOSR-UHFFFAOYSA-N	1.0×10^{-1}		Hilal et al. (2008)	Q	
decanenitrile $C_{10}H_{19}N$ [1975-78-6] HBZDPWBWBJMYRY-UHFFFAOYSA-N	8.0×10^{-2}		Hilal et al. (2008)	Q	
undecanenitrile $C_{11}H_{21}N$ [2244-07-7] SZKKNEOUHLFYNA-UHFFFAOYSA-N	6.1×10^{-2}		Hilal et al. (2008)	Q	
cyclohexanecarbonitrile $C_7H_{11}N$ [766-05-2] VBWIZSYFQSOUFQ-UHFFFAOYSA-N	7.3×10^{-1}		Hilal et al. (2008)	Q	
ethanedinitrile C_2N_2 (cyanogen) [460-19-5] JMANVNJQNLATNU-UHFFFAOYSA-N	1.8×10^{-3} 1.8×10^{-3} 1.9×10^{-3} 1.9×10^{1} 1.8×10^{-3} 2.6×10^{-3} 2.9×10^{-2} 1.9×10^{-3} 1.8×10^{-3}		Duchowicz et al. (2020) HSDB (2015) Yaws (2003) Duchowicz et al. (2020) Gharagheizi et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Yaws (1999) Yaws and Yang (1992)	V V X Q Q Q Q ? ?	186 237, 12 246 67 21, 12 21, 12
pentanedinitrile $C_5H_6N_2$ [544-13-8] ZTOMUSMDRMJOTH-UHFFFAOYSA-N	7.8×10^{2}	7600	Plyasunov et al. (2006)	L	

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Table A4.3: Nitriles (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexanedinitrile	1.5×10^{3}	8000	Plyasunov et al. (2006)	L	
$C_6H_8N_2$	8.2×10^{3}		Duchowicz et al. (2020)	V	186
(adiponitrile)	8.2×10^{3}		HSDB (2015)	V	
[111-69-3]	2.4×10^{2}		Mackay et al. (2006d)	V	
BTGRAWJCKBQKAO-UHFFFAOYSA-N	2.4×10^{2}		Mackay et al. (1995)	V	
	2.3×10^{1}		Duchowicz et al. (2020)	Q	
	2.2×10^{3}		Hilal et al. (2008)	Q	
2-methylpentanedinitrile	3.3×10^{2}		HSDB (2015)	Q	99
$C_6H_8N_2$					
[4553-62-2]					
FPPLREPCQJZDAQ-UHFFFAOYSA-N					
tetramethylbutanedinitrile	1.9×10^{2}		HSDB (2015)	Q	99
$C_8H_{12}N_2$					
[3333-52-6]					
ZVQXQPNJHRNGID-UHFFFAOYSA-N					
2-propenenitrile	1.0×10^{-1}	3900	Brockbank (2013)	L	1
C_3H_3N	1.2×10^{-1}	6800	Hiatt (2013)	M	
(acrylonitrile)	7.6×10^{-2}		Hovorka et al. (2002)	M	38
[107-13-1]	3.1×10^{-2}		Welke et al. (1998)	M	
NLHHRLWOUZZQLW-UHFFFAOYSA-N	1.3×10^{-1}		Mackay et al. (2006d)	V	
	8.2×10^{-2}	3400	Fogg and Sangster (2003)	V	
	9.1×10^{-2}		Lide and Frederikse (1995)	V	
	1.3×10^{-1}		Mackay et al. (1995)	V	
	9.8×10^{-2}		Hwang et al. (1992)	V	
	1.1×10^{-1}	2800	Goldstein (1982)	X	298
	1.1×10^{-1}		Mackay et al. (1995)	C	
	1.1×10^{-1}		Ryan et al. (1988)	C	
	9.2×10^{-2}		Keshavarz et al. (2022)	Q	
	4.3×10^{-1}		Duchowicz et al. (2020)	Q	184
	2.2×10^{-2}		Hilal et al. (2008)	Q	
	4.6×10^{-1}		Modarresi et al. (2007)	Q	67
		3600	Kühne et al. (2005)	Q	
	7.2×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	9.0×10^{-2}		Mackay et al. (2006d)	?	
		3600	Kühne et al. (2005)	?	
	1.0×10^{-1}		Yaws (1999)	?	21, 12
2-butenenitrile	8.8×10^{-2}		Duchowicz et al. (2020)	V	186
C_4H_5N	1.5×10^{-1}		Duchowicz et al. (2020)	Q	
(crotononitrile)	2.7×10^{-1}		Modarresi et al. (2007)	Q	67
[4786-20-3]					
NKKMVIVFRUYPLQ-NSCUHMNNSA-N					

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Table A4.3: Nitriles (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-butenenitrile C_4H_5N (vinylacetonitrile) [109-75-1] SJNALLRHIVGIBI-UHFFFAOYSA-N	2.0×10^{-1}	4900	Brockbank (2013)	L	1
2-methyl-2-propene nitrile	3.6×10^{-2}	4200	Brockbank (2013)	L	1
C_4H_5N	5.4×10^{-2}	6700	Hiatt (2013)	M	
(methacrylonitrile)	4.0×10^{-2}		Duchowicz et al. (2020)	V	186
[126-98-7]	4.0×10^{-2}		HSDB (2015)	V	
GYCMBHHDWRMZGG-UHFFFAOYSA-N	1.2×10^{-1}		Duchowicz et al. (2020)	Q	
	1.7×10^{-2}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Modarresi et al. (2007)	Q	67
		4000	Kühne et al. (2005)	Q	
		4600	Kühne et al. (2005)	?	
benzenenitrile	3.5×10^{-1}	5600	Brockbank (2013)	L	1
C_6H_5CN	2.9×10^{-1}	5100	Lee et al. (2013)	M	
(benzonitrile)	1.9×10^{-1}		Duchowicz et al. (2020)	V	186
[100-47-0]	1.9×10^{-1}		HSDB (2015)	V	
JFDZBHWFFUWGJE-UHFFFAOYSA-N	1.9×10^{-1}		Mackay et al. (2006d)	V	
	3.9×10^{-1}		Schüürmann (2000)	V	
	1.9×10^{-1}		Mackay et al. (1995)	V	
	1.9×10^{-1}		Mackay et al. (1995)	V	
	5.0×10^{-1}		Abraham et al. (1994a)	R	
	2.3×10^{-1}		Duchowicz et al. (2020)	Q	
	1.3×10^{-1}		Li et al. (2014)	Q	241
	2.4×10^{-1}		Hilal et al. (2008)	Q	
	6.7×10^{-1}		Modarresi et al. (2007)	Q	67
		5900	Kühne et al. (2005)	Q	
	5.2×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.3		Katritzky et al. (1998)	Q	
	1.5×10^{-1}		Nirmalakhandan et al. (1997)	Q	
		6400	Kühne et al. (2005)	?	
	9.6×10^{-1}		Yaws (1999)	?	21, 415
	1.8×10^{-2}		Yaws and Yang (1992)	?	21, 415
	4.1×10^{-1}		Abraham et al. (1990)	?	
2-pyridinecarbonitrile $C_6H_4N_2$ [100-70-9] FFNVQNRYTPFDDP-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	99
3,3'-iminobispropanenitrile $C_6H_9N_3$ [111-94-4] SBAJRGRUGUQKAF-UHFFFAOYSA-N	2.0×10^{6}		HSDB (2015)	Q	99

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Table A4.3: Nitriles (C, H, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methylbenzonitrile C_8H_7N (o-tolunitrile) [529-19-1] NWPNXBQSRGKSJB-UHFFFAOYSA-N	7.6×10^{-1}		Schüürmann (2000)	V	
3-methylbenzonitrile	1.7×10^{-1}		Zhang et al. (2010)	Q	287, 288
C_8H_7N	3.4×10^{-1}		Zhang et al. (2010)	Q	287, 289
(m-tolunitrile)	8.8×10^{-1}		Zhang et al. (2010)	Q	287, 290
[620-22-4]	1.8×10^{-1}		Zhang et al. (2010)	Q	287, 291
BOHCMQZJWOGWTA-UHFFFAOYSA-N					
benzeneacetonitrile	1.1	6800	Brockbank (2013)	L	1
C_8H_7N	7.0×10^{-2}		HSDB (2015)	V	
(phenylacetonitrile)	1.0×10^{1}		Hilal et al. (2008)	Q	
[140-29-4]		6200	Kühne et al. (2005)	Q	
SUSQOBVLVYHIEX-UHFFFAOYSA-N		5100	Kühne et al. (2005)	?	
1,2-benzenedicarbonitrile $C_8H_4N_2$ [91-15-6] XQZYPMVTSDWCCE-UHFFFAOYSA-N	2.0×10^{1}		HSDB (2015)	Q	99
3,7-dimethyl-2,6-octadienenitrile $C_{10}H_{15}N$ (geranyl nitrile) [5146-66-7] HLCSDJLATUNSSI-JXMROGBWSA-N	2.9×10^{-2}		Helburn et al. (2008)	M	
2,2'-azobis(2-methylbutyronitrile)	4.5×10^{4}		Zhang et al. (2010)	Q	287, 288
$C_{10}H_{16}N_4$	9.2×10^{1}		Zhang et al. (2010)	Q	287, 289
[13472-08-7]	1.5×10^{1}		Zhang et al. (2010)	Q	287, 290
AVTLBBWTUPQRAY-UHFFFAOYSA-N	4.4×10^{-1}		Zhang et al. (2010)	Q	287, 291

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A4.4 Amines, amides, amino acids (C, H, O, N)

Table A4.4: Amines, amides, amino acids (C, H, O, N)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
formamide	7.1×10^{3}		Duchowicz et al. (2020)	V	186
CH_3NO	7.0×10^{3}		HSDB (2015)	V	
[75-12-7]	2.3×10^{2}		Duchowicz et al. (2020)	Q	
ZHNUHDYFZUAESO-UHFFFAOYSA-N					
methyl nitrite	1.5×10^{-1}		HSDB (2015)	Q	99
CH_3ONO					
[624-91-9]					
BLLFVUPNHCTMSV-UHFFFAOYSA-N					
urea	5.7×10^{6}		Duchowicz et al. (2020)	V	186
CH_4N_2O	5.7×10^{6}		HSDB (2015)	V	
[57-13-6]	1.0×10^{7}		Mackay et al. (2006d)	V	
XSQUKJJJFZCRTK-UHFFFAOYSA-N	1.0×10^{7}		Mackay et al. (1995)	V	
	1.1×10^{5}		Duchowicz et al. (2020)	Q	
ethanolamine	4.2×10^{3}	8300	Kim et al. (2008)	M	550
$HOC_2H_4NH_2$	6.0×10^{4}		Bone et al. (1983)	M	12
[141-43-5]	1.1×10^{4}		Modarresi et al. (2007)	Q	67
HZAXFHJVJLSVMW-UHFFFAOYSA-N	9.7×10^{2}	5800	Nguyen (2013)	?	565, 11
1,1'-azodiformamide	1.2×10^{7}		HSDB (2015)	V	
$C_2H_4N_4O_2$					
[123-77-3]					
XOZUGNYVDXMRKW-UHFFFAOYSA-N					
ethyl nitrite	1.1×10^{-1}		HSDB (2015)	Q	99
C_2H_5ONO					
[109-95-5]					
QQZWEECEMNQSTG-UHFFFAOYSA-N					
carbamic acid, methyl ester	2.5×10^{2}		HSDB (2015)	Q	99
$C_2H_5NO_2$					
[598-55-0]					
GTCAXTIRRLKXRU-UHFFFAOYSA-N					
acetaldoxime	1.7		HSDB (2015)	Q	447
C_2H_5NO					
(acetaldehyde oxime)					
[107-29-9]					
FZENGILVLUJGJX-UHFFFAOYSA-N					

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethanamide	5.3×10^3		Wolfenden (1976)	M	
C_2H_5NO	2.8×10^3		Mackay et al. (2006d)	V	
(acetamide)	2.8×10^3		Mackay et al. (1995)	V	
[60-35-5]	3.8×10^3		Yaws (2003)	X	237
DLFVBJFMPXGRIB-UHFFFAOYSA-N	9.0×10^2		HSDB (2015)	Q	99
	2.8×10^3		Gharagheizi et al. (2012)	Q	
	3.7×10^3		Gharagheizi et al. (2010)	Q	246
	4.2×10^3		Hilal et al. (2008)	Q	
	5.1×10^3		Modarresi et al. (2007)	Q	67
	2.2×10^3		Yaffe et al. (2003)	Q	248, 249
	2.2×10^2		Katritzky et al. (1998)	Q	
N-methylmethanamide	1.4×10^3	7200	Burkholder et al. (2019)	L	
C_2H_5NO	1.4×10^3	7200	Burkholder et al. (2015)	L	
(N-methylformamide)	1.4×10^3	7200	Brockbank (2013)	L	1
[123-39-7]	1.5×10^3	7600	Bernauer and Dohnal (2008)	M	1
ATHHXGZTWNVVOU-UHFFFAOYSA-N	5.0×10^2		Duchowicz et al. (2020)	V	186
	4.9×10^2		HSDB (2015)	V	
	9.7×10^1		Duchowicz et al. (2020)	Q	
	5.6×10^2		Hilal et al. (2008)	Q	
	1.6×10^2		Modarresi et al. (2007)	Q	67
N-nitrosodimethylamine	3.9		Burkholder et al. (2019)	L	
$C_2H_6N_2O$	3.9		Burkholder et al. (2015)	L	
[62-75-9]	2.9×10^{-1}	13000	Thompson et al. (2018)	M	
UMFJAHHVKNCGLG-UHFFFAOYSA-N	4.1		Haruta et al. (2011)	M	12
	6.1	6400	Klein (1982)	M	
	5.2		Mirvish et al. (1976)	M	14
	3.0×10^{-1}		Mackay et al. (1995)	C	
	9.5		Hilal et al. (2008)	Q	
	3.6		Modarresi et al. (2007)	Q	67
	3.0×10^{-1}		Mackay et al. (2006d)	?	
methylnitrosourea	$>1.9\times10^2$		Mirvish et al. (1976)	M	14
$C_2H_5N_3O_2$					
[684-93-5]					
ZRKWMRDKSOPRRS-UHFFFAOYSA-N					
ethanediamide	5.0×10^5		Duchowicz et al. (2020)	V	186
$C_2H_4N_2O_2$	2.2×10^6		Duchowicz et al. (2020)	Q	
[471-46-5]					
YIKSCQDJHCMVMK-UHFFFAOYSA-N					
nitrosoazetidine	$>1.9\times10^2$		Mirvish et al. (1976)	M	14
$C_3H_6N_2O$					
[15216-10-1]					
SNKTZBNDUVWOAZ-UHFFFAOYSA-N					

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methylnitrosoacetamide $C_3H_6N_2O_2$ [7417-67-6] FFLFWNRFMZRFKU-UHFFFAOYSA-N	8.6×10^{-2}		Mirvish et al. (1976)	M	14
ethylnitrosocyanamide $C_3H_5N_3O$ [38434-77-4] LMIMSGCBKHFTDY-UHFFFAOYSA-N	2.6×10^{-1}		Mirvish et al. (1976)	M	14
2-propenamide	5.8×10^{3}		Duchowicz et al. (2020)	V	186
C_3H_5NO	5.5×10^{3}		HSDB (2015)	V	
(acrylamide)	6.9×10^{3}		Mackay et al. (2006d)	V	
[79-06-1]	3.1×10^{4}		Lide and Frederikse (1995)	V	
HRPVXLWXLXDGHG-UHFFFAOYSA-N	6.9×10^{3}		Mackay et al. (1995)	V	
	2.9×10^{4}		Yaws (2003)	X	237, 38
	4.1×10^{2}		Duchowicz et al. (2020)	Q	
	7.3×10^{2}		Gharagheizi et al. (2012)	Q	
	2.9×10^{4}		Gharagheizi et al. (2010)	Q	246
	4.1×10^{3}		Hilal et al. (2008)	Q	
	7.3×10^{3}		Modarresi et al. (2007)	Q	67
		8400	Kühne et al. (2005)	Q	
		7900	Kühne et al. (2005)	?	
methylvinylnitrosamine $C_3H_6N_2O$ (N-nitrosomethylvinylamine) [4549-40-0] AWZVYNHQGTZJIH-UHFFFAOYSA-N	2.7		HSDB (2015)	Q	99
urethane	1.5×10^{2}		Duchowicz et al. (2020)	V	186
$C_3H_7NO_2$	1.5×10^{2}		HSDB (2015)	V	
[51-79-6]	2.5×10^{1}		Duchowicz et al. (2020)	Q	
JOYRKODLDBILNP-UHFFFAOYSA-N	1.1×10^{1}		Hilal et al. (2008)	Q	
	6.4×10^{1}		Modarresi et al. (2007)	Q	67
	7.3×10^{1}		Katritzky et al. (1998)	Q	
propanamide C_3H_7NO (propionamide) [79-05-0] QLNJFJADRCOGBJ-UHFFFAOYSA-N	3.3×10^{3}	8800	Plyasunov et al. (2001)	T	
N,N-dimethylmethanamide	1.3×10^{2}	6600	Burkholder et al. (2019)	L	
C_3H_7NO	1.3×10^{2}	6600	Burkholder et al. (2015)	L	
(N,N-dimethylformamide)	1.4×10^{2}	7700	Brockbank (2013)	L	1, 566
[68-12-2]	1.6×10^{2}	7500	Bernauer and Dohnal (2008)	M	1
ZMXDDKWLCZADIW-UHFFFAOYSA-N	2.2×10^{2}		Abraham et al. (1994a)	R	
	4.5×10^{1}		Hilal et al. (2008)	Q	
	5.8		Modarresi et al. (2007)	Q	67

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.6×10^{1}		Katritzky et al. (1998)	Q	
	2.2×10^{2}		Nirmalakhandan et al. (1997)	Q	
	1.6×10^{2}		Taft et al. (1985)	Q	
N-methylacetamide C_3H_7NO [79-16-3] OHLUUHNLEMFGTQ-UHFFFAOYSA-N	2.1×10^{3}	7600	Burkholder et al. (2019)	L	
	2.1×10^{3}	7600	Burkholder et al. (2015)	L	
	3.2×10^{3}	8900	Bernauer and Dohnal (2008)	M	1
	2.3×10^{2}		Duchowicz et al. (2020)	V	186
	2.3×10^{2}		HSDB (2015)	V	
	3.8×10^{1}		Duchowicz et al. (2020)	Q	
	1.4×10^{2}		Modarresi et al. (2007)	Q	67
N-methyl-N-nitrosoethanamine $C_3H_8N_2O$ (N-nitrosomethylethylamine) [10595-95-6] RTDCJKARQCRONF-UHFFFAOYSA-N	6.9		HSDB (2015)	Q	447
2-methoxyethanamine C_3H_9NO (2-methoxyethylamine) [109-85-3] ASUDFOJKTJLAIK-UHFFFAOYSA-N	2.5×10^{1}	7600	Cabani et al. (1978)	T	
2-(methylamino)ethanol C_3H_9NO [109-83-1] OPKOKAMJFNKNAS-UHFFFAOYSA-N	9.0×10^{1}		HSDB (2015)	V	
1-amino-2-propanol C_3H_9NO [78-96-6] HXKKHQJGJAFBHI-UHFFFAOYSA-N	4.2×10^{4}		HSDB (2015)	Q	545
2-amino-1-propanol C_3H_9NO (alaninol) [6168-72-5] BKMMTJMQCTUHRP-UHFFFAOYSA-N	1.3×10^{3}	7700	Nguyen (2013)	M	11
N-nitroso-N-methylurethane $C_4H_8N_2O_3$ (N-nitroso-N-methylurethane) [615-53-2] CAUBWLYZCDDYEF-UHFFFAOYSA-N	3.9×10^{-1}		Mirvish et al. (1976)	M	14
	1.8		Duchowicz et al. (2020)	V	186
	1.8		HSDB (2015)	V	
	1.6×10^{1}		Duchowicz et al. (2020)	Q	
	3.2×10^{1}		Modarresi et al. (2007)	Q	67
dinitrosopiperazine $C_4H_8N_4O_2$ [140-79-4] WNSYEWGYAFFSSQ-UHFFFAOYSA-N	$>1.9\times10^{2}$		Mirvish et al. (1976)	M	14

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-amino-3(methylamino)propionic acid $C_4H_{10}N_2O_2$ (3-(methylamino)-(DL)-alanine) [16676-91-8] UJVHVMNGOZXSOZ-UHFFFAOYSA-N	2.9×10^{7}		HSDB (2015)	Q	99
N-nitrosodiethanolamine $C_4H_{10}N_2O_3$ [1116-54-7] YFCDLVPYFMHRQZ-UHFFFAOYSA-N	2.0×10^{6}		HSDB (2015)	Q	447
N-nitrosodiethylamine $C_4H_{10}N_2O$ [55-18-5] WBNQDOYYEUMPFS-UHFFFAOYSA-N	1.2×10^{-2}	3800	Thompson et al. (2018)	M	
	5.6	6300	Klein (1982)	M	
	1.4		Mirvish et al. (1976)	M	14
	7.1×10^{-1}		Keshavarz et al. (2022)	Q	
	7.5		Duchowicz et al. (2020)	Q	184
	3.9		Hilal et al. (2008)	Q	
	2.6		Modarresi et al. (2007)	Q	67
	2.7		Duchowicz et al. (2020)	?	185, 21
diethanolamine $C_4H_{11}NO_2$ [111-42-2] ZBCBWPMODOFKDW-UHFFFAOYSA-N	3.3×10^{3}	1300	Nguyen (2013)	M	11
	2.6×10^{5}		Duchowicz et al. (2020)	V	186
	2.5×10^{5}		HSDB (2015)	V	
	1.0×10^{4}		Duchowicz et al. (2020)	Q	
diglycolamine $C_4H_{11}NO_2$ [929-06-6] GIAFURWZWWWBQT-UHFFFAOYSA-N	6.1×10^{3}	3700	Nguyen (2013)	M	33, 11
3-methoxy-1-propanamine $C_4H_{11}NO$ (3-methoxypropylamine) [5332-73-0] FAXDZWQIWUSWJH-UHFFFAOYSA-N	2.1×10^{1}		Du et al. (2017)	M	478
	4.8×10^{1}	8700	Cabani et al. (1978)	T	
	4.9×10^{1}		Du et al. (2017)	Q	549
	1.4×10^{1}		Du et al. (2017)	Q	
2-amino-2-methyl-1-propanol $C_4H_{11}NO$ [124-68-5] CBTVGIZVANVGBH-UHFFFAOYSA-N	2.1×10^{2}		Du et al. (2017)	M	478
	7.0×10^{2}	8500	Nguyen (2013)	M	11
	1.8×10^{2}		Du et al. (2017)	Q	549
	9.3×10^{1}		Du et al. (2017)	Q	
N,N-dimethylaminoethanol $C_4H_{11}NO$ (dimethylethanolamine) [108-01-0] UEEJHVSXFDXPFK-UHFFFAOYSA-N	9.3×10^{1}	7900	Nguyen (2013)	M	11
	2.6×10^{1}		Duchowicz et al. (2020)	V	186
	4.4×10^{2}		Duchowicz et al. (2020)	Q	

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-[(2-aminoethyl)amino]ethanol $C_4H_{12}N_2O$ [111-41-1] LHIJANUOQQMGNT-UHFFFAOYSA-N	9.0×10^{7}		HSDB (2015)	Q	99
tetramethylammonium hydroxide $C_4H_{13}NO$ [75-59-2] WGTYBPLFGIVFAS-UHFFFAOYSA-M	2.3×10^{10}		HSDB (2015)	Q	99
methacrylamide C_4H_7NO [79-39-0] FQPSGWSUVKBHSU-UHFFFAOYSA-N	8.8×10^{3}		Ebert et al. (2023)	?	316
acetone cyanohydrin C_4H_7NO [75-86-5] MWFMGBPGAXYFAR-UHFFFAOYSA-N	8.0×10^{1}		HSDB (2015)	V	
carbamic acid, 1-methylethyl ester $C_4H_9NO_2$ [1746-77-6] OVPLZYJGTGDFNB-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	99
propylcarbamate $C_4H_9NO_2$ [627-12-3] YNTOKMNHRPSGFU-UHFFFAOYSA-N	1.0×10^{2}		HSDB (2015)	V	
butanamide C_4H_9NO [541-35-5] DNSISZSEWVHGLH-UHFFFAOYSA-N	3.6×10^{3}		Ebert et al. (2023)	?	316
N,N-dimethylacetamide C_4H_9NO [127-19-5] FXHOOIRPVKKKFG-UHFFFAOYSA-N	6.1×10^{1} 6.1×10^{1} 4.4×10^{2} 4.4×10^{2} 1.7×10^{2} 1.3×10^{1} 3.6×10^{2}	7800 7800 8000 8600	Burkholder et al. (2019) Burkholder et al. (2015) Brockbank (2013) Bernauer and Dohnal (2008) Hilal et al. (2008) Modarresi et al. (2007) Taft et al. (1985)	L L L M Q Q Q	 1 1 67
2-butanone, oxime C_4H_9NO [96-29-7] WHIVNJATOVLWBW-UHFFFAOYSA-N	8.1		HSDB (2015)	V	

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
nitrosoethylurethane $C_5H_{10}N_2O_3$ (N-ethyl-N-nitrosourethane) [614-95-9] RAUQLNDTFONODT-UHFFFAOYSA-N	5.2×10^2		HSDB (2015)	Q	99
N,N-diethylmethanamide $C_5H_{11}NO$ (N,N-diethylformamide) [617-84-5] SUAKHGWARZSWIH-UHFFFAOYSA-N	1.3×10^2		Yaffe et al. (2003)	Q	248, 249
N-nitroso-N-butylurea $C_5H_{11}N_3O_2$ [869-01-2] LSWOCDLIYSKTRX-UHFFFAOYSA-N	4.3×10^4		HSDB (2015)	Q	99
N-methyldiethanolamine	3.3×10^3		Du et al. (2017)	M	478
$C_5H_{13}NO_2$	3.9×10^3	3800	Nguyen (2013)	M	11
[105-59-9]	4.0×10^5	12000	Kim et al. (2008)	M	550
CRVGTESFCCXCTH-UHFFFAOYSA-N	3.1×10^5		Duchowicz et al. (2020)	V	186
	3.2×10^5		HSDB (2015)	V	
	1.3×10^5		Duchowicz et al. (2020)	Q	
	2.4×10^3		Du et al. (2017)	Q	549
	1.9×10^3		Du et al. (2017)	Q	
methylbutylnitrosamine $C_5H_{12}N_2O$ [7068-83-9] PKTSCJXWLVREKX-UHFFFAOYSA-N	1.7		Mirvish et al. (1976)	M	14
2-(isopropylamino)ethanol	1.1×10^2		Du et al. (2017)	M	478
$C_5H_{13}NO$	1.4×10^1		Du et al. (2017)	Q	549
[109-56-8]	5.4×10^1		Du et al. (2017)	Q	
RILLZYSZSDGYGV-UHFFFAOYSA-N					
3-(dimethylamino)-1,2-propanediol	6.7×10^2		Du et al. (2017)	M	478
$C_5H_{13}NO_2$	6.1×10^3		Du et al. (2017)	Q	549
[623-57-4]	6.4×10^2		Du et al. (2017)	Q	
QCMHUGYTOGXZIW-UHFFFAOYSA-N					
2-amino-2-ethyl-1,3-propanediol	7.1×10^2		Du et al. (2017)	M	478
$C_5H_{13}NO_2$	4.0×10^4		Du et al. (2017)	Q	549
[115-70-8]	2.7×10^3		Du et al. (2017)	Q	
IOAOAKDONABGPZ-UHFFFAOYSA-N					
daminozide	2.3×10^4		Duchowicz et al. (2020)	V	186
$C_6H_{11}NO_3$	4.1×10^3		Duchowicz et al. (2020)	Q	
[1596-84-5]	7.0×10^1		Maniere et al. (2011)	?	165
NOQGZXFMHARMLW-UHFFFAOYSA-N					

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methylpentylnitrosamine $C_6H_{14}N_2O$ [13256-07-0] KSFCDINBDBFFSI-UHFFFAOYSA-N	2.0		Mirvish et al. (1976)	M	14
ethylbutylnitrosamine $C_6H_{14}N_2O$ [4549-44-4] ZGMCNGHHUQZNIH-UHFFFAOYSA-N	9.9×10^{-1}		Mirvish et al. (1976)	M	14
nitrosohexamethyleneimine $C_6H_{12}N_2O$ [932-83-2] UZMVSVHUTOAPTD-UHFFFAOYSA-N	4.3×10^{1}		Mirvish et al. (1976)	M	14
2,6-dimethylnitrosomorpholine $C_6H_{12}N_2O_2$ [1456-28-6] DPYMAXOKJUBANR-UHFFFAOYSA-N	3.5×10^{1}		Mirvish et al. (1976)	M	14
2,6-dimethyldinitrosopiperazine $C_6H_{12}N_4O_2$ [55380-34-2] JIWAGFGPBKDFQN-UHFFFAOYSA-N	$>1.9\times10^{2}$		Mirvish et al. (1976)	M	14
N-(1-methylethyl)-2-propenamide $C_6H_{11}NO$ (N-isopropylacrylamide) [2210-25-5] QNILTEGFHQSKFF-UHFFFAOYSA-N	4.3×10^{2}		HSDB (2015)	Q	99
hexanamide $C_6H_{13}NO$ [628-02-4] ALBYIUDWACNRRB-UHFFFAOYSA-N	1.8×10^{3}		Ebert et al. (2023)	?	316
N-butylacetamide $C_6H_{13}NO$ [1119-49-9] GYLDXXLJMRTVSS-UHFFFAOYSA-N	2.7×10^{3} 5.2×10^{2}		Gibbs et al. (1991) Hilal et al. (2008)	M Q	
N-(1-methylethyl)-N-nitroso-2-propanamine $C_6H_{14}N_2O$ (nitrosodiisopropylamine) [601-77-4] AUIKJTGFPFLMFP-UHFFFAOYSA-N	1.2 3.4×10^{-1} 1.1		Mirvish et al. (1976) Hilal et al. (2008) Modarresi et al. (2007)	M Q Q	14 67

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-nitrosodipropylamine	1.8		Mirvish et al. (1976)	M	14
$C_6H_{14}N_2O$	2.8		Mackay et al. (2006d)	V	
(N,N-dipropylnitrosamine)	2.8		Mackay et al. (1995)	V	
[621-64-7]	1.6		Mackay et al. (1995)	C	
YLKFDHTUAUWZPQ-UHFFFAOYSA-N	5.8		Hilal et al. (2008)	Q	
	1.3		Modarresi et al. (2007)	Q	67
N-(2-hydroxyethyl)piperazine	2.9×10^3	6400	Nguyen (2013)	M	33, 11
$C_6H_{14}N_2O$					
[103-76-4]					
WFCSWCVEJLETKA-UHFFFAOYSA-N					
N-ethyldiethanolamine	9.0×10^4		HSDB (2015)	Q	99
$C_6H_{15}NO_2$					
[139-87-7]					
AKNUHUCEWALCOI-UHFFFAOYSA-N					
triethanolamine	1.4×10^7		Duchowicz et al. (2020)	V	186
$C_6H_{15}NO_3$	1.4×10^7		HSDB (2015)	V	
[102-71-6]	3.3×10^7		Duchowicz et al. (2020)	Q	
GSEJCLTVZPLZKY-UHFFFAOYSA-N					
o-aminophenol	4.9×10^4		HSDB (2015)	Q	99
C_6H_7NO					
(2-aminophenol)					
[95-55-6]					
CDAWCLOXVUBKRW-UHFFFAOYSA-N					
4-aminophenol	2.7×10^4		Duchowicz et al. (2020)	V	186
C_6H_7NO	2.7×10^4		HSDB (2015)	V	
[123-30-8]	1.8×10^4		Duchowicz et al. (2020)	Q	
PLIKAWJENQZMHA-UHFFFAOYSA-N					
3-aminophenol	3.7×10^4		HSDB (2015)	Q	99
C_6H_7NO					
[591-27-5]					
CWLKGDAVCFYWJK-UHFFFAOYSA-N					
4-(2-hydroxyethyl)morpholine	1.4×10^3		Du et al. (2017)	M	478
$C_6H_{13}NO_2$	6.0×10^1		Du et al. (2017)	Q	549
[622-40-2]	1.7×10^3		Du et al. (2017)	Q	
KKFDCBRMNNSAAW-UHFFFAOYSA-N					
4-hydroxy-N-methylpiperidine	1.3×10^3		Du et al. (2017)	M	478
$C_6H_{13}NO$	4.6×10^3		Du et al. (2017)	Q	549
[106-52-5]	1.1×10^3		Du et al. (2017)	Q	
BAUWRHPMUVYFOD-UHFFFAOYSA-N					

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dimethylaminoethoxyethanol	8.3×10^2		Du et al. (2017)	M	478
$C_6H_{15}NO_2$	4.3×10^3	8500	Nguyen (2013)	M	11
[1704-62-7]	5.6×10^2		Du et al. (2017)	Q	549
YSAANLSYLSUVHB-UHFFFAOYSA-N	6.2×10^2		Du et al. (2017)	Q	
2-(diethylamino)ethanol	5.9		Du et al. (2017)	M	478
$C_6H_{15}NO$	3.2		Du et al. (2017)	Q	549
[100-37-8]	1.8×10^1		Du et al. (2017)	Q	
BFSVOASYOCHEOV-UHFFFAOYSA-N					
bis(2-methoxyethyl)amine	1.1×10^2		Du et al. (2017)	M	478
$C_6H_{15}NO_2$	2.3×10^2		Du et al. (2017)	Q	549
[111-95-5]	1.5×10^2		Du et al. (2017)	Q	
IBZKBSXREAQDTO-UHFFFAOYSA-N					
cyclohexanone oxime	4.3×10^1		Duchowicz et al. (2020)	V	186
$C_6H_{11}NO$	1.4×10^1		Duchowicz et al. (2020)	Q	
[100-64-1]					
VEZUQRBDRNJBJY-UHFFFAOYSA-N					
p-diaminoanisole	2.5×10^5		HSDB (2015)	Q	99
$C_7H_{10}N_2O$					
(2-methoxy-1,4-benzenediamine)					
[5307-02-8]					
HGUYBLVGLMAUFF-UHFFFAOYSA-N					
4-methoxy-1,3-benzenediamine	1.4×10^4		HSDB (2015)	Q	99
$C_7H_{10}N_2O$					
[615-05-4]					
BAHPQISAXRFLCL-UHFFFAOYSA-N					
2-cyano-N-[(ethylamino)carbonyl]-2-(methoxyimino)acetamide	3.0×10^4		Duchowicz et al. (2020)	V	186
$C_7H_{10}N_4O_3$	3.0×10^4		HSDB (2015)	V	
(cymoxanil)	6.2×10^2		Barcelo and Hennion (1997)	X	567
[57966-95-7]	9.9×10^8		Duchowicz et al. (2020)	Q	
XERJKGMBORTKEO-UHFFFAOYSA-N	3.2×10^1		Goodarzi et al. (2010)	Q	568, 569
	2.6×10^4		Maniere et al. (2011)	?	241, 493, 165
	3.0×10^4		Maniere et al. (2011)	?	241, 570, 165
isocyanatocyclohexane	5.8×10^{-3}		HSDB (2015)	Q	99
$C_7H_{11}NO$					
[3173-53-3]					
KQWGXHWJMSMDJJ-UHFFFAOYSA-N					

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
L-theanine $C_7H_{14}N_2O_3$ [3081-61-6] DATAGRPVKZEWHA-YFKPBYRVSA-N	1.1×10^{10}		HSDB (2015)	Q	447
tetryl $C_7H_5N_5O_8$ [479-45-8] AGUIVNYEYSCPNI-UHFFFAOYSA-N	3.7×10^{3}		HSDB (2015)	Q	99
anthranilic acid $C_7H_7NO_2$ [118-92-3] RWZYAGGXGHYGMB-UHFFFAOYSA-N	2.6×10^{5}		HSDB (2015)	Q	99
3-aminobenzoic acid $C_7H_7NO_2$ [99-05-8] XFDUHJPVQKIXHO-UHFFFAOYSA-N	3.7×10^{6}		Ebert et al. (2023)	?	316
4-aminobenzoic acid $C_7H_7NO_2$ [150-13-0] ALYNCZNDIQEVRV-UHFFFAOYSA-N	6.6×10^{4}		HSDB (2015)	V	
salicylamide $C_7H_7NO_2$ [65-45-2] SKZKKFZAGNVIMN-UHFFFAOYSA-N	2.0×10^{4} 3.4×10^{4}		Abraham et al. (2019) HSDB (2015)	Q Q	 99
mesalamine $C_7H_7NO_3$ [89-57-6] KBOPZPXVLCULAV-UHFFFAOYSA-N	2.0×10^{6}		HSDB (2015)	Q	99
N-phenylformamide C_7H_7NO [103-70-8] DYDNPESBYVVLBO-UHFFFAOYSA-N	1.2×10^{3}		HSDB (2015)	Q	99
benzamide C_7H_7NO [55-21-0] KXDAEFPNCMNJSK-UHFFFAOYSA-N	 2.2×10^{4} 4.7×10^{4} 5.2×10^{3} 9.0×10^{2} 3.8×10^{3} 2.7×10^{4} 8.2×10^{3} 4.0×10^{4} 4.0×10^{4}		Mackay et al. (2006d) Mackay et al. (1995) Abraham et al. (1994a) Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Nirmalakhandan et al. (1997) Duchowicz et al. (2020) HSDB (2015)	V V R Q Q Q Q Q ? ?	558 299 67 185, 21 419

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
anthranilamide $C_7H_8N_2O$ (2-aminobenzamide) [88-68-6] PXBFMLJZNCDSMP-UHFFFAOYSA-N	1.3×10^7		HSDB (2015)	Q	99
N-methyl-N-nitrosobenzenamine $C_7H_8N_2O$ [614-00-6] MAXCWSIJKVASQC-UHFFFAOYSA-N	2.0		HSDB (2015)	Q	99
2-methoxy-benzenamine C_7H_9NO (2-methoxyaniline) [90-04-0] VMPITZXILSNTON-UHFFFAOYSA-N	1.1×10^1 1.2×10^1 6.7×10^1 1.1×10^1 2.8×10^1 5.6 1.5×10^1		Duchowicz et al. (2020) Abraham et al. (1994a) Duchowicz et al. (2020) HSDB (2015) Hilal et al. (2008) Modarresi et al. (2007) Nirmalakhandan et al. (1997)	V R Q Q Q Q Q	186 99 67
3-methoxy-benzenamine C_7H_9NO (3-methoxyaniline) [536-90-3] NCBZRJODKRCREW-UHFFFAOYSA-N	9.0×10^1 9.0×10^1 1.8×10^2 2.8×10^1 6.4×10^1 1.5×10^1		Abraham et al. (1994a) HSDB (2015) Hilal et al. (2008) Modarresi et al. (2007) English and Carroll (2001) Nirmalakhandan et al. (1997)	R Q Q Q Q Q	 99 67 230, 231
4-methoxy-benzenamine C_7H_9NO (4-methoxyaniline) [104-94-9] BHAAPTBBJKJZER-UHFFFAOYSA-N	1.5×10^2 1.2×10^2 1.8×10^2 5.8×10^1 1.4×10^2 2.8×10^1 9.9×10^1 1.5×10^1 1.5×10^2		Altschuh et al. (1999) Abraham et al. (1994a) Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) English and Carroll (2001) Nirmalakhandan et al. (1997) Duchowicz et al. (2020)	M R Q Q Q Q Q Q ?	 67 230, 231 185, 21
4-(methylamino)phenol C_7H_9NO (N-methyl-4-aminophenol) [150-75-4] ZFIQGRISGKSVAG-UHFFFAOYSA-N	2.2×10^4		HSDB (2015)	Q	99
3-(diethylamino)-1,2-propanediol $C_7H_{17}NO_2$ [621-56-7] LTACQVCHVAUOKN-UHFFFAOYSA-N	5.4×10^2 7.0×10^2 2.6×10^2		Du et al. (2017) Du et al. (2017) Du et al. (2017)	M Q Q	478 549

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-(2-hydroxyethyl)piperidine $C_7H_{15}NO$ (2-piperidinoethanol) [3040-44-6] KZTWONRVIPPDKH-UHFFFAOYSA-N	5.1×10^{1} 6.1×10^{-1} 4.9×10^{1}		Du et al. (2017) Du et al. (2017) Du et al. (2017)	M Q Q	478 549
2-piperidineethanol $C_7H_{15}NO$ [1484-84-0] PTHDBHDZSMGHKF-UHFFFAOYSA-N	3.9×10^{2} 1.2×10^{2} 2.3×10^{2}		Du et al. (2017) Du et al. (2017) Du et al. (2017)	M Q Q	478 549
emylcamate $C_7H_{15}NO_2$ [78-28-4] SLWGJZPKHAXZQL-UHFFFAOYSA-N	3.0×10^{-1} 8.7		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
defenuron $C_8H_{10}N_2O$ [1007-36-9] SQBHGDSDVWCPHN-UHFFFAOYSA-N	8.5×10^{5}		MacBean (2012a)	?	12
N-methyl-N- nitrosobenzenemethanamine $C_8H_{10}N_2O$ [937-40-6] NGXUJKBJBFLCAR-UHFFFAOYSA-N	7.9×10^{-1} 1.2×10^{2} 3.8×10^{1}		Mirvish et al. (1976) Hilal et al. (2008) Modarresi et al. (2007)	M Q Q	14 67
norepinephrine $C_8H_{11}NO_3$ [51-41-2] SFLSHLFXELFNJZ-QMMMGPOBSA-N	3.1×10^{13}		HSDB (2015)	Q	99
2,4-dimethoxyaniline $C_8H_{11}NO_2$ [2735-04-8] GEQNZVKIDIPGCO-UHFFFAOYSA-N	1.6×10^{1}		Ebert et al. (2023)	?	318
4-methoxy-2-methylbenzenamine $C_8H_{11}NO$ (m-cresidine) [102-50-1] CDGNLUSBENXDGG-UHFFFAOYSA-N	8.2×10^{1}		HSDB (2015)	Q	99
p-cresidine $C_8H_{11}NO$ [120-71-8] WXWCDTXEKCVRRO-UHFFFAOYSA-N	8.0×10^{1}		HSDB (2015)	Q	99

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-nitrosodi-N-butylamine	7.2×10^{-1}		Mirvish et al. (1976)	M	14
$C_8H_{18}N_2O$	7.5×10^{-1}		Hilal et al. (2008)	Q	
[924-16-3]	1.1		Modarresi et al. (2007)	Q	67
YGJHZCLPZAZIHH-UHFFFAOYSA-N					
(diisopropylamino)-ethanol	2.2		Du et al. (2017)	M	478
$C_8H_{19}NO$	2.3		Du et al. (2017)	Q	549
[96-80-0]	2.4		Du et al. (2017)	Q	
ZYWUVGFIXPNBDL-UHFFFAOYSA-N	1.9×10^{2}		Hilal et al. (2008)	Q	
	8.2×10^{1}		Modarresi et al. (2007)	Q	67
phthalamide	7.0×10^{6}		HSDB (2015)	Q	99
$C_8H_8N_2O_2$					
[88-96-0]					
NAYYNDKKHOIIOD-UHFFFAOYSA-N					
acetaminophen	1.5×10^{7}		HSDB (2015)	Q	99
$C_8H_9NO_2$					
[103-90-2]					
RZVAJINKPMORJF-UHFFFAOYSA-N					
methyl anthranilate	5.2		Duchowicz et al. (2020)	V	186
$C_8H_9NO_2$	5.2		HSDB (2015)	V	
[134-20-3]	3.6		Dupeux et al. (2022)	Q	259
VAMXMNNIEUEQDV-UHFFFAOYSA-N	2.6×10^{2}		Duchowicz et al. (2020)	Q	
4'-aminoacetophenone	2.2×10^{3}		HSDB (2015)	Q	99
C_8H_9NO					
(4-acetylaniline)					
[99-92-3]					
GPRYKVSEZCQIHD-UHFFFAOYSA-N					
N-phenylacetamide	4.7×10^{2}		Yaws (2003)	X	258
C_8H_9NO	1.5×10^{3}		Dupeux et al. (2022)	Q	259
(acetanilide)	1.6×10^{3}		HSDB (2015)	Q	99
[103-84-4]					
FZERHIULMFGESH-UHFFFAOYSA-N					
tropine	1.3×10^{3}		Du et al. (2017)	M	478
$C_8H_{15}NO$	2.6×10^{3}		Du et al. (2017)	Q	549
[120-29-6]	5.6×10^{2}		Du et al. (2017)	Q	
CYHOMWAPJJPNMW-UHFFFAOYSA-N					
bis[2-(N,N-dimethylamino)ethyl]	7.9×10^{1}		Du et al. (2017)	M	478
ether					
$C_8H_{20}N_2O$	2.4×10^{2}		Du et al. (2017)	Q	549
[3033-62-3]	7.9×10^{1}		Du et al. (2017)	Q	
GTEXIOINCJRBIO-UHFFFAOYSA-N					

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methylcarbamic acid, 3-methylphenyl ester $C_9H_{11}NO_2$ (metolcarb) [1129-41-5] VOEYXMAFNDNNED-UHFFFAOYSA-N	1.2×10^4		HSDB (2015)	V	
phenylcarbamic acid, ethyl ester $C_9H_{11}NO_2$ [101-99-5] LBKPGNUOUPTQKA-UHFFFAOYSA-N	3.4×10^2		HSDB (2015)	Q	99
ethyl anthranilate $C_9H_{11}NO_2$ [87-25-2] TWLLPUMZVVGILS-UHFFFAOYSA-N	6.2×10^2		HSDB (2015)	Q	99
benzocaine $C_9H_{11}NO_2$ [94-09-7] BLFLLBZGZJTVJG-UHFFFAOYSA-N	6.2×10^2		HSDB (2015)	Q	99
1-(4-aminophenyl)-1-propanone $C_9H_{11}NO$ (4-aminopropiophenone) [70-69-9] FSWXOANXOQPCFF-UHFFFAOYSA-N	2.1×10^3		HSDB (2015)	Q	99
(4-ethoxyphenyl)urea $C_9H_{12}N_2O_2$ (dulcin) [150-69-6] GGLIEWRLXDLBBF-UHFFFAOYSA-N	6.2×10^5		HSDB (2015)	Q	447
fenuron $C_9H_{12}N_2O$ [101-42-8] XXOYNJXVWVNOOJ-UHFFFAOYSA-N	4.9×10^3 8.7×10^2 3.7×10^3 3.6×10^1 9.6 1.0×10^4 4.4		Duchowicz et al. (2020) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Duchowicz et al. (2020) HSDB (2015) Goodarzi et al. (2010)	V V V X Q Q Q	186 12 567 99 568, 571
epinephrine $C_9H_{13}NO_3$ [51-43-4] UCTWMZQNUQWSLP-UHFFFAOYSA-N	1.4×10^{13}		HSDB (2015)	Q	99
meprobamate $C_9H_{18}N_2O_4$ [57-53-4] NPPQSCRMBWNHMW-UHFFFAOYSA-N	5.5×10^4		HSDB (2015)	Q	99

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
propamocarb	2.1×10^{3}		Keshavarz et al. (2022)	Q	
$C_9H_{20}N_2O_2$	1.6×10^{3}		Duchowicz et al. (2020)	Q	184
[24579-73-5]	1.6×10^{3}		Hilal et al. (2008)	Q	
WZZLDXDUQPOXNW-UHFFFAOYSA-N	3.3×10^{2}		Modarresi et al. (2007)	Q	67
	6.7×10^{3}		Duchowicz et al. (2020)	?	185, 21
	1.2×10^{8}		Maniere et al. (2011)	?	241, 165
proximpham	3.9×10^{3}		MacBean (2012a)	?	12
$C_{10}H_{12}N_2O_2$					
[2828-42-4]					
LATYTXGNKNKTDS-UHFFFAOYSA-N					
dioxacarb	6.7×10^{5}		Duchowicz et al. (2020)	V	186
$C_{10}H_{13}NO_4$	2.2×10^{4}		Duchowicz et al. (2020)	Q	
[6988-21-2]	6.7×10^{5}		MacBean (2012a)	?	
SDKQRNRRDYRQKY-UHFFFAOYSA-N					
phenol, 3,5-dimethyl-, methylcarbamate	5.5×10^{1}		Duchowicz et al. (2020)	V	186
$C_{10}H_{13}NO_2$	9.1		Duchowicz et al. (2020)	Q	
(3,5-xylyl methylcarbamate)	2.5×10^{2}		HSDB (2015)	Q	99
[2655-14-3]	4.3×10^{2}		MacBean (2012a)	?	
CVQODEWAPZVVBU-UHFFFAOYSA-N					
phenylcarbamic acid, 1-methylethyl ester	5.4×10^{1}		Duchowicz et al. (2020)	V	186
$C_{10}H_{13}NO_2$	5.5×10^{1}		HSDB (2015)	V	
[122-42-9]	3.2×10^{-2}		Duchowicz et al. (2020)	Q	
VXPLXMJHHKHSOA-UHFFFAOYSA-N					
xylylcarb	9.1×10^{1}		Watanabe (1993)	M	
$C_{10}H_{13}NO_2$	9.4×10^{1}		Duchowicz et al. (2020)	V	186
[2425-10-7]	9.1		Duchowicz et al. (2020)	Q	
WCJYTPVNMWIZCG-UHFFFAOYSA-N					
phenacetin	4.6×10^{4}		Duchowicz et al. (2020)	V	186
$C_{10}H_{13}NO_2$	4.7×10^{4}		HSDB (2015)	V	
[62-44-2]	2.7		Duchowicz et al. (2020)	Q	
CPJSUEIXXCENMM-UHFFFAOYSA-N					
ephedrine	1.1×10^{5}		HSDB (2015)	Q	447
$C_{10}H_{15}NO$					
[299-42-3]					
KWGRBVOPPLSCSI-PSASIEDQSA-N					

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
m-cumenyl methylcarbamate $C_{11}H_{15}NO_2$ (3-isopropylphenyl methyl carbamate) [64-00-6] GYKXQTKSWLAUIT-UHFFFAOYSA-N	1.6×10^{2}		HSDB (2015)	Q	99
propoxur $C_{11}H_{15}NO_3$ [114-26-1] ISRUGXGCCGIOQO-UHFFFAOYSA-N	2.9×10^{3} 5.1×10^{5} 7.1×10^{3} 7.7 7.6×10^{-2} 1.4		HSDB (2015) Mackay et al. (2006d) Siebers et al. (1994) Suntio et al. (1988) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V V V X Q	 12 567 568
methocarbamol $C_{11}H_{15}NO_5$ [532-03-6] GNXFOGHNGIVQEH-UHFFFAOYSA-N	1.5×10^{10}		HSDB (2015)	Q	99
aminocarb $C_{11}H_{16}N_2O_2$ [2032-59-9] IMIDOCRTMDIQIJ-UHFFFAOYSA-N	1.9×10^{3} 1.8×10^{4}		Mackay et al. (2006d) HSDB (2015)	V Q	 99
monodesmethylisoproturon $C_{11}H_{16}N_2O$ [34123-57-4] DOULWWSSZVEPIN-UHFFFAOYSA-N	2.8×10^{5}		Otto et al. (1997)	V	
cycluron $C_{11}H_{22}N_2O$ [2163-69-1] DQZCVNGCTZLGAQ-UHFFFAOYSA-N	8.2×10^{2}		HSDB (2015)	Q	99
methylneodecanamide $C_{11}H_{23}NO$ [105726-67-8] GELCOLZWXWHMIB-UHFFFAOYSA-N	4.1×10^{1}		HSDB (2015)	Q	99
isoprocarb $C_{11}H_{15}NO_2$ [2631-40-5] QBSJMKIUCUGGNG-UHFFFAOYSA-N	7.4×10^{2} 7.6		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
4-(phenylazo)phenol $C_{12}H_{10}N_2O$ (4-hydroxyazobenzene) [1689-82-3] BEYOBVMPDRKTNR-UHFFFAOYSA-N	1.5×10^{4} 1.5×10^{4} 1.0×10^{4}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-naphthaleneacetamide $C_{12}H_{11}NO$ [86-86-2] XFNJVKMNNVCYEK-UHFFFAOYSA-N	9.8×10^{7}		Maniere et al. (2011)	?	12, 165
carbetamide $C_{12}H_{16}N_2O_3$ [16118-49-3] AMRQXHFXNZFDCH-UHFFFAOYSA-N	1.1 3.7 5.2×10^{7}		Barcelo and Hennion (1997) Goodarzi et al. (2010) Maniere et al. (2011)	X Q ?	567 568 12, 165
N-nitrosodiphenylamine $C_{12}H_{10}N_2O$ (N,N-Diphenylnitrosamine) [86-30-6] UBUCNCOMADRQHX-UHFFFAOYSA-N	8.7×10^{-3} 8.7×10^{-3} 1.5×10^{-2} 8.2		Mackay et al. (2006d) Mackay et al. (1995) Mackay et al. (1995) HSDB (2015)	V V C Q	 99
carbaryl $C_{12}H_{11}NO_2$ [63-25-2] CVXBEEMKQHEXEN-UHFFFAOYSA-N	$>9.9\times10^{1}$ 3.6×10^{3} 3.0×10^{3} 2.2×10^{4} 2.3×10^{3} 7.7×10^{2} 7.6×10^{1} 2.3×10^{3} 3.5×10^{3} 1.2×10^{2} 8.1 1.4×10^{3} 3.1×10^{3}		Mabury and Crosby (1996) Watanabe (1993) Duchowicz et al. (2020) Mackay et al. (2006d) Meylan and Howard (1991) Suntio et al. (1988) Barcelo and Hennion (1997) Howard and Meylan (1997) Armbrust (2000) Duchowicz et al. (2020) Goodarzi et al. (2010) Hilal et al. (2008) Meylan and Howard (1991)	M M V V V V X X C Q Q Q Q	 186 12 567 446 568, 571
4,4'-oxybisbenzenamine $C_{12}H_{12}N_2O$ (bis(4-aminophenyl) ether) [101-80-4] HLBLWEWZXPIGSM-UHFFFAOYSA-N	6.6×10^{5}		HSDB (2015)	Q	99
carbofuran $C_{12}H_{15}NO_3$ [1563-66-2] DUEPRVBVGDRKAG-UHFFFAOYSA-N	2.4×10^{1} $>9.9\times10^{1}$ 2.2×10^{4} 2.0×10^{4} 2.0×10^{3} 1.9×10^{1} 4.6×10^{1}		Chao et al. (2017) Mabury and Crosby (1996) HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Goodarzi et al. (2010)	M M V V V X Q	 12 567 568

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
phenol, 3-methyl-5-(1-methylethyl)-, methylcarbamate $C_{12}H_{16}NO_2$ (promecarb) [2631-37-0] DTAPQAJKAFRNJB-UHFFFAOYSA-N	1.1×10^2 1.1×10^2 4.1 3.1×10^2		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) MacBean (2012a)	V V Q ?	186
fenobucarb $C_{12}H_{17}NO_2$ [3766-81-2] DIRFUJHNVNOBMY-UHFFFAOYSA-N	1.5×10^2 1.7×10^2 8.2		Watanabe (1993) Duchowicz et al. (2020) Duchowicz et al. (2020)	M V Q	 186
diethyltoluamide $C_{12}H_{17}NO$ (DEET) [134-62-3] MMOXZBCLCQITDF-UHFFFAOYSA-N	4.7×10^2		HSDB (2015)	Q	99
N,N-dimethyl-N'-[4-(1-methylethyl)phenyl]-urea $C_{12}H_{18}N_2O$ (isoproturon) [34123-59-6] PUIYMUZLKQOUOZ-UHFFFAOYSA-N	8.8×10^4 8.1×10^4 9.5×10^4 1.1×10^5 2.3		Duchowicz et al. (2020) Mackay et al. (2006d) Otto et al. (1997) Siebers et al. (1994) Duchowicz et al. (2020)	V V V V Q	186
dimorpholinodiethyl ether $C_{12}H_{24}N_2O_3$ [6425-39-4] ZMSQJSMSLXVTKN-UHFFFAOYSA-N	1.8×10^3	2600	Nguyen (2013)	M	11
carisoprodol $C_{12}H_{24}N_2O_4$ [78-44-4] OFZCIYFFPZCNJE-UHFFFAOYSA-N	1.4×10^4		HSDB (2015)	Q	99
4-hydroxy-4'-nitroazobenzene $C_{12}H_9N_3O_3$ [1435-60-5] NRJPVIOTANUINF-YPKPFQOOSA-N	4.0×10^5 1.4×10^6		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
2,4-dinitro-N-phenyl-benzenamine $C_{12}H_9N_3O_4$ [961-68-2] RHTVQEPJVKUMPI-UHFFFAOYSA-N	1.3×10^4 6.6×10^5		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
N-(2,4-dinitrophenyl)-N-(4-hydroxyphenyl)amine $C_{12}H_9N_3O_5$ [119-15-3] BCPQALWAROJVLE-UHFFFAOYSA-N	6.8×10^6 1.4×10^9		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
disperse orange 3 $C_{12}H_{10}N_4O_2$ [730-40-5] UNBOSJFEZZJZLR-UHFFFAOYSA-N	3.5×10^4 1.9×10^5		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
diethylpropion $C_{13}H_{19}NO$ [90-84-6] XXEPPPIWZFICOJ-UHFFFAOYSA-N	4.3×10^1		HSDB (2015)	Q	99
salbutamol $C_{13}H_{21}NO_3$ (albuterol) [18559-94-9] NDAUXUAQIAJITI-UHFFFAOYSA-N	1.5×10^{10}		HSDB (2015)	Q	99
disperse blue 1 $C_{14}H_{12}N_4O_2$ [2475-45-8] JSFUMBWFPQSADC-UHFFFAOYSA-N	4.7×10^1		HSDB (2015)	V	
3,3'-dimethoxybenzidine $C_{14}H_{16}N_2O_2$ [119-90-4] JRBJSXQPQWSCCF-UHFFFAOYSA-N	2.1×10^5		HSDB (2015)	Q	99
aspartame $C_{14}H_{18}N_2O_5$ [22839-47-0] IAOZJIPTCAWIRG-QWRGUYRKSA-N	3.9×10^{12}		HSDB (2015)	Q	99
dinobuton $C_{14}H_{18}N_2O_7$ (dessin) [973-21-7] HDWLUGYOLUHEMN-UHFFFAOYSA-N	6.2×10^2		HSDB (2015)	Q	99
N-(2-methylcyclohexyl)-N'-phenylurea $C_{14}H_{20}N_2O$ (siduron) [1982-49-6] JXVIIQLNUPXOII-UHFFFAOYSA-N	1.5×10^5		HSDB (2015)	V	
butralin $C_{14}H_{21}N_3O_4$ [33629-47-9] SPNQRCTZKIBOAX-UHFFFAOYSA-N	2.0 2.0		HSDB (2015) Mackay et al. (2006d)	V V	

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
lauramine oxide $C_{14}H_{31}NO$ [1643-20-5] SYELZBGXAIXKHU-UHFFFAOYSA-N	1.5×10^{5}		HSDB (2015)	Q	99
2-aminoanthraquinone $C_{14}H_9NO_2$ [117-79-3] XOGPDSATLSAZEK-UHFFFAOYSA-N	1.1×10^{5} 1.1×10^{5} 3.1×10^{5}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
1-amino-9,10-anthracenedione $C_{14}H_9NO_2$ [82-45-1] KHUFHLFHOQVFGB-UHFFFAOYSA-N	2.0×10^{3} 9.8×10^{4}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
1-amino-4-hydroxy-9,10-anthracenedione $C_{14}H_9NO_3$ [116-85-8] AQXYVFBSOOBBQV-UHFFFAOYSA-N	3.8×10^{5} 4.2×10^{5}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
1,4-diamino-9,10-anthracenedione $C_{14}H_{10}N_2O_2$ [128-95-0] FBMQNRKSAWNXBT-UHFFFAOYSA-N	2.1×10^{4} 1.3×10^{7}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
N,N-dimethyl-4-[(4-nitrophenyl)azo]-benzenamine $C_{14}H_{14}N_4O_2$ [2491-74-9] LSFRFLVWCKLQTO-UHFFFAOYSA-N	1.5×10^{2} 1.0×10^{4}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
karbutilate $C_{14}H_{21}N_3O_3$ [4849-32-5] OWNAXTAAAQTBSP-UHFFFAOYSA-N	1.8×10^{8}		Ebert et al. (2023)	?	318
diethofencarb $C_{14}H_{21}NO_4$ [87130-20-9] LNJNFVJKDJYTEU-UHFFFAOYSA-N	1.2×10^{1} 1.3×10^{-1}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
1-amino-2-methyl-9,10-anthracenedione $C_{15}H_{11}NO_2$ (1-amino-2-methylanthraquinone) [82-28-0] ZLCUIOWQYBYEBG-UHFFFAOYSA-N	8.2×10^{6}		HSDB (2015)	Q	99

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-2-fluorenylacetamide $C_{15}H_{13}NO$ (2-acetylaminofluorene) [53-96-3] CZIHNRWJTSTCEX-UHFFFAOYSA-N	5.2×10^{4}		HSDB (2015)	Q	99
tebutam $C_{15}H_{23}NO$ [35256-85-0] RJKCKKDSSSRYCB-UHFFFAOYSA-N	3.8×10^{1} 1.5×10^{-1} 6.7×10^{1}		Duchowicz et al. (2020) Duchowicz et al. (2020) MacBean (2012a)	V Q ?	186
isopropalin $C_{15}H_{23}N_3O_4$ [33820-53-0] NEKOXWSIMFDGMA-UHFFFAOYSA-N	1.9×10^{-1}		Mackay et al. (2006d)	V	
dodine $C_{15}H_{33}N_3O_2$ (doguadine) [2439-10-3] YIKWKLYQRFRGPM-UHFFFAOYSA-N	1.1×10^{5} 9.9×10^{5} 1.1×10^{5}		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	186 241, 165
metalaxyl $C_{15}H_{21}NO_4$ [57837-19-1] ZQEIXNIJLIKNTD-UHFFFAOYSA-N	3.3×10^{3} 4.0×10^{4} 8.5×10^{4}		HSDB (2015) Mackay et al. (2006d) Burkhard and Guth (1981)	V V V	
metalaxyl-m $C_{15}H_{21}NO_4$ [70630-17-0] ZQEIXNIJLIKNTD-GFCCVEGCSA-N	2.8×10^{4} 2.1×10^{2} 2.9×10^{4}		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	186 165
metoprolol $C_{15}H_{25}NO_3$ [37350-58-6] IUBSYMUCCVWXPE-UHFFFAOYSA-N	4.7×10^{5}		HSDB (2015)	Q	99
1-(methylamino)anthraquinone $C_{15}H_{11}NO_2$ [82-38-2] SVTDYSXXLJYUTM-UHFFFAOYSA-N	3.3×10^{2} 7.1×10^{4}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
4'-[(2-hydroxy-5-methylphenyl)azo]acetanilide $C_{15}H_{15}N_3O_2$ [2832-40-8] PXOZAFXVEWKXED-UHFFFAOYSA-N	6.6×10^{5} 3.2×10^{5}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
desmedipham $C_{16}H_{16}N_2O_4$ [13684-56-5] WZJZMXBKUWKXTQ-UHFFFAOYSA-N	2.3×10^{6}		Ebert et al. (2023)	?	365
phenmedipham $C_{16}H_{16}N_2O_4$ (betanal) [13684-63-4] IDOWTHOLJBTAFI-UHFFFAOYSA-N	1.2×10^{7} 1.2×10^{7} 1.2×10^{5} 4.5 5.3×10^{2} 2.0×10^{7}		Duchowicz et al. (2020) HSDB (2015) Barcelo and Hennion (1997) Duchowicz et al. (2020) Goodarzi et al. (2010) Maniere et al. (2011)	V V X Q Q ?	186 567 568, 569 12, 165
fenam $C_{16}H_{17}NO$ [957-51-7] QAHFOPIILNICLA-UHFFFAOYSA-N	2.7×10^{5} 4.1×10^{5} 2.7×10^{5} 4.9×10^{1}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Duchowicz et al. (2020)	V V V Q	186
difenoxuron $C_{16}H_{18}N_2O_3$ [14214-32-5] AMVYOVYGIJXTQB-UHFFFAOYSA-N	5.6×10^{7}		MacBean (2012a)	?	
butacarb $C_{16}H_{25}NO_2$ [2655-19-8] SLZWBCGZQRRUNG-UHFFFAOYSA-N	2.2×10^{2}		HSDB (2015)	V	
oseltamivir $C_{16}H_{28}N_2O_4$ [196618-13-0] VSZGPKBBMSAYNT-RRFJBIMHSA-N	3.4×10^{10}		HSDB (2015)	Q	99
N,N-bis(2-hydroxyethyl)dodecanamide $C_{16}H_{33}NO_3$ [120-40-1] AOMUHOFOVNGZAN-UHFFFAOYSA-N	4.6×10^{6}		HSDB (2015)	Q	99
1,4-bis(methylamino)-9,10-anthracenedione $C_{16}H_{14}N_2O_2$ [2475-44-7] QOSTVEDABRQTSU-UHFFFAOYSA-N	5.2×10^{4} 7.5×10^{6}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
metominostrobin $C_{16}H_{16}N_2O_3$ [133408-50-1] HIIRDDUVRXCDBN-SDXDJHTJSA-N	2.5×10^{4} 8.6×10^{6}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-[(2-methoxyphenyl)azo]-2-naphthol $C_{17}H_{14}N_2O_2$ [1229-55-6] ALLOLPOYFRLCCX-VHEBQXMUSA-N	9.0×10^4		HSDB (2015)	Q	99
furalaxyl $C_{17}H_{19}NO_4$ [57646-30-7] CIEXPHRYOLIQQD-UHFFFAOYSA-N	1.1×10^4		MacBean (2012a)	?	
fenoxycarb $C_{17}H_{19}NO_4$ [72490-01-8] HJUFTIJOISQSKQ-UHFFFAOYSA-N	2.3×10^4 2.5×10^4 2.3×10^7 1.2×10^4 8.4×10^2 8.4×10^2 3.0×10^4		Duchowicz et al. (2020) Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V V V V Q Q ?	186 186 241, 165
bifenazate $C_{17}H_{20}N_2O_3$ [149877-41-8] VHLKTXFWDRXILV-UHFFFAOYSA-N	1.0×10^3 $>9.9\times10^2$		MacBean (2012b) Maniere et al. (2011)	X ?	350 12, 165
napropamide $C_{17}H_{21}NO_2$ [15299-99-7] WXZVAROIGSFCFJ-UHFFFAOYSA-N	1.2×10^4 1.2×10^4		HSDB (2015) Maniere et al. (2011)	V ?	 241, 165
napropamide-M $C_{17}H_{21}NO_2$ [41643-35-0] WXZVAROIGSFCFJ-CYBMUJFWSA-N	3.8×10^4		Ebert et al. (2023)	?	318
padimate O $C_{17}H_{27}NO_2$ [21245-02-3] WYWZRNAHINYAEF-UHFFFAOYSA-N	2.5		HSDB (2015)	Q	447
nadolol $C_{17}H_{27}NO_4$ [42200-33-9] VWPOSFSPZNDTMJ-UHFFFAOYSA-N	7.0×10^8		HSDB (2015)	Q	99
2,6-di-*tert*-butyl-4-(dimethylaminomethyl)phenol $C_{17}H_{29}NO$ [88-27-7] VMZVBRIIHDRYGK-UHFFFAOYSA-N	4.8×10^3 2.4×10^2 1.3 4.8×10^1		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
mepronil $C_{17}H_{19}NO_2$ [55814-41-0] BCTQJXQXJVLSIG-UHFFFAOYSA-N	8.4×10^2 4.7		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
daimuron $C_{17}H_{20}N_2O$ [42609-52-9] NNYRZQHKCHEXSD-UHFFFAOYSA-N	9.9×10^3 2.6×10^1		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
naptalam $C_{18}H_{13}NO_3$ [132-66-1] JXTHEWSKYLZVJC-UHFFFAOYSA-N	$>2.3\times10^{10}$		MacBean (2012a)	?	
citrus red 2 $C_{18}H_{16}N_2O_3$ [6358-53-8] ULLJIFAIUSUJBP-ZZEZOPTASA-N	1.9×10^7		HSDB (2015)	Q	99
kresoxim-methyl $C_{18}H_{19}NO_4$ [143390-89-0] ZOTBXTZVPHCKPN-UHFFFAOYSA-N	2.7×10^3 2.8×10^3		HSDB (2015) Maniere et al. (2011)	V ?	 241, 165
dinocap $C_{18}H_{24}N_2O_6$ [39300-45-3] RNDNTTTUTQAXII-GORDUTHDSA-N	2.1×10^3		HSDB (2015)	V	
orysastrobin $C_{18}H_{25}N_5O_5$ [248593-16-0] JHIPUJPTQJYEQK-ZLHHXESBSA-N	2.9×10^5		Ebert et al. (2023)	?	318
spiroxamine $C_{18}H_{35}NO_2$ [118134-30-8] PUYXTUJWRLOUCW-UHFFFAOYSA-N	4.0×10^2 2.0×10^2		Maniere et al. (2011) Maniere et al. (2011)	? ?	12, 165 12, 165
capsaicin $C_{18}H_{27}NO_3$ [404-86-4] YKPUWZUDDOIDPM-SOFGYWHQSA-N	9.9×10^7		HSDB (2015)	Q	99
mandestrobin $C_{19}H_{23}NO_3$ [173662-97-0] PDPWCKVFIFAQIQ-UHFFFAOYSA-N	1.5×10^6		Maniere et al. (2011)	?	12, 165

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dimoxystrobin $C_{19}H_{22}N_2O_3$ [149961-52-4] WXUZAHCNPWONDH-DYTRJAOYSA-N	2.2×10^{7}		Maniere et al. (2011)	?	241, 165
(*RS*)-α-2-naphthoxypropionanilide $C_{19}H_{17}NO_2$ (naproanilide) [52570-16-8] LVKTWOXHRYGDMM-UHFFFAOYSA-N	1.6×10^{5}		Hilal et al. (2008)	Q	
	7.5×10^{4}		Modarresi et al. (2007)	Q	67
phenylbutazone $C_{19}H_{20}N_2O_2$ [50-33-9] VYMDGNCVAMGZFE-UHFFFAOYSA-N	1.5×10^{3}		HSDB (2015)	Q	99
phenisopham $C_{19}H_{22}N_2O_4$ [57375-63-0] PWEOEHNGYFXZLI-UHFFFAOYSA-N	1.3×10^{4}		MacBean (2012a)	?	
formoterol $C_{19}H_{24}N_2O_4$ [73573-87-2] BPZSYCZIITTYBL-ORAYPTAESA-N	1.1×10^{17}		HSDB (2015)	Q	99
benalaxyl-m $C_{20}H_{23}NO_3$ [98243-83-5] CJPQIRJHIZUAQP-MRXNPFEDSA-N	4.3×10^{3}		Maniere et al. (2011)	?	12, 165
benalaxyl $C_{20}H_{23}NO_3$ [71626-11-4] CJPQIRJHIZUAQP-UHFFFAOYSA-N	8.5×10^{1}		Duchowicz et al. (2020)	V	186
	8.3×10^{1}		Mackay et al. (2006d)	V	
	5.1×10^{1}		Duchowicz et al. (2020)	Q	
	1.5×10^{2}		Maniere et al. (2011)	?	12, 165
tralkoxydim $C_{20}H_{27}NO_3$ [87820-88-0] SOTLWPHEAQOHHC-UHFFFAOYSA-N	4.1×10^{4}		HSDB (2015)	V	
neotame $C_{20}H_{30}N_2O_5$ [165450-17-9] HLIAVLHNDJUHFG-HOTGVXAUSA-N	4.3×10^{3}		HSDB (2015)	Q	99
colchicine $C_{22}H_{25}NO_6$ [64-86-8] IAKHMKGGTNLKSZ-MRXNPFEDSA-N	5.5×10^{11}		HSDB (2015)	Q	99

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tebufenozide $C_{22}H_{28}N_2O_2$ [112410-23-8] QYPNKSZPJQQLRK-UHFFFAOYSA-N	7.6×10^{2} $>1.5\times10^{4}$		HSDB (2015) Maniere et al. (2011)	V ?	 165
methoxyfenozide $C_{22}H_{28}N_2O_3$ [161050-58-4] QCAWEPFNJXQPAN-UHFFFAOYSA-N	2.6×10^{6} $>6.1\times10^{3}$		HSDB (2015) Maniere et al. (2011)	Q ?	99 12, 165
propoxyphene $C_{22}H_{29}NO_2$ [469-62-5] XLMALTXPSGQGBX-PGRDOPGGSA-N	4.3×10^{3}		HSDB (2015)	Q	99
(Z)-13-docosenamide $C_{22}H_{43}NO$ (erucamide) [112-84-5] UAUDZVJPLUQNMU-KTKRTIGZSA-N	3.5		HSDB (2015)	Q	545
butroxydim $C_{24}H_{33}NO_4$ [138164-12-2] ZOGDSYNXUXQGHF-XIEYBQDHSA-N	1.7×10^{4}		MacBean (2012a)	?	
2,2-bis[4-(4-aminophenoxy)phenyl]propane $C_{27}H_{26}N_2O_2$ [13080-86-9] KMKWGXGSGPYISJ-UHFFFAOYSA-N	2.0×10^{8} 2.8×10^{8} 1.0×10^{8} 3.1×10^{10}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
1,4-bis[(4-methylphenyl)amino]-9,10-anthracenedione $C_{28}H_{22}N_2O_2$ (D&C Green No. 6) [128-80-3] TVRGPOFMYCMNRB-UHFFFAOYSA-N	6.6×10^{10}		HSDB (2015)	Q	99
mifepristone $C_{29}H_{35}NO_2$ [84371-65-3] VKHAHZOOUSRJNA-GCNJZUOMSA-N	2.0×10^{-1}		HSDB (2015)	Q	99
2'-anilino-6'-[ethyl(3-methylbutyl)amino]-3'-methylspiro[isobenzofuran-1(3H),9'-[9H]xanthene]-3-one $C_{34}H_{34}N_2O_3$ [70516-41-5] HUSIBQLZEMMTCQ-UHFFFAOYSA-N	2.0×10^{8} 3.5×10^{8} 8.0×10^{8}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q	287, 288 287, 289 287, 290 287, 291

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
spinetoram	1.0×10^{2}		Maniere et al. (2011)	?	241, 570, 165
$C_{42}H_{69}NO_{10}$	1.1×10^{4}		Maniere et al. (2011)	?	241, 570, 165
[935545-74-7]	1.6×10^{2}		Maniere et al. (2011)	?	241, 572, 165
GOENIMGKWNZVDA-OAMCMWGQSA-N	2.0×10^{3}		Maniere et al. (2011)	?	241, 165
	2.9×10^{2}		Maniere et al. (2011)	?	241, 493, 165
	2.9×10^{3}		Maniere et al. (2011)	?	241, 493, 165
	4.3×10^{1}		Maniere et al. (2011)	?	241, 572, 165
	2.5×10^{2}		Maniere et al. (2011)	?	241, 165
spinosad	5.3×10^{6}		Maniere et al. (2011)	?	241, 165
$C_{42}H_{71}NO_9$	4.3×10^{4}		Maniere et al. (2011)	?	241, 165
[168316-95-8]					
RQOIAWYOVOXMST-UHFFFAOYSA-N					
emamectin benzoate	5.8×10^{3}		HSDB (2015)	V	
$C_{56}H_{81}NO_{15}$	2.5×10^{1}		Maniere et al. (2011)	?	241, 573, 165
[155569-91-8]	5.9×10^{3}		Maniere et al. (2011)	?	241, 493, 165
GCKZANITAMOIAR-UHFFFAOYSA-N	7.7×10^{4}		Maniere et al. (2011)	?	241, 570, 165
glutamic acid	9.0×10^{7}		Yaws (2003)	X	237
$C_5H_9NO_4$	1.8×10^{10}		Gharagheizi et al. (2012)	Q	
[617-65-2]	9.6×10^{7}		Gharagheizi et al. (2010)	Q	246
WHUUTDBJXJRKMK-UHFFFAOYSA-N	9.9×10^{10}		Saxena and Hildemann (1996)	E	401
asparagine	9.9×10^{10}		Saxena and Hildemann (1996)	E	401
$C_4H_8N_2O_3$					
[70-47-3]					
DCXYFEDJOCDNAF-UWTATZPHSA-N					
serine	3.9×10^{10}		Saxena and Hildemann (1996)	E	401
$C_3H_7NO_3$					
[302-84-1]					
MTCFGRXMJLQNBG-UHFFFAOYSA-N					
glutamine	3.3×10^{10}		HSDB (2015)	Q	447
$C_5H_{10}N_2O_3$	9.9×10^{10}		Saxena and Hildemann (1996)	E	401
[56-85-9]					
ZDXPYRJPNDTMRX-GSVOUGTGSA-N					

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Table A4.4: Amines, amides, amino acids (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
glycine $C_2H_5NO_2$ [56-40-6] DHMQDGOQFOQNFH-UHFFFAOYSA-N	1.2×10^{11} 8.9×10^{5}	16000	Brimblecombe et al. (1992) Saxena and Hildemann (1996)	V E	 401
arginine $C_6H_{14}N_4O_2$ [74-79-3] ODKSFYDXXFIFQN-SCSAIBSYSA-N	9.9×10^{14}		Saxena and Hildemann (1996)	E	401
alanine $C_3H_7NO_2$ [302-72-7] QNAYBMKLOCPYGJ-UHFFFAOYSA-N	3.5×10^{10} 5.9×10^{5}	16000	Brimblecombe et al. (1992) Saxena and Hildemann (1996)	V E	 401
leucine $C_6H_{13}NO_2$ [328-39-2] ROHFNLRQFUQHCH-UHFFFAOYSA-N	2.0×10^{5}		Saxena and Hildemann (1996)	E	401

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A4.5 Heterocycles with oxygen and nitrogen (C, H, O, N)

Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyanuric acid	1.1×10^{9}		HSDB (2015)	Q	99
$C_3H_3N_3O_3$	1.1×10^{9}		Zhang et al. (2010)	Q	287, 288
[108-80-5]	3.4×10^{5}		Zhang et al. (2010)	Q	287, 289
ZFSLODLOARCGLH-UHFFFAOYSA-N	4.2×10^{10}		Zhang et al. (2010)	Q	287, 290
	4.0×10^{7}		Zhang et al. (2010)	Q	287, 291
isoxazole	4.0×10^{-1}		Duchowicz et al. (2020)	V	186
C_3H_3NO	5.4×10^{-1}		Duchowicz et al. (2020)	Q	
[288-14-2]	2.4×10^{-1}		Hilal et al. (2008)	Q	
CTAPFRYPJLPFDF-UHFFFAOYSA-N	2.1×10^{-1}		Modarresi et al. (2007)	Q	67
glycidamide	7.7×10^{4}		HSDB (2015)	Q	99
$C_3H_5NO_2$					
[5694-00-8]					
FMAZQSYXRGRESX-UHFFFAOYSA-N					
cyclonite	4.9×10^{5}		HSDB (2015)	V	
$C_3H_6N_6O_6$					
[121-82-4]					
XTFIVUDBNACUBN-UHFFFAOYSA-N					
5-methyl-3-(2H)-isoxazolone	4.7×10^{3}		Duchowicz et al. (2020)	V	186
$C_4H_5NO_2$	4.7×10^{2}		Duchowicz et al. (2020)	Q	
(hymexazol)	5.0×10^{3}		Hilal et al. (2008)	Q	
[10004-44-1]	1.6×10^{2}		Modarresi et al. (2007)	Q	67
KGVPNLBXJKTABS-UHFFFAOYSA-N	7.1×10^{3}		Maniere et al. (2011)	?	241, 165
3-amino-1H-pyridazin-6-one	1.2×10^{7}		Ebert et al. (2023)	?	318
$C_4H_5N_3O$					
(maleic hydrazide)					
[10071-13-3]					
MMZLICVOTDAZOX-UHFFFAOYSA-N					
maleic hydrazide	2.5×10^{7}		Maniere et al. (2011)	?	12, 165
$C_4H_4N_2O_2$					
[123-33-1]					
BGRDGMRNKXEXQD-UHFFFAOYSA-N					
allantoin	2.9×10^{12}		HSDB (2015)	Q	99
$C_4H_6N_4O_3$					
[97-59-6]					
POJWUDADGALRAB-UHFFFAOYSA-N					
2-pyrrolidinone	9.3×10^{3}		Duchowicz et al. (2020)	V	186
C_4H_7NO	9.3×10^{3}		HSDB (2015)	V	
[616-45-5]	1.2×10^{3}		Duchowicz et al. (2020)	Q	
HNJBEVLQSNELDL-UHFFFAOYSA-N					

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Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-nitrosomorpholine	3.9×10^{2}		Mirvish et al. (1976)	M	14
$C_4H_8N_2O_2$	9.0×10^{2}		Hilal et al. (2008)	Q	
[59-89-2]	1.5×10^{2}		Modarresi et al. (2007)	Q	67
ZKXDGKXYMTYWTB-UHFFFAOYSA-N					
N-nitrosopyrrolidine	1.5×10^{2}	8500	Klein (1982)	M	
$C_4H_8N_2O$	1.9×10^{2}		Mirvish et al. (1976)	M	14
[930-55-2]	3.4×10^{1}		Hilal et al. (2008)	Q	
WNYADZVDBIBLJJ-UHFFFAOYSA-N					
cyclotetramethylenetetranitramine	1.1×10^{4}		HSDB (2015)	Q	99
$C_4H_8N_8O_8$					
[2691-41-0]					
UZGLIIJVICEWHF-UHFFFAOYSA-N					
1-oxa-4-azacyclohexane	1.9×10^{2}	7800	Nguyen (2013)	M	11
C_4H_9NO	8.5		Duchowicz et al. (2020)	V	186
(morpholine)	8.2		HSDB (2015)	V	
[110-91-8]	7.3×10^{1}	8400	Cabani et al. (1975a)	T	
YNAVUWVOSKDBBP-UHFFFAOYSA-N	2.2×10^{1}		Duchowicz et al. (2020)	Q	
	1.6×10^{2}		Hilal et al. (2008)	Q	
	8.1×10^{1}		Modarresi et al. (2007)	Q	67
	9.5×10^{1}		English and Carroll (2001)	Q	230, 274
	1.0×10^{1}		Nirmalakhandan et al. (1997)	Q	
	4.2×10^{1}		Yaws (1999)	?	21, 12
1-aziridineethanol	1.3×10^{4}		HSDB (2015)	Q	99
C_4H_9NO					
[1072-52-2]					
VYONOYYDEFODAJ-UHFFFAOYSA-N					
2-ethyl-3-methoxypyrazine	6.7×10^{-1}		Buttery et al. (1971)	M	
$C_4N_2H_3(C_2H_5)OCH_3$	2.5×10^{1}		Hilal et al. (2008)	Q	
[25680-58-4]	2.6		Modarresi et al. (2007)	Q	67
DPCILIMHENXHQX-UHFFFAOYSA-N					
2-isobutyl-3-methoxypyrazine	1.7×10^{-1}		Karl et al. (2003)	M	
$C_4N_2H_3(C_4H_9)OCH_3$	2.0×10^{-1}		Buttery et al. (1971)	M	
[24683-00-9]	1.3		Modarresi et al. (2007)	Q	67
UXFSPRAGHGMRSQ-UHFFFAOYSA-N					
N-nitrosopiperidine	1.1×10^{1}		Mirvish et al. (1976)	M	14
$C_5H_{10}N_2O$	2.9×10^{1}		Hilal et al. (2008)	Q	
[100-75-4]	9.6		Modarresi et al. (2007)	Q	67
UWSDONTXWQOZFN-UHFFFAOYSA-N	3.4		Katritzky et al. (1998)	Q	
butyl carbamate	1.1×10^{2}		HSDB (2015)	Q	99
$C_5H_{11}NO_2$					
[592-35-8]					
SKKTUOZKZKCGTB-UHFFFAOYSA-N					

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Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methyl-1-oxa-4-azacyclohexane	5.0		Du et al. (2017)	M	478
$C_5H_{11}NO$	1.2×10^1	10000	Leng et al. (2015a)	M	
(N-methylmorpholine;	1.8×10^1	8300	Cabani et al. (1975a)	T	
4-methylmorpholine)					
[109-02-4]	9.6		Du et al. (2017)	Q	549
SJRJJKPEHAURKC-UHFFFAOYSA-N	3.6		Du et al. (2017)	Q	
	5.7		Hilal et al. (2008)	Q	
	6.4		Modarresi et al. (2007)	Q	67
	1.4×10^1		English and Carroll (2001)	Q	230, 231
	1.7×10^1		Nirmalakhandan et al. (1997)	Q	
allopurinol	4.9×10^8		HSDB (2015)	Q	99
$C_5H_4N_4O$					
[315-30-0]					
OFCNXPDARWKPPY-UHFFFAOYSA-N					
4-methoxypyridine		7100	Arnett and Chawla (1979)	?	559
$C_5H_4NOCH_3$					
[620-08-6]					
XQABVLBGNWBWIV-UHFFFAOYSA-N					
N-methyl-2-pyrrolidone	3.1×10^3	11000	Brockbank (2013)	L	1
C_5H_9NO	2.1×10^3	9100	Bernauer and Dohnal (2009)	M	
[872-50-4]	3.1×10^3		Kim et al. (2000)	M	
SECXISVLQFMRJM-UHFFFAOYSA-N	2.8×10^3		Keshavarz et al. (2022)	Q	
	1.0×10^1		Duchowicz et al. (2020)	Q	184
	3.7×10^1		Modarresi et al. (2007)	Q	67
	3.1×10^3		Duchowicz et al. (2020)	?	185, 21
5,5-dimethyl-2,4-	3.5×10^3		HSDB (2015)	Q	99
imidazolidinedione					
$C_5H_8N_2O_2$	3.6×10^3		Zhang et al. (2010)	Q	287, 288
[77-71-4]	1.6×10^5		Zhang et al. (2010)	Q	287, 289
YIROYDNZEPTFOL-UHFFFAOYSA-N	5.1×10^6		Zhang et al. (2010)	Q	287, 290
	1.6×10^5		Zhang et al. (2010)	Q	287, 291
1-methyluracil	2.3×10^3		Duchowicz et al. (2020)	V	186
$C_5H_6N_2O_2$	2.1×10^5		Duchowicz et al. (2020)	Q	
[615-77-0]					
XBCXJKGHPABGSD-UHFFFAOYSA-N					
2-azacycloheptanone	1.8×10^5		HSDB (2015)	V	
$C_6H_{11}NO$	2.0×10^3		Hwang et al. (1992)	V	
(caprolactam)	3.9×10^4		Abraham et al. (2019)	Q	
[105-60-2]					
JBKVHLHDHHXQEQ-UHFFFAOYSA-N					

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Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-acetylpyrrolidine $C_6H_{11}NO$ [4030-18-6] LNWWQYYLZVZXKS-UHFFFAOYSA-N	6.2×10^{3}		Gibbs et al. (1991)	M	
glucosamine $C_6H_{13}NO_5$ [3416-24-8] MSWZFWKMSRAUBD-IVMDWMLBSA-N	1.3×10^{10}		HSDB (2015)	Q	99
N-ethylmorpholine $C_6H_{13}NO$ [100-74-3] HVCNXQOWACZAFN-UHFFFAOYSA-N	4.0×10^{2}		HSDB (2015)	Q	99
3-formylpyridine C_6H_5NO [500-22-1] QJZUKDFHGGYHMC-UHFFFAOYSA-N	6.5×10^{1}		Abraham et al. (1994a)	R	
	6.5×10^{1}		Keshavarz et al. (2022)	Q	
	1.5×10^{1}		Duchowicz et al. (2020)	Q	
	1.0×10^{2}		Hilal et al. (2008)	Q	
	2.7×10^{1}		Modarresi et al. (2007)	Q	67
	6.5×10^{1}		Yaffe et al. (2003)	Q	248, 249
	1.2×10^{2}		English and Carroll (2001)	Q	230, 274
	3.8×10^{1}		Nirmalakhandan et al. (1997)	Q	
	6.6×10^{1}		Duchowicz et al. (2020)	?	185, 21
4-formylpyridine C_6H_5NO [872-85-5] BGUWFUQJCDRPTL-UHFFFAOYSA-N	5.6×10^{1}		Abraham et al. (1994a)	R	
	6.5×10^{1}		Keshavarz et al. (2022)	Q	
	1.5×10^{1}		Duchowicz et al. (2020)	Q	299
	1.0×10^{2}		Hilal et al. (2008)	Q	
	2.2×10^{1}		Modarresi et al. (2007)	Q	67
	6.5×10^{1}		Yaffe et al. (2003)	Q	248, 272
	6.4×10^{1}		English and Carroll (2001)	Q	230, 231
	3.8×10^{1}		Nirmalakhandan et al. (1997)	Q	
	5.6×10^{1}		Duchowicz et al. (2020)	?	185, 21
niacinamide $C_6H_6N_2O$ [98-92-0] DFPAKSUCGFBDDF-UHFFFAOYSA-N	3.4×10^{6}		HSDB (2015)	Q	99
metronidazole $C_6H_9N_3O_3$ [443-48-1] VAOCPAMSLUNLGC-UHFFFAOYSA-N	5.8×10^{5}		HSDB (2015)	Q	99
nicotinic acid $C_6H_5NO_2$ [59-67-6] PVNIIMVLHYAWGP-UHFFFAOYSA-N	2.5×10^{4}		Abraham et al. (2019)	Q	

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Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
isonicotinic acid $C_6H_5NO_2$ [55-22-1] TWBYWOBDOCUKOW-UHFFFAOYSA-N	1.6×10^4		Abraham et al. (2019)	Q	
1-methylthymine $C_6H_8N_2O_2$ [4160-72-9] GKMIDMKPBOUSBQ-UHFFFAOYSA-N	1.7×10^4		Ebert et al. (2023)	?	365
glydant $C_7H_{12}N_2O_4$ (1,3-dimethylol-5,5-dimethylhydantoin) [6440-58-0] WSDISUOETYTPRL-UHFFFAOYSA-N	1.4×10^6		HSDB (2015)	Q	99
3-quinuclidinol $C_7H_{13}NO$ [1619-34-7] IVLICPVPXWEGCA-UHFFFAOYSA-N	1.7×10^3 1.8×10^4 5.1×10^3 1.2×10^4		Du et al. (2017) Du et al. (2017) Du et al. (2017) HSDB (2015)	M Q Q Q	478 549 99
dinotefuran $C_7H_{14}N_4O_3$ [165252-70-0] YKBZOVFACRVRJN-UHFFFAOYSA-N	1.5×10^8		HSDB (2015)	V	
1,2,3-benzotriazin-4(1H)-one $C_7H_5N_3O$ [90-16-4] DMSSTTLDFWKBSX-UHFFFAOYSA-N	3.1×10^4		HSDB (2015)	Q	99
4-acetylpyridine C_7H_7NO [1122-54-9] WMQUKDQWMMOHSA-UHFFFAOYSA-N	1.6×10^2 8.8×10^1 5.0 1.9×10^2 4.1×10^1 8.0×10^1 2.7×10^1 1.6×10^2		Abraham et al. (1994a) Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) English and Carroll (2001) Nirmalakhandan et al. (1997) Duchowicz et al. (2020)	R Q Q Q Q Q Q ?	 299 67 230, 231 185, 21
3-acetylpyridine C_7H_7NO [350-03-8] WEGYGNROSJDEIW-UHFFFAOYSA-N	4.6×10^2 8.8×10^1 5.0 1.9×10^2 5.2×10^1 2.7×10^1 4.6×10^2		Abraham et al. (1994a) Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Nirmalakhandan et al. (1997) Duchowicz et al. (2020)	R Q Q Q Q Q ?	 299 67 185, 21

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Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
theophylline $C_7H_8N_4O_2$ [58-55-9] ZFXYFBGIUFBOJW-UHFFFAOYSA-N	5.5×10^{8}		HSDB (2015)	Q	99
theobromine $C_7H_8N_4O_2$ [83-67-0] YAPQBXQYLJRXSA-UHFFFAOYSA-N	6.2×10^{5}		HSDB (2015)	Q	99
2-pyridineethanol C_7H_9NO [103-74-2] BXGYBSJAZFGIPX-UHFFFAOYSA-N	6.6×10^{4}		HSDB (2015)	Q	99
caffeine $C_8H_{10}N_4O_2$ [58-08-2] RYYVLZVUVIJVGH-UHFFFAOYSA-N	9.0×10^{5}		HSDB (2015)	V	
acyclovir $C_8H_{11}N_5O_3$ [59277-89-3] MKUXAQIIEYXACX-UHFFFAOYSA-N	3.1×10^{16}		HSDB (2015)	Q	99
2-methoxy-3-(1-methylethyl)-pyrazine $C_8H_{12}N_2O$ [25773-40-4] NTOPKICPEQUPPH-UHFFFAOYSA-N	2.1×10^{1} 1.5×10^{1}		Wu et al. (2022a) Hilal et al. (2008)	Q Q	413
simeton $C_8H_{15}N_5O$ [673-04-1] HKAMKLBXTLTVCN-UHFFFAOYSA-N	1.5×10^{4} 2.5×10^{4}		Hilal et al. (2008) Abraham et al. (2007)	Q Q	
N-isobutylmorpholine $C_8H_{17}NO$ [10315-98-7] QKVSMSABRNCNRS-UHFFFAOYSA-N		8100 6000	Kühne et al. (2005) Kühne et al. (2005)	Q ?	
phthalimide $C_8H_5NO_2$ [85-41-6] XKJCHHZQLQNZHY-UHFFFAOYSA-N	9.9×10^{2}		HSDB (2015)	Q	99
furazolidone $C_8H_7N_3O_5$ [67-45-8] PLHJDBGFXBMTGZ-UHFFFAOYSA-N	3.0×10^{5}		HSDB (2015)	Q	99

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1,2,3,6-tetrahydrophthalimide $C_8H_9NO_2$ [85-40-5] CIFFBTOJCKSRJY-UHFFFAOYSA-N	3.3×10^{2}		HSDB (2015)	Q	99
N-nitrosonornicotine $C_9H_{11}N_3O$ [16543-55-8] XKABJYQDMJTNGQ-UHFFFAOYSA-N	5.8×10^{4}		HSDB (2015)	Q	447
9-[(1,3-dihydroxy-2-propoxy)methyl]guanine $C_9H_{13}N_5O_4$ (ganciclovir) [82410-32-0] IRSCQMHQWWYFCW-UHFFFAOYSA-N	6.6×10^{17}		HSDB (2015)	Q	99
2-*sec*-butyl-3-methoxypyrazine $C_9H_{14}N_2O$ [24168-70-5] QMQDJVIJVPEQHE-UHFFFAOYSA-N	2.0×10^{-1}		Ebert et al. (2023)	?	365
atraton $C_9H_{17}N_5O$ [1610-17-9] PXWUKZGIHQRDHL-UHFFFAOYSA-N	6.4×10^{3} 1.1×10^{4} 2.2×10^{3}		Hilal et al. (2008) Abraham et al. (2007) MacBean (2012a)	Q Q ?	
4-hydroxy-2,2,6,6-tetramethyl-1-piperidinyloxy $C_9H_{18}NO_2$ [2226-96-2] UZFMOKQJFYMBGY-UHFFFAOYSA-N	3.3×10^{9}		HSDB (2015)	Q	99
8-hydroxyquinoline C_9H_7NO [148-24-3] MCJGNVYPOGVAJF-UHFFFAOYSA-N	1.7×10^{1} 1.7×10^{1} 8.9×10^{1} 5.5×10^{2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Maniere et al. (2011)	V V Q ?	186 241, 165
carbendazim $C_9H_9N_3O_2$ [10605-21-7] TWFZGCMQGLPBSX-UHFFFAOYSA-N	4.7×10^{5} 6.5×10^{5}		HSDB (2015) Mackay et al. (2006d)	V V	
metamitron $C_{10}H_{10}N_4O$ [41394-05-2] VHCNQEUWZYOAEV-UHFFFAOYSA-N	1.0×10^{6} 2.2×10^{6} 4.5×10^{3} 2.8×10^{7} 1.6×10^{7} 1.1×10^{7}		Barcelo and Hennion (1997) Delgado and Alderete (2003) Goodarzi et al. (2010) Delgado and Alderete (2003) Delgado and Alderete (2003) Maniere et al. (2011)	X C Q Q Q ?	567 568 241, 165

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pymetrozin $C_{10}H_{11}N_5O$ [123312-89-0] QHMTXANCGGJZRX-UHFFFAOYSA-N	3.3×10^{5}		HSDB (2015)	V	
3-oxo-N-phenylbutanamide $C_{10}H_{11}NO_2$ (acetoacetanilide) [102-01-2] DYRDKSSFIWVSNM-UHFFFAOYSA-N	2.3×10^{6}		HSDB (2015)	Q	99
2,3'-didehydro-3'-deoxythymidine (stavudine) $C_{10}H_{12}N_2O_4$ (stavudine) [3056-17-5] XNKLLVCARDGLGL-JGVFFNPUSA-N	4.3×10^{9}		HSDB (2015)	Q	99
cotinine $C_{10}H_{12}N_2O$ [486-56-6] UIKROCXWUNQSPJ-UHFFFAOYSA-N	3.0×10^{6}		HSDB (2015)	Q	99
4-(N-nitroso-N-methylamino)-1-(3-pyridyl)-1-butanone $C_{10}H_{13}N_3O_2$ [64091-91-4] FLAQQSHRLBFIEZ-UHFFFAOYSA-N	1.2×10^{8}		HSDB (2015)	Q	99
9-(4-hydroxy-3-hydroxymethylbut-1-yl)guanine $C_{10}H_{15}N_5O_3$ (penciclovir) [39809-25-1] JNTOCHDNEULJHD-UHFFFAOYSA-N	1.0×10^{26}		HSDB (2015)	Q	99
anatoxin A $C_{10}H_{15}NO$ [64285-06-9] SGNXVBOIDPPRJJ-UHFFFAOYSA-N	1.5×10^{3}		HSDB (2015)	Q	99
dimetilan $C_{10}H_{16}N_4O_3$ [644-64-4] RDBIYWSVMRVKSG-UHFFFAOYSA-N	2.4×10^{5}		HSDB (2015)	Q	99
isolan $C_{10}H_{17}N_3O_2$ [119-38-0] RNNBHZYEKNHLKT-UHFFFAOYSA-N	4.9×10^{3}		HSDB (2015)	Q	99

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Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
amicarbazone $C_{10}H_{19}N_5O_2$ [129909-90-6] ORFPWVRKFLOQHK-UHFFFAOYSA-N	1.5×10^{7}		MacBean (2012b)	X	350
prometone	1.1×10^{4}		HSDB (2015)	V	
$C_{10}H_{19}N_5O$	1.1×10^{4}		Mackay et al. (2006d)	V	
(prometon)	1.1×10^{4}		Suntio et al. (1988)	V	12
[1610-18-0]	1.1×10^{2}		Barcelo and Hennion (1997)	X	567
ISEUFVQQFVOBCY-UHFFFAOYSA-N	6.9×10^{1}		Goodarzi et al. (2010)	Q	568
	2.7×10^{3}		Hilal et al. (2008)	Q	
	5.1×10^{3}		Abraham et al. (2007)	Q	
secbumeton	2.8×10^{3}		Mackay et al. (2006d)	V	
$C_{10}H_{19}N_5O$	2.9×10^{3}		Suntio et al. (1988)	V	12
[26259-45-0]	5.0×10^{3}		Hilal et al. (2008)	Q	
ZJMZZNVGNSWOOM-UHFFFAOYSA-N	7.2×10^{3}		Abraham et al. (2007)	Q	
	2.7×10^{3}		MacBean (2012a)	?	
terbumeton	2.1×10^{3}		Mackay et al. (2006d)	V	
$C_{10}H_{19}N_5O$	2.4×10^{3}		Hilal et al. (2008)	Q	
[33693-04-8]	1.6×10^{3}		Abraham et al. (2007)	Q	
BCQMBFHBDZVHKU-UHFFFAOYSA-N					
kinetin $C_{10}H_9N_5O$ [525-79-1] QANMHLXAZMSUEX-UHFFFAOYSA-N	8.2×10^{8}		HSDB (2015)	Q	99
isouron	7.3×10^{4}		Duchowicz et al. (2020)	V	186
$C_{10}H_{17}N_3O_2$	3.3×10^{1}		Duchowicz et al. (2020)	Q	
[55861-78-4]					
JLLJHQLUZAKJFH-UHFFFAOYSA-N					
fuberidazole $C_{11}H_8N_2O$ [3878-19-1] UYJUZNLFJAWNEZ-UHFFFAOYSA-N	1.9×10^{5}		Ebert et al. (2023)	?	318
carbadox $C_{11}H_{10}N_4O_4$ [6804-07-5] OVGGLBAWFMIPPY-WUXMJOGZSA-N	2.2×10^{17}		HSDB (2015)	Q	99
bendiocarb	2.5×10^{2}		Duchowicz et al. (2020)	V	186
$C_{11}H_{13}NO_4$	2.5×10^{2}		HSDB (2015)	V	
[22781-23-3]	2.7×10^{2}		Mackay et al. (2006d)	V	
XEGGRYVFLWGFHI-UHFFFAOYSA-N	2.0×10^{2}		Duchowicz et al. (2020)	Q	

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Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,5-trimethylphenol, methylcarbamate $C_{11}H_{15}NO_2$ (2,3,5-trimethacarb) [2655-15-4] NYOKZHDTNBDPOB-UHFFFAOYSA-N	4.5×10^{1}		HSDB (2015)	V	
butalbital $C_{11}H_{16}N_2O_3$ [77-26-9] UZVHFVZFNXBMQJ-UHFFFAOYSA-N	1.6×10^{7}		HSDB (2015)	Q	99
dexrazoxane $C_{11}H_{16}N_4O_4$ [24584-09-6] BMKDZUISNHGIBY-ZETCQYMHSA-N	4.7×10^{13}		HSDB (2015)	Q	99
pentobarbital $C_{11}H_{18}N_2O_3$ [76-74-4] WEXRUCMBJFQVBZ-UHFFFAOYSA-N	1.2×10^{7}		HSDB (2015)	Q	99
pirimor $C_{11}H_{18}N_4O_2$ (pirimicarb) [23103-98-2] YFGYUFNIOHWBOB-UHFFFAOYSA-N	1.2×10^{4} 3.1×10^{3} 5.0×10^{3} 5.9×10^{3} 3.1×10^{3} 3.4×10^{4} 3.0×10^{4} 3.0×10^{4} 2.8×10^{4}		HSDB (2015) Mackay et al. (2006d) Siebers and Mattusch (1996) Siebers et al. (1994) Suntio et al. (1988) Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011)	V V V V V ? ? ? ?	 12 12 12, 574, 165 12, 575, 165 12, 576, 165 12, 165
ethirimol $C_{11}H_{19}N_3O$ [23947-60-6] BBXXLROWFHWFQY-UHFFFAOYSA-N	3.6×10^{3}		Mackay et al. (2006d)	V	
pyroquilon $C_{11}H_{11}NO$ [57369-32-1] XRJLAOUDSILTFT-UHFFFAOYSA-N	5.1×10^{3}		Ebert et al. (2023)	?	318
fenfuram $C_{12}H_{11}NO_2$ [24691-80-3] JFSPBVWPKOEZCB-UHFFFAOYSA-N	2.5×10^{4}		Mackay et al. (2006d)	V	

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Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
oxabetrinil $C_{12}H_{12}N_2O_3$ [74782-23-3] WFVUIONFJOAYPK-UHFFFAOYSA-N	8.6×10^{1}		Ebert et al. (2023)	?	318
phenobarbital $C_{12}H_{12}N_2O_3$ [50-06-6] DDBREPKUVSBGFI-UHFFFAOYSA-N	5.8×10^{8}		HSDB (2015)	Q	99
triaziquone $C_{12}H_{13}N_3O_2$ [68-76-8] PXSOHRWMIRDKMP-UHFFFAOYSA-N	1.1×10^{10}		HSDB (2015)	Q	99
triallyl cyanurate $C_{12}H_{15}N_3O_3$ [101-37-1] BJELTSYBAHKXRW-UHFFFAOYSA-N	2.3×10^{1} 1.8×10^{3} 1.9×10^{2} 4.1×10^{4}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
entecavir $C_{12}H_{15}N_5O_3$ [142217-69-4] QDGZDCVAUDNJFG-FXQIFTODSA-N	6.2×10^{15}		HSDB (2015)	Q	99
metaxalone $C_{12}H_{15}NO_3$ [1665-48-1] IMWZZHHPURKASS-UHFFFAOYSA-N	3.7×10^{4}		HSDB (2015)	Q	99
phendimetrazine $C_{12}H_{17}NO$ [634-03-7] MFOCDFTXLCYLKU-UHFFFAOYSA-N	3.7×10^{2}		HSDB (2015)	Q	99
hexazinone $C_{12}H_{20}N_4O_2$ [51235-04-2] CAWXEEYDBZRFPE-UHFFFAOYSA-N	$>9.9\times10^{1}$ 4.4×10^{6}		Mabury and Crosby (1996) HSDB (2015)	M V	
picaridin $C_{12}H_{23}NO_3$ [119515-38-7] QLHULAHOXSSASE-UHFFFAOYSA-N	3.3×10^{5}		HSDB (2015)	Q	99
lenacil $C_{13}H_{18}N_2O_2$ [2164-08-1] ZTMKADLOSYKWCA-UHFFFAOYSA-N	1.3×10^{5} 3.8×10^{4} 7.7×10^{6}		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	186 241, 165

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Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pyrinuron $C_{13}H_{12}N_4O_3$ (pyriminil) [53558-25-1] CLKZWXHKFXZIMA-UHFFFAOYSA-N	5.4×10^{10}		HSDB (2015)	Q	99
melatonin $C_{13}H_{16}N_2O_2$ [73-31-4] DRLFMBDRBRZALE-UHFFFAOYSA-N	3.8×10^{8}		HSDB (2015)	Q	447
dibenz[b,f]][1,4]oxazepine $C_{13}H_9NO$ [257-07-8] NPUACKRELIJTFM-UHFFFAOYSA-N	2.4×10^{-3}		HSDB (2015)	Q	99
oxadixyl $C_{14}H_{18}N_2O_4$ [77732-09-3] UWVQIROCRJWDKL-UHFFFAOYSA-N	2.0×10^{6}		Ebert et al. (2023)	?	318
benomyl $C_{14}H_{18}N_4O_3$ [17804-35-2] RIOXQFHNBCKOKP-UHFFFAOYSA-N	5.2×10^{5} 3.1×10^{5} 1.8×10^{5} 2.0×10^{6}		Mackay et al. (2006d) Keshavarz et al. (2022) Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q Q ?	 185, 21
trimethoprim $C_{14}H_{18}N_4O_3$ [738-70-5] IEDVJHCEMCRBQM-UHFFFAOYSA-N	4.1×10^{8}		HSDB (2015)	Q	99
ethoxyquin $C_{14}H_{19}NO$ [91-53-2] DECIPOUIJURFOJ-UHFFFAOYSA-N	8.0		Ebert et al. (2023)	?	318
famciclovir $C_{14}H_{19}N_5O_4$ [104227-87-4] GGXKWVWZWMLJEH-UHFFFAOYSA-N	1.0×10^{8}		HSDB (2015)	Q	99
furmecyclox $C_{14}H_{21}NO_3$ [60568-05-0] QTDRLOKFLJJHTG-UHFFFAOYSA-N	1.4×10^{2}		MacBean (2012a)	?	
oxcarbazepine $C_{15}H_{12}N_2O_2$ [28721-07-5] CTRLABGOLIVAIY-UHFFFAOYSA-N	1.4×10^{7}		HSDB (2015)	Q	99

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Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
phenytoin $C_{15}H_{12}N_2O_2$ [57-41-0] CXOFVDLJLONNDW-UHFFFAOYSA-N	9.7×10^{5}		HSDB (2015)	Q	99
carbamazepine $C_{15}H_{12}N_2O$ [298-46-4] FFGPTBGBLSHEPO-UHFFFAOYSA-N	9.0×10^{4}		HSDB (2015)	Q	99
propylthiouracil $C_{15}H_{12}N_2O$ [51-52-5] KNAHARQHSZJURB-UHFFFAOYSA-N	9.0×10^{3}		HSDB (2015)	Q	99
ancymidol $C_{15}H_{16}N_2O_2$ [12771-68-5] HUTDUHSNJYTCAR-UHFFFAOYSA-N	9.1×10^{5} 1.5×10^{6} 4.7×10^{6} 6.3×10^{5}		Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Duchowicz et al. (2020)	Q Q Q ?	 185, 21
imazethapyr $C_{15}H_{19}N_3O_3$ [81335-77-5] XVOKUMIPKHGGTN-UHFFFAOYSA-N	9.9×10^{10}		HSDB (2015)	Q	99
imazamox $C_{15}H_{19}N_3O_4$ [114311-32-9] NUPJIGQFXCQJBK-UHFFFAOYSA-N	1.1×10^{13} 2.0×10^{11}		HSDB (2015) Maniere et al. (2011)	Q ?	99 241, 165
cycloheximide $C_{15}H_{23}NO_4$ [66-81-9] YPHMISFOHDHNIV-FSZOTQKASA-N	2.8×10^{9}		HSDB (2015)	Q	99
oxymatrine $C_{15}H_{24}N_2O_2$ [16837-52-8] XVPBINOPNYFXID-LHDUFFHYSA-N	9.9×10^{12}		HSDB (2015)	Q	99
triapenthenol $C_{15}H_{25}N_3O$ [76608-88-3] CNFMJLVJDNGPHR-UKTHLTGXSA-N	4.0×10^{4}		Ebert et al. (2023)	?	318
mebendazole $C_{16}H_{13}N_3O_3$ [31431-39-7] OPXLLQIJSORQAM-UHFFFAOYSA-N	1.8×10^{10}		HSDB (2015)	Q	99

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Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
imazamethabenz-methyl $C_{16}H_{20}N_2O_3$ [81405-85-8] FFCCBBNQPIMUJI-UHFFFAOYSA-N	2.6×10^{6}		HSDB (2015)	V	
nifedipine $C_{17}H_{18}N_2O_6$ [21829-25-4] HYIMSNHJOBLJNT-UHFFFAOYSA-N	1.4×10^{8}		HSDB (2015)	Q	99
oxymorphone $C_{17}H_{19}NO_4$ [76-41-5] UQCNKQCJZOAFTQ-UHFFFAOYSA-N	2.4×10^{13}		HSDB (2015)	Q	99
desomorphine $C_{17}H_{21}NO_2$ [427-00-9] LNNWVNGFPYWNQE-UHFFFAOYSA-N	2.4×10^{6}		HSDB (2015)	Q	99
cocaine $C_{17}H_{21}NO_4$ [50-36-2] ZPUCINDJVBIVPJ-PFSRBDOWSA-N	2.3×10^{5} 2.3×10^{5} 7.9×10^{4}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
N-(2-ethylhexyl)-5-norbornene-2,3-dicarboximide $C_{17}H_{25}NO_2$ [113-48-4] WLLGXSLBOPFWQV-UHFFFAOYSA-N	3.5×10^{1}		HSDB (2015)	Q	99
imazaquin $C_{17}H_{17}N_3O_3$ [81335-37-7] CABMTIJINOIHOD-UHFFFAOYSA-N	2.7×10^{11}		Maniere et al. (2011)	?	12, 165
(*E*)-pyriminobac-methyl $C_{17}H_{19}N_3O_6$ [147411-69-6] USSIUIGPBLPCDF-KEBDBYFISA-N	7.3×10^{2}		Ebert et al. (2023)	?	318
(*Z*)-pyriminobac-methyl $C_{17}H_{19}N_3O_6$ [147411-70-9] USSIUIGPBLPCDF-JMIUGGIZSA-N	1.9×10^{4}		Ebert et al. (2023)	?	318
imiprothrin $C_{17}H_{22}N_2O_4$ [72963-72-5] VPRAQYXPZIFIOH-UHFFFAOYSA-N	1.6×10^{5} 6.9×10^{3}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186

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Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
iprovalicarb $C_{18}H_{28}N_2O_3$ [140923-17-7] NWUWYYSKZYIQAE-LBAUFKAWSA-N	7.1×10^{5}		Maniere et al. (2011)	?	12, 165
quinophthalone $C_{18}H_{11}NO_2$ [8003-22-3] IZMJMCDDWKSTTK-UHFFFAOYSA-N	1.6×10^{8}		HSDB (2015)	Q	99
pefurazoate $C_{18}H_{23}N_3O_4$ [101903-30-4] WBTYBAGIHOISOQ-UHFFFAOYSA-N	1.8×10^{3}		Ebert et al. (2023)	?	318
tetramethrin $C_{19}H_{25}NO_4$ [7696-12-0] CXBMCYHAMVGWJQ-UHFFFAOYSA-N	5.8		HSDB (2015)	V	
isoxaben $C_{19}H_{25}NO_4$ [82558-50-7] PMHURSZHKKJGBM-UHFFFAOYSA-N	7.8×10^{3} 7.8×10^{3} 5.3×10^{3} 5.1×10^{3}		Duchowicz et al. (2020) MacBean (2012b) Duchowicz et al. (2020) Maniere et al. (2011)	V X Q ?	186 350 12, 165
alfuzosin $C_{19}H_{27}N_5O_4$ [81403-80-7] WNMJYKCGWZFFKR-UHFFFAOYSA-N	1.0×10^{14}		HSDB (2015)	Q	99
2,6-dimethyl-4-tridecylmorpholine $C_{19}H_{39}NO$ (tridemorph) [24602-86-6] YTOPFCCWCSOHFV-UHFFFAOYSA-N	5.8×10^{-2}		Ebert et al. (2023)	?	318
pyriproxyfen $C_{20}H_{19}NO_3$ [95737-68-1] NHDHVHZZCFYRSB-UHFFFAOYSA-N	1.6×10^{4} $>1.4\times10^{1}$		HSDB (2015) Maniere et al. (2011)	Q ?	99 72, 165
papaverine $C_{20}H_{21}NO_4$ [58-74-2] XQYZDYMELSJDRZ-UHFFFAOYSA-N	1.3×10^{7}		HSDB (2015)	Q	99
fenazaquin $C_{20}H_{22}N_2O$ [120928-09-8] DMYHGDXADUDKCQ-UHFFFAOYSA-N	2.1×10^{2} 9.9×10^{1} 4.7×10^{1} 1.8×10^{1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Maniere et al. (2011)	V V Q ?	186 241, 165

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Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bitertanol $C_{20}H_{23}N_3O_2$ [55179-31-2] VGPIBGGRCVEHQZ-UHFFFAOYSA-N	1.2×10^{4}		Mackay et al. (2006d)	V	
bitertanol diastereoisomer a $C_{20}H_{23}N_3O_2$ [70585-36-3] VGPIBGGRCVEHQZ-OALUTQOASA-N	3.1×10^{6}		Mackay et al. (2006d)	V	
bitertanol diastereoisomer b $C_{20}H_{23}N_3O_2$ [70585-38-5] VGPIBGGRCVEHQZ-RBUKOAKNSA-N	1.5×10^{6}		Mackay et al. (2006d)	V	
naltrexone $C_{20}H_{23}NO_4$ [16590-41-3] DQCKKXVULJGBQN-UHFFFAOYSA-N	2.3×10^{13}		HSDB (2015)	Q	99
D-lysergic acid N,N-diethylamide $C_{20}H_{25}N_3O$ (LSD) [50-37-3] VAYOSLLFUXYJDT-UHFFFAOYSA-N	6.6×10^{10}		HSDB (2015)	Q	99
ibogaine $C_{20}H_{26}N_2O$ [83-74-9] HSIBGVUMFOSJPD-UHFFFAOYSA-N	8.2×10^{5}		HSDB (2015)	Q	99
fenpropimorph $C_{20}H_{33}NO$ [67564-91-4] RYAUSSKQMZRMAI-ALOPSCKCSA-N	6.2 6.2×10^{-2} 7.9×10^{-2} 3.6×10^{-1}		Mackay et al. (2006d) Barcelo and Hennion (1997) Goodarzi et al. (2010) Maniere et al. (2011)	V X Q ?	 567 568 241, 165
strychnine $C_{21}H_{22}N_2O_2$ [57-24-9] QMGVPVSNSZLJIA-UHFFFAOYSA-N	1.6×10^{8}		HSDB (2015)	Q	99
nalmefene $C_{21}H_{25}NO_3$ [55096-26-9] WJBLNOPPDWQMCH-UHFFFAOYSA-N	5.5×10^{10}		HSDB (2015)	Q	99
benztropine $C_{21}H_{25}NO$ [86-13-5] GIJXKZJWITVLHI-UHFFFAOYSA-N	4.5×10^{3}		HSDB (2015)	Q	99

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Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
stanozolol $C_{21}H_{32}N_2O$ [10418-03-8] LKAJKIOFIWVMDJ-KIWJEFSTSA-N	9.0×10^{2}		HSDB (2015)	Q	99
spirotetramat	1.4×10^{7}		Maniere et al. (2011)	?	241, 493, 165
$C_{21}H_{27}NO_5$	1.6×10^{7}		Maniere et al. (2011)	?	241, 577, 165
[203313-25-1]	9.2×10^{6}		Maniere et al. (2011)	?	241, 573, 165
CLSVJBIHYWPGQY-GGYDESQDSA-N					
diacetylmorphine	1.6×10^{7}		Duchowicz et al. (2020)	V	186
$C_{21}H_{23}NO_5$	2.7×10^{5}		Duchowicz et al. (2020)	Q	
(heroin) [561-27-3] GVGLGOZIDCSQPN-PVHGPHFFSA-N					
pyrametostrobin $C_{21}H_{23}N_3O_4$ [915410-70-7] DWTVBEZBWMDXIY-UHFFFAOYSA-N	2.2×10^{4}		Ebert et al. (2023)	?	318
azoxystrobin	1.4×10^{8}		HSDB (2015)	V	
$C_{22}H_{17}N_3O_5$	1.4×10^{8}		Maniere et al. (2011)	?	241, 165
[131860-33-8] WFDXOXNFNRHQEC-GHRIWEEISA-N					
famoxadone	2.1×10^{2}		HSDB (2015)	V	
$C_{22}H_{18}N_2O_4$	2.2×10^{2}		Maniere et al. (2011)	?	241, 165
[131807-57-3] PCCSBWNGDMYFCW-UHFFFAOYSA-N					
tadalafil $C_{22}H_{19}N_3O_4$ [171596-29-5] WOXKDUGGOYFFRN-IIBYNOLFSA-N	2.0×10^{12}		HSDB (2015)	Q	99
bisacodyl $C_{22}H_{19}NO_4$ [603-50-9] KHOITXIGCFIULA-UHFFFAOYSA-N	1.4×10^{6}		HSDB (2015)	Q	99
fentanyl $C_{22}H_{28}N_2O$ [437-38-7] PJMPHNIQZUBGLI-UHFFFAOYSA-N	1.1×10^{6}		HSDB (2015)	Q	99

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Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-(triphenylmethyl)morpholine $C_{23}H_{23}NO$ (trifenmorph) [1420-06-0] ZJMLMBICUVVJDX-UHFFFAOYSA-N	7.6×10^{4} 3.2		HSDB (2015) MacBean (2012a)	Q ?	99
brucine $C_{23}H_{26}N_2O_4$ [357-57-3] RRKTZKIUPZVBMF-UHFFFAOYSA-N	4.7×10^{10}		HSDB (2015)	Q	99
mycophenolate mofetil $C_{23}H_{31}NO_7$ [128794-94-5] RTGDFNSFWBGLEC-SYZQJQIISA-N	1.8×10^{9}		HSDB (2015)	Q	99
pinoxaden $C_{23}H_{32}N_2O_4$ [243973-20-8] MGOHCFMYLBAPRN-UHFFFAOYSA-N	1.1×10^{6} 1.1×10^{6}		HSDB (2015) Maniere et al. (2011)	V ?	 165
fenpyroximate $C_{24}H_{27}N_3O_4$ [134098-61-6] YYJNOYZRYGDPNH-MFKUBSTISA-N	4.6 7.6 5.8×10^{4}		Duchowicz et al. (2020) MacBean (2012b) Duchowicz et al. (2020)	V X Q	186 350
valsartan $C_{24}H_{29}N_5O_3$ [137862-53-4] ACWBQPMHZXGDFX-QFIPXVFZSA-N	3.2×10^{12}		HSDB (2015)	Q	99
donepezil $C_{24}H_{29}NO_3$ [120014-06-4] ADEBPBSSDYVVLD-UHFFFAOYSA-N	8.2×10^{6}		HSDB (2015)	Q	99
chromafenozide $C_{24}H_{30}N_2O_3$ [143807-66-3] HPNSNYBUADCFDR-UHFFFAOYSA-N	5.1×10^{5} 6.2×10^{5} 5.6×10^{5}		Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011)	? ? ?	12, 493, 165 12, 577, 165 12, 573, 165
cyenopyrafen $C_{24}H_{31}N_3O_2$ [560121-52-0] APJLTUBHYCOZJI-VZCXRCSSSA-N	1.6×10^{3}		Ebert et al. (2023)	?	318

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Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-[4-[4-(2-benzoxazolyl)styryl]phenyl]-5-methylbenzoxazole	7.5×10^{8}		Zhang et al. (2010)	Q	287, 288
$C_{29}H_{20}N_2O_2$	6.2×10^{6}		Zhang et al. (2010)	Q	287, 289
[5242-49-9]	1.2×10^{5}		Zhang et al. (2010)	Q	287, 290
SOTPOQQKAUOHRO-BQYQJAHWSA-N	9.5×10^{7}		Zhang et al. (2010)	Q	287, 291
2-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol	7.2×10^{9}		Zhang et al. (2010)	Q	287, 288
$C_{30}H_{29}N_3O$	5.8×10^{5}		Zhang et al. (2010)	Q	287, 289
[70321-86-7]	1.4×10^{7}		Zhang et al. (2010)	Q	287, 290
OLFNXLXEGXRUOI-UHFFFAOYSA-N	8.8×10^{6}		Zhang et al. (2010)	Q	287, 291
fenpicoxamid $C_{31}H_{38}N_2O_{11}$ [517875-34-2] QGTOTYJSCYHYFK-RBODFLQRSA-N	4.2×10^{2}		Maniere et al. (2011)	?	165
norbormide $C_{33}H_{25}N_3O_3$ [991-42-4] DNTHHIVFNQZZRD-UHFFFAOYSA-N	3.7×10^{17}		HSDB (2015)	Q	99
reserpine $C_{33}H_{40}N_2O_9$ [50-55-5] QEVHRUUCFGRFIF-UHFFFAOYSA-N	1.8×10^{17}		HSDB (2015)	Q	99
telmisartan $C_{33}H_{30}N_4O_2$ [144701-48-4] RMMXLENWKUUMAY-UHFFFAOYSA-N	1.9×10^{14}		Abraham et al. (2019)	Q	
telaprevir $C_{36}H_{53}N_7O_6$ [402957-28-2] BBAWEDCPNXPBQM-GDEBMMAJSA-N	1.3×10^{25}		HSDB (2015)	Q	99
lopinavir $C_{37}H_{48}N_4O_5$ [192725-17-0] KJHKTHWMRKYKJE-WRHCQWCJSA-N	2.3×10^{22}		HSDB (2015)	Q	99
atazanavir $C_{38}H_{52}N_6O_7$ [198904-31-3] AXRYRYVKAWYZBR-GASGPIRDSA-N	2.7×10^{26}		HSDB (2015)	Q	99

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Table A4.5: Heterocycles with oxygen and nitrogen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tylosin $C_{46}H_{77}NO_{17}$ [1401-69-0] WBPYTXDJUQJLPQ-SNQVITFCSA-N	1.7×10^{32}		HSDB (2015)	Q	99
nystatin $C_{47}H_{75}NO_{17}$ [1400-61-9] VQOXZBDYSJBXMA-QFHUWGMOSA-N	4.9×10^{4}		HSDB (2015)	Q	99
1,3,5-tris(3,5-di-*tert*-butyl-4-hydroxybenzyl)-1,3,5-triazinane-2,4,6-trione	6.1×10^{20}		Zhang et al. (2010)	Q	287, 288
$C_{48}H_{69}N_3O_6$	1.3×10^{12}		Zhang et al. (2010)	Q	287, 289
[27676-62-6]	3.4×10^{10}		Zhang et al. (2010)	Q	287, 290
VNQNXQYZMPJLQX-UHFFFAOYSA-N	8.2×10^{14}		Zhang et al. (2010)	Q	287, 291

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A4.6 Nitrates ($RONO_2$)

Table A4.6: Nitrates ($RONO_2$)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
urea nitrate $CH_5N_3O_4$ [124-47-0] AYTGUZPQPXGYFS-UHFFFAOYSA-N	5.8×10^{11}		HSDB (2015)	Q	99
methyl nitrate CH_3ONO_2 [598-58-3] LRMHVVPPGGOAJQ-UHFFFAOYSA-N	2.0×10^{-2}	4700	Burkholder et al. (2019)	L	
	2.0×10^{-2}	4700	Burkholder et al. (2015)	L	
	2.0×10^{-2}	4700	Sander et al. (2011)	L	
	2.0×10^{-2}	4700	Sander et al. (2006)	L	
	2.0×10^{-2}	4700	Kames and Schurath (1992)	M	
	2.6×10^{-2}		Schwartz (1986)	C	87
	1.6×10^{-2}		Wang et al. (2017)	Q	80, 238
	1.3×10^{-1}		Wang et al. (2017)	Q	80, 239
	1.0×10^{-3}		Wang et al. (2017)	Q	80, 240
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.2×10^{-2}		Hilal et al. (2008)	Q	
		4900	Kühne et al. (2005)	Q	
		4800	Kühne et al. (2005)	?	
ethyl nitrate $C_2H_5ONO_2$ [625-58-1] IDNUEBSJWINEMI-UHFFFAOYSA-N	1.6×10^{-2}	5400	Burkholder et al. (2019)	L	
	1.6×10^{-2}	5400	Burkholder et al. (2015)	L	
	1.6×10^{-2}	5400	Sander et al. (2011)	L	
	1.6×10^{-2}	5400	Sander et al. (2006)	L	
	1.6×10^{-2}	5400	Kames and Schurath (1992)	M	
	1.2×10^{-2}		Wang et al. (2017)	Q	80, 238
	6.5×10^{-2}		Wang et al. (2017)	Q	80, 239
	9.1×10^{-4}		Wang et al. (2017)	Q	80, 240
	3.3×10^{-2}		HSDB (2015)	Q	99
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-2}		Hilal et al. (2008)	Q	
1-propyl nitrate $C_3H_7ONO_2$ [627-13-4] JNTOKFNBDFMTIV-UHFFFAOYSA-N	1.1×10^{-2}	5500	Burkholder et al. (2019)	L	
	1.1×10^{-2}	5500	Burkholder et al. (2015)	L	
	1.1×10^{-2}	5500	Sander et al. (2011)	L	
	1.1×10^{-2}	5500	Sander et al. (2006)	L	
	9.0×10^{-3}	5600	Staudinger and Roberts (2001)	L	
	7.4×10^{-3}	4600	Hauff et al. (1998)	M	
	1.1×10^{-2}	5500	Kames and Schurath (1992)	M	
	1.1×10^{-2}		Hauff et al. (1998)	V	
	3.6×10^{-3}		Keshavarz et al. (2022)	Q	
	6.9×10^{-3}		Duchowicz et al. (2020)	Q	184
	1.0×10^{-2}		Wang et al. (2017)	Q	80, 238

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	3.1×10^{-2}		Wang et al. (2017)	Q	80, 239
	6.2×10^{-4}		Wang et al. (2017)	Q	80, 240
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-2}		Hilal et al. (2008)	Q	
	5.3×10^{-2}		Modarresi et al. (2007)	Q	67
		5600	Kühne et al. (2005)	Q	
	7.8×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4600	Kühne et al. (2005)	?	
2-propyl nitrate $C_3H_7ONO_2$ (isopropyl nitrate) [1712-64-7] GAPFWGOSHOCNBM-UHFFFAOYSA-N	7.8×10^{-3}	5400	Burkholder et al. (2019)	L	
	7.8×10^{-3}	5400	Burkholder et al. (2015)	L	
	7.8×10^{-3}	5400	Sander et al. (2011)	L	
	7.8×10^{-3}	5400	Sander et al. (2006)	L	
	6.6×10^{-3}	5400	Staudinger and Roberts (2001)	L	
	5.5×10^{-3}	4300	Hauff et al. (1998)	M	
	7.8×10^{-3}	5400	Kames and Schurath (1992)	M	
	8.1×10^{-3}		Hauff et al. (1998)	V	
	3.6×10^{-3}		Keshavarz et al. (2022)	Q	
	2.7×10^{-3}		Duchowicz et al. (2020)	Q	184
	1.1×10^{-2}		Wang et al. (2017)	Q	80, 238
	2.4×10^{-2}		Wang et al. (2017)	Q	80, 239
	7.1×10^{-4}		Wang et al. (2017)	Q	80, 240
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	4.9		Raventos-Duran et al. (2010)	Q	245
	1.7×10^{-2}		Hilal et al. (2008)	Q	
	4.9×10^{-2}		Modarresi et al. (2007)	Q	67
		4600	Kühne et al. (2005)	Q	
	6.1×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4300	Kühne et al. (2005)	?	
1-butyl nitrate $C_4H_9ONO_2$ [928-45-0] QQHZPQUHCAKSOL-UHFFFAOYSA-N	1.0×10^{-2}	5800	Burkholder et al. (2019)	L	
	1.0×10^{-2}	5800	Burkholder et al. (2015)	L	
	1.0×10^{-2}	5800	Sander et al. (2011)	L	
	1.0×10^{-2}	5800	Sander et al. (2006)	L	
	8.8×10^{-3}	6000	Staudinger and Roberts (2001)	L	
	6.3×10^{-3}	5200	Hauff et al. (1998)	M	
	1.0×10^{-2}	5800	Kames and Schurath (1992)	M	
	1.0×10^{-2}	6000	Luke et al. (1989)	M	
	8.5×10^{-3}		Hauff et al. (1998)	V	
	4.8×10^{-3}		Keshavarz et al. (2022)	Q	
	1.0×10^{-2}		Duchowicz et al. (2020)	Q	
	8.9×10^{-3}		Wang et al. (2017)	Q	80, 238
	2.0×10^{-2}		Wang et al. (2017)	Q	80, 239
	3.0×10^{-4}		Wang et al. (2017)	Q	80, 240
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.7×10^{-2}		Hilal et al. (2008)	Q	
	4.2×10^{-2}		Modarresi et al. (2007)	Q	67
		5900	Kühne et al. (2005)	Q	
	6.4×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		5800	Kühne et al. (2005)	?	
2-butyl nitrate $C_4H_9ONO_2$ [924-52-7] DYONNFFVDNILGI-UHFFFAOYSA-N	6.4×10^{-3}	5400	Burkholder et al. (2019)	L	
	6.4×10^{-3}	5400	Burkholder et al. (2015)	L	
	6.4×10^{-3}	5400	Sander et al. (2011)	L	
	6.4×10^{-3}	5400	Sander et al. (2006)	L	
	6.4×10^{-3}	6100	Staudinger and Roberts (2001)	L	
	4.4×10^{-3}		Hauff et al. (1998)	M	
	6.4×10^{-3}	5400	Kames and Schurath (1992)	M	
	6.3×10^{-3}	5600	Luke et al. (1989)	M	
	6.4×10^{-3}		Hauff et al. (1998)	V	
	8.9×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.5×10^{-2}		Wang et al. (2017)	Q	80, 239
	5.5×10^{-4}		Wang et al. (2017)	Q	80, 240
		4900	Kühne et al. (2005)	Q	
		5400	Kühne et al. (2005)	?	
isobutyl nitrate $C_4H_9ONO_2$ [543-29-3] LNNXFUZKZLXPOF-UHFFFAOYSA-N	7.0×10^{-3}	5200	Kames and Schurath (1992)	M	
	4.8×10^{-3}		Keshavarz et al. (2022)	Q	
	3.9×10^{-3}		Duchowicz et al. (2020)	Q	
	8.9×10^{-3}		Wang et al. (2017)	Q	80, 238
	2.0×10^{-2}		Wang et al. (2017)	Q	80, 239
	4.6×10^{-4}		Wang et al. (2017)	Q	80, 240
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-2}		Hilal et al. (2008)	Q	
	4.4×10^{-2}		Modarresi et al. (2007)	Q	67
	4.4×10^{-3}		Duchowicz et al. (2020)	?	185, 21
1-pentyl nitrate $C_5H_{11}ONO_2$ (amyl nitrate) [1002-16-0] HSNWZBCBUUSSQD-UHFFFAOYSA-N	6.6×10^{-3}	6300	Hauff et al. (1998)	M	
	1.2×10^{-2}		Kames and Schurath (1992)	M	12
	4.0×10^{-3}		Hauff et al. (1998)	V	
	6.5×10^{-3}		Keshavarz et al. (2022)	Q	
	1.3×10^{-2}		Duchowicz et al. (2020)	Q	
	6.9×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.4×10^{-2}		Wang et al. (2017)	Q	80, 239
	4.8×10^{-4}		Wang et al. (2017)	Q	80, 240
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.3×10^{-2}		Hilal et al. (2008)	Q	
	3.8×10^{-2}		Modarresi et al. (2007)	Q	67

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
		6300	Kühne et al. (2005)	Q	
	5.9×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		6300	Kühne et al. (2005)	?	
2-pentyl nitrate	3.7×10^{-3}	6400	Staudinger and Roberts (2001)	L	
$C_5H_{11}ONO_2$	3.7×10^{-3}	5100	Hauff et al. (1998)	M	
(MCM:PEBNO3)	3.6×10^{-3}	6300	Kames and Schurath (1992)	M	
[21981-48-6]	4.8×10^{-3}		Hauff et al. (1998)	V	
RWRBSYOTDDOXKC-UHFFFAOYSA-N	3.4×10^{-3}	6000	Wieser et al. (2023)	Q	437
	6.5×10^{-3}		Keshavarz et al. (2022)	Q	
	5.0×10^{-3}		Duchowicz et al. (2020)	Q	299
	8.3×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.0×10^{-2}		Wang et al. (2017)	Q	80, 239
	4.8×10^{-4}		Wang et al. (2017)	Q	80, 240
	9.5×10^{-3}		Hilal et al. (2008)	Q	
	3.6×10^{-2}		Modarresi et al. (2007)	Q	67
		5300	Kühne et al. (2005)	Q	
	3.3×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		5100	Kühne et al. (2005)	?	
3-pentyl nitrate	3.8×10^{-3}	5300	Hauff et al. (1998)	M	
$C_5H_{13}ONO_2$	4.9×10^{-3}		Hauff et al. (1998)	V	
[82944-59-0]	6.5×10^{-3}		Keshavarz et al. (2022)	Q	
WQZKKVJFBZPJSU-UHFFFAOYSA-N	5.0×10^{-3}		Duchowicz et al. (2020)	Q	299
	8.3×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.0×10^{-2}		Wang et al. (2017)	Q	80, 239
	3.7×10^{-4}		Wang et al. (2017)	Q	80, 240
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	9.2×10^{-3}		Hilal et al. (2008)	Q	
	4.0×10^{-2}		Modarresi et al. (2007)	Q	67
		5300	Kühne et al. (2005)	Q	
	3.6×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		5300	Kühne et al. (2005)	?	
3-methyl-1-butanol nitrate	5.0×10^{-3}	5900	Hauff et al. (1998)	M	
$C_5H_{11}ONO_2$	6.5×10^{-3}		Keshavarz et al. (2022)	Q	
(isoamyl nitrate)	5.0×10^{-3}		Duchowicz et al. (2020)	Q	184
[543-87-3]	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
NTHGIYFSMNNHSC-UHFFFAOYSA-N	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	3.8×10^{-2}		Modarresi et al. (2007)	Q	67
		6300	Kühne et al. (2005)	Q	
	4.5×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		5900	Kühne et al. (2005)	?	

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pentaerythritol tetranitrate	7.6×10^{3}		HSDB (2015)	V	
$C_5H_8N_4O_{12}$	1.2		Yaws (2003)	X	237
[78-11-5]	8.2×10^{5}		Zhang et al. (2010)	Q	287, 288
TZRXHJWUDPFEEY-UHFFFAOYSA-N	1.1×10^{4}		Zhang et al. (2010)	Q	287, 289
	7.9×10^{4}		Zhang et al. (2010)	Q	287, 290
	3.6×10^{3}		Zhang et al. (2010)	Q	287, 291
	1.2		Gharagheizi et al. (2010)	Q	246
1-hexyl nitrate	7.6×10^{-3}	6700	Hauff et al. (1998)	M	
$C_6H_{13}ONO_2$	3.6×10^{-3}		Hauff et al. (1998)	V	
[20633-11-8]	8.8×10^{-3}		Keshavarz et al. (2022)	Q	
AGDYNDJUZRMYRG-UHFFFAOYSA-N	1.5×10^{-2}		Duchowicz et al. (2020)	Q	184
	5.8×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.0×10^{-2}		Wang et al. (2017)	Q	80, 239
	2.4×10^{-4}		Wang et al. (2017)	Q	80, 240
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	9.5×10^{-3}		Hilal et al. (2008)	Q	
	3.1×10^{-2}		Modarresi et al. (2007)	Q	67
		6600	Kühne et al. (2005)	Q	
	6.6×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		6700	Kühne et al. (2005)	?	
2-nitrooxyethanol	3.9×10^{2}		Burkholder et al. (2019)	L	
$HOC_2H_4ONO_2$	3.9×10^{2}		Burkholder et al. (2015)	L	
[16051-48-2]	3.9×10^{2}		Sander et al. (2011)	L	
HTKIMWYSDZQQBP-UHFFFAOYSA-N	3.9×10^{2}		Sander et al. (2006)	L	
	3.8×10^{2}	8600	Shepson et al. (1996)	M	
	3.9×10^{2}		Kames and Schurath (1992)	M	12
	5.7×10^{1}		Keshavarz et al. (2022)	Q	
	9.0×10^{-1}		Duchowicz et al. (2020)	Q	299
	4.2×10^{1}		Wang et al. (2017)	Q	80, 238
	5.5×10^{2}		Wang et al. (2017)	Q	80, 239
	7.6		Wang et al. (2017)	Q	80, 240
	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{2}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{2}		Raventos-Duran et al. (2010)	Q	245
	1.7×10^{2}		Hilal et al. (2008)	Q	
	8.5×10^{1}		Modarresi et al. (2007)	Q	67
		9200	Kühne et al. (2005)	Q	
	3.8×10^{2}		Duchowicz et al. (2020)	?	185, 21
		8700	Kühne et al. (2005)	?	

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1-nitrooxy-2-propanol	6.6×10^{1}		Burkholder et al. (2019)	L	
$C_3H_7O_4N$	6.6×10^{1}		Burkholder et al. (2015)	L	
[20266-65-3]	6.6×10^{1}		Sander et al. (2011)	L	
OMDFJTSKBNDDRM-UHFFFAOYSA-N	6.6×10^{1}		Sander et al. (2006)	L	
	1.1×10^{2}	10000	Shepson et al. (1996)	M	
	6.6×10^{1}		Kames and Schurath (1992)	M	578, 12
	7.2×10^{1}		Kames and Schurath (1992)	M	578, 12
	7.7×10^{1}		Keshavarz et al. (2022)	Q	
	9.3×10^{-1}		Duchowicz et al. (2020)	Q	
	3.9×10^{1}		Wang et al. (2017)	Q	80, 238
	3.6×10^{2}		Wang et al. (2017)	Q	80, 239
	1.7		Wang et al. (2017)	Q	80, 240
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{2}		Raventos-Duran et al. (2010)	Q	245
	9.5×10^{1}		Hilal et al. (2008)	Q	
	5.5×10^{1}		Modarresi et al. (2007)	Q	67
	1.1×10^{2}		Duchowicz et al. (2020)	?	185, 21
2-nitrooxy-1-propanol	7.2×10^{1}		Burkholder et al. (2019)	L	
$C_3H_7O_4N$	7.2×10^{1}		Burkholder et al. (2015)	L	
[20266-74-4]	7.2×10^{1}		Sander et al. (2011)	L	
HGCMMKIIGJXXMW-UHFFFAOYSA-N	7.2×10^{1}		Sander et al. (2006)	L	
	4.4×10^{1}	8800	Shepson et al. (1996)	M	
	6.6×10^{1}		Kames and Schurath (1992)	M	578, 12
	7.2×10^{1}		Kames and Schurath (1992)	M	578, 12
	7.7×10^{1}		Keshavarz et al. (2022)	Q	
	9.3×10^{-1}		Duchowicz et al. (2020)	Q	184
	3.9×10^{1}		Wang et al. (2017)	Q	80, 238
	2.7×10^{2}		Wang et al. (2017)	Q	80, 239
	1.6		Wang et al. (2017)	Q	80, 240
	3.1×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{2}		Raventos-Duran et al. (2010)	Q	245
	8.6×10^{1}		Hilal et al. (2008)	Q	
	6.9×10^{1}		Modarresi et al. (2007)	Q	67
	4.4×10^{1}		Duchowicz et al. (2020)	?	185, 21
1-nitrooxy-2-butanol	8.9×10^{1}		Treves et al. (2000)	M	28
$C_4H_9O_4N$	5.7×10^{1}	9200	Shepson et al. (1996)	M	
[147794-11-4]	1.0×10^{2}		Keshavarz et al. (2022)	Q	
KNUQGVIXAYDSOX-UHFFFAOYSA-N	1.7		Duchowicz et al. (2020)	Q	299
	3.2×10^{1}		Wang et al. (2017)	Q	80, 238
	1.9×10^{2}		Wang et al. (2017)	Q	80, 239
	1.1		Wang et al. (2017)	Q	80, 240
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	245

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.1×10^{1}		Hilal et al. (2008)	Q	
	5.4×10^{1}		Modarresi et al. (2007)	Q	67
	5.7×10^{1}		Duchowicz et al. (2020)	?	185, 21
2-nitrooxy-1-butanol	8.8×10^{1}		Treves et al. (2000)	M	28
$C_4H_9O_4N$	5.9×10^{1}	9600	Shepson et al. (1996)	M	
[147794-12-5]	1.0×10^{2}		Keshavarz et al. (2022)	Q	
YXMNEYKMHSBVTD-UHFFFAOYSA-N	1.7		Duchowicz et al. (2020)	Q	299
	3.2×10^{1}		Wang et al. (2017)	Q	80, 238
	1.6×10^{2}		Wang et al. (2017)	Q	80, 239
	1.6		Wang et al. (2017)	Q	80, 240
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{1}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	245
	6.0×10^{1}		Hilal et al. (2008)	Q	
	5.4×10^{1}		Modarresi et al. (2007)	Q	67
	5.9×10^{1}		Duchowicz et al. (2020)	?	185, 21
2-nitrooxy-3-butanol	1.0×10^{2}	9500	Shepson et al. (1996)	M	
$C_4H_9O_4N$	1.0×10^{2}		Keshavarz et al. (2022)	Q	
[147794-10-3]	6.8×10^{-1}		Duchowicz et al. (2020)	Q	299
CGFCSKMZZXPWEY-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	80, 238
	2.0×10^{2}		Wang et al. (2017)	Q	80, 239
	9.3×10^{-1}		Wang et al. (2017)	Q	80, 240
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	271, 243
	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	245
	5.4×10^{1}		Hilal et al. (2008)	Q	
	7.4×10^{1}		Modarresi et al. (2007)	Q	67
	1.0×10^{2}		Duchowicz et al. (2020)	?	185, 21
3-nitrooxy-1-butanol	1.4×10^{2}		Treves et al. (2000)	M	28
$C_4H_9O_4N$	2.6×10^{1}		Wang et al. (2017)	Q	80, 238
FOHXKGXDMSQVTH-UHFFFAOYSA-N	5.1×10^{2}		Wang et al. (2017)	Q	80, 239
	5.0		Wang et al. (2017)	Q	80, 240
4-nitrooxy-1-butanol	2.9×10^{2}		Treves et al. (2000)	M	28
$C_4H_9O_4N$	2.2×10^{1}		Wang et al. (2017)	Q	80, 238
[22911-39-3]	7.4×10^{2}		Wang et al. (2017)	Q	80, 239
FBOGSWRRYABFKU-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	80, 240
4-nitrooxy-2-butanol	1.3×10^{2}		Treves et al. (2000)	M	28
$C_4H_9O_4N$	2.6×10^{1}		Wang et al. (2017)	Q	80, 238
(3-hydroxy-1-nitrooxy-butane)	6.5×10^{2}		Wang et al. (2017)	Q	80, 239
[141299-18-5]	3.4		Wang et al. (2017)	Q	80, 240
WUKDMTQXKGFHBU-UHFFFAOYSA-N					

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
4-nitrooxy-1-pentanol $C_5H_{11}O_4N$ SVIFKHUNGQLAEN-UHFFFAOYSA-N	2.0×10^2 2.0×10^1 3.4×10^2 1.3×10^1		Treves et al. (2000) Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	M Q Q Q	28 80, 238 80, 239 80, 240
5-nitrooxy-1-pentanol $C_5H_{11}O_4N$ DVOSRLSVEOCANS-UHFFFAOYSA-N	2.0×10^2		Ebert et al. (2023)	?	579
5-nitrooxy-2-pentanol $C_5H_{11}O_4N$ (MCM:HO2C5NO3) RIQPKERROQFFJK-UHFFFAOYSA-N	3.6×10^2 2.1×10^1 2.0×10^1 4.4×10^2 6.5	9900	Treves et al. (2000) Wieser et al. (2023) Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	M Q Q Q Q	28 437 80, 238 80, 239 80, 240
1-nitrooxy-2-propanone $CH_3COCH_2ONO_2$ (nitrooxyacetone) [6745-71-7] ISWXYJQANHQYSR-UHFFFAOYSA-N	1.0×10^1 1.0×10^1 1.0×10^1 1.0×10^1 1.0×10^1 7.6 1.4×10^2 5.0×10^{-1} 2.5×10^1 3.9×10^1 7.8×10^1 1.2×10^2		Burkholder et al. (2019) Burkholder et al. (2015) Sander et al. (2011) Sander et al. (2006) Kames and Schurath (1992) Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Hilal et al. (2008)	L L L L M Q Q Q Q Q Q Q	 12 80, 238 80, 239 80, 240 242, 243 244 245
ISOP1N6CO $C_5H_7NO_5$ XXORYENTKCFFSM-UHFFFAOYSA-N	2.1×10^5	14000	Wieser et al. (2023)	Q	437
C52COCONO2 $C_5H_7NO_5$ QJXLMYNMVOSKND-UHFFFAOYSA-N	6.7×10^1	11000	Wieser et al. (2023)	Q	437
ISOP1N23O4CO $C_5H_7NO_5$ WBVYILWVTRBTDJ-UHFFFAOYSA-N	1.5×10^3	12000	Wieser et al. (2023)	Q	437
ROO6R7ONO2 $C_6H_{11}NO_5$ COKJDYWOSQONMU-UHFFFAOYSA-N	7.5×10^4	13000	Wieser et al. (2023)	Q	437
2-heptyl nitrate $C_7H_{15}NO_3$ (C7H15ONO2) HHXLSUKHLTZWKR-UHFFFAOYSA-N	2.3×10^{-3}	6600	Wieser et al. (2023)	Q	437

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
C7OHONO2 $C_7H_{15}NO_4$ MZJHMUSTUUJGSJ-UHFFFAOYSA-N	1.2×10^{1}	11000	Wieser et al. (2023)	Q	437
C622CONO2 $C_7H_{11}NO_5$ DJCVHBPUJHAWIU-UHFFFAOYSA-N	9.9×10^{2}	14000	Wieser et al. (2023)	Q	437
2-octyl nitrate $C_8H_{17}NO_3$ (C8H17ONO2) QCOKASLKYUXYJH-UHFFFAOYSA-N	6.8	7000	Wieser et al. (2023)	Q	437
C8OHONO2 $C_8H_{17}NO_4$ UEQWMROPIQKFIM-UHFFFAOYSA-N	9.0	11000	Wieser et al. (2023)	Q	437
C824ONO2 $C_8H_{13}NO_5$ YMYILPYDFNRVBZ-UHFFFAOYSA-N	9.5×10^{6}	14000	Wieser et al. (2023)	Q	437
C819ONO2 $C_8H_{13}NO_6$ XLUWXWLWQTYVOF-UHFFFAOYSA-N	3.9×10^{6}	16000	Wieser et al. (2023)	Q	437
C92ONO2 $C_9H_{15}NO_5$ PNFDSIMYWKOAKE-UHFFFAOYSA-N	4.7×10^{5}	15000	Wieser et al. (2023)	Q	437
NORLIMONO2 $C_9H_{15}NO_6$ MUTWZANDXPDWFF-UHFFFAOYSA-N	3.8×10^{8}	16000	Wieser et al. (2023)	Q	437
C822CONO2 $C_9H_{13}NO_5$ RVFLVBTUEWAABB-UHFFFAOYSA-N	6.2×10^{1}	13000	Wieser et al. (2023)	Q	437
C817CONO2 $C_9H_{13}NO_6$ LHFXXFGIVAQFTO-UHFFFAOYSA-N	1.2×10^{5}	15000	Wieser et al. (2023)	Q	437
C9CONO2 $C_{10}H_{15}NO_5$ FNVMVXZLPDKVAS-UHFFFAOYSA-N	8.0×10^{1}	20000	Wieser et al. (2023)	Q	437
LIMONO2 $C_{10}H_{15}NO_5$ DEKWHDOXDJNWRD-UHFFFAOYSA-N	3.8×10^{4}	14000	Wieser et al. (2023)	Q	437

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1,2-ethanediol dinitrate	6.3		Burkholder et al. (2019)	L	
$O_3NCH_2CH_2ONO_2$	6.3		Burkholder et al. (2015)	L	
(1,2-ethane dinitrate)	6.3		Sander et al. (2011)	L	
[628-96-6]	6.3		Sander et al. (2006)	L	
UQXKXGWGFRWILX-UHFFFAOYSA-N	7.8×10^{-1}		Fischer and Ballschmiter (1998b)	M	580
	6.3		Kames and Schurath (1992)	M	12
	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	9.9		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	245
	8.2		Hilal et al. (2008)	Q	
	4.9×10^{-1}		Modarresi et al. (2007)	Q	67
1,2-propanediol dinitrate	1.7		Burkholder et al. (2019)	L	
$C_3H_6(ONO_2)_2$	1.7		Burkholder et al. (2015)	L	
(1,2-propane dinitrate)	1.7		Sander et al. (2011)	L	
[6423-43-4]	1.7		Sander et al. (2006)	L	
PSXCGTLGGVDWFU-UHFFFAOYSA-N	3.2×10^{-1}		Fischer and Ballschmiter (1998b)	M	580
	1.7		Kames and Schurath (1992)	M	12
	1.0×10^{1}		HSDB (2015)	Q	99
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	3.1		Raventos-Duran et al. (2010)	Q	244
	9.9		Raventos-Duran et al. (2010)	Q	245
	2.7		Hilal et al. (2008)	Q	
1,3-propanediol dinitrate	1.6		Burkholder et al. (2019)	L	581
$C_3H_6N_2O_6$	1.6		Burkholder et al. (2015)	L	582
[3457-90-7]	1.3		Fischer and Ballschmiter (1998b)	M	580
KOSAMXZBGUIISK-UHFFFAOYSA-N	1.2		Raventos-Duran et al. (2010)	Q	242, 243
	3.9		Raventos-Duran et al. (2010)	Q	244
	9.9		Raventos-Duran et al. (2010)	Q	245
	4.4		Hilal et al. (2008)	Q	
1,2,3-propanetriol trinitrate	2.3×10^{2}		HSDB (2015)	V	
$C_3H_5N_3O_9$	1.9×10^{2}		Yaws (2003)	X	237, 12
(nitroglycerin)	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
[55-63-0]	3.9×10^{2}		Raventos-Duran et al. (2010)	Q	244
SNIOPGDIGTZGOP-UHFFFAOYSA-N	3.9×10^{3}		Raventos-Duran et al. (2010)	Q	245
	1.9×10^{2}		Gharagheizi et al. (2010)	Q	246
	3.9×10^{1}		Hilal et al. (2008)	Q	
	1.0×10^{2}		Yaws (1999)	?	21, 12
1,2-butanediol dinitrate	2.1×10^{-1}		Fischer and Ballschmiter (1998b)	M	580
$C_4H_8N_2O_6$	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
[20820-41-1]	1.6		Raventos-Duran et al. (2010)	Q	244
CTISQZXTUUHJNC-UHFFFAOYSA-N	7.8		Raventos-Duran et al. (2010)	Q	245

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3-butanediol dinitrate	5.7×10^{-1}		Fischer and Ballschmiter (1998b)	M	580
$C_4H_8N_2O_6$	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
[6423-44-5]	1.6		Raventos-Duran et al. (2010)	Q	244
DGFBULNMARLFTH-UHFFFAOYSA-N	7.8		Raventos-Duran et al. (2010)	Q	245
1,4-butanediol dinitrate	1.6		Fischer and Ballschmiter (1998b)	M	580
$C_4H_8N_2O_6$	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
[3457-91-8]	3.1		Raventos-Duran et al. (2010)	Q	244
QELUAJBXJAWSRC-UHFFFAOYSA-N	7.8		Raventos-Duran et al. (2010)	Q	245
	2.7		Hilal et al. (2008)	Q	
2,3-butanediol dinitrate	1.2×10^{-1}		Fischer and Ballschmiter (1998b)	M	580
$C_4H_8N_2O_6$	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
[6423-45-6]	1.6		Raventos-Duran et al. (2010)	Q	244
RVDDYBGRQLZMSB-UHFFFAOYSA-N	7.8		Raventos-Duran et al. (2010)	Q	245
1,2-pentanediol dinitrate $C_5H_{10}N_2O_6$ [89365-05-9] MZWHVGLDAWPHHW-UHFFFAOYSA-N	1.3×10^{-1}		Fischer and Ballschmiter (1998b)	M	580
1,4-pentanediol dinitrate $C_5H_{10}N_2O_6$ [25385-63-1] IUTIKUKYGRINOD-UHFFFAOYSA-N	3.9×10^{-1}		Fischer and Ballschmiter (1998b)	M	580
1,5-pentanediol dinitrate	1.2		Fischer and Ballschmiter (1998b)	M	580
$C_5H_{10}N_2O_6$	9.9×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
[3457-92-9]	2.0		Raventos-Duran et al. (2010)	Q	244
MIYIEPHJPVBSEV-UHFFFAOYSA-N	6.2		Raventos-Duran et al. (2010)	Q	245
(2R,4S)-2,4-pentanediol dinitrate $C_5H_{10}N_2O_6$ (*cis*-2,4-pentanediol dinitrate) [208252-05-5]	2.2×10^{-1}		Fischer and Ballschmiter (1998b)	M	580
(2R,4R)-2,4-pentanediol dinitrate $C_5H_{10}N_2O_6$ (*trans*-2,4-pentanediol dinitrate) [208252-04-4]	1.4×10^{-1}		Fischer and Ballschmiter (1998b)	M	580
1,2-hexanediol dinitrate $C_6H_{12}N_2O_6$ [110539-07-6] UJKJGCZXZPXTGS-UHFFFAOYSA-N	9.6×10^{-2}		Fischer and Ballschmiter (1998b)	M	580
1,5-hexanediol dinitrate $C_6H_{12}N_2O_6$ [206443-83-6] PGDWEAOSOZNKFU-UHFFFAOYSA-N	2.7×10^{-1}		Fischer and Ballschmiter (1998b)	M	580

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,6-hexanediol dinitrate $C_6H_{12}N_2O_6$ [3457-93-0] GCVAYIWGKFFWEU-UHFFFAOYSA-N	1.5		Fischer and Ballschmiter (1998b)	M	580
2,5-hexanediol dinitrate $C_6H_{12}N_2O_6$ [99115-63-6] ISSLCMSTXXUOEU-UHFFFAOYSA-N	3.1×10^{-1} 6.2×10^{-1} 6.2×10^{-1} 4.9		Fischer and Ballschmiter (1998b) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010)	M Q Q Q	580 271, 243 244 245
(1R,2S)-1,2-cyclohexanediol dinitrate $C_6H_{10}N_2O_6$ (*cis*-1,2-cyclohexanediol dinitrate) [32342-28-2]	1.3		Fischer and Ballschmiter (1998b)	M	580
(1R,2R)-1,2-cyclohexanediol dinitrate $C_6H_{10}N_2O_6$ (*trans*-1,2-cyclohexanediol dinitrate) [32342-29-3]	5.2×10^{-1}		Fischer and Ballschmiter (1998b)	M	580
(1R,3S)-1,3-cyclohexanediol dinitrate $C_6H_{10}N_2O_6$ (*cis*-1,3-cyclohexanediol dinitrate) [170994-36-2]	3.4		Fischer and Ballschmiter (1998b)	M	580
(1R,3R)-1,3-cyclohexanediol dinitrate $C_6H_{10}N_2O_6$ (*trans*-1,3-cyclohexanediol dinitrate) [170994-41-9]	6.8×10^{-1}		Fischer and Ballschmiter (1998b)	M	580
1,7-heptanediol dinitrate $C_7H_{14}N_2O_6$ [3457-94-1] KIERETFMVSIXIJ-UHFFFAOYSA-N	1.1		Fischer and Ballschmiter (1998b)	M	580
(1R,2R)-1,2-cycloheptanediol dinitrate $C_7H_{12}N_2O_6$ (*trans*-1,2-cycloheptanediol dinitrate) [208252-06-6]	8.8×10^{-1}		Fischer and Ballschmiter (1998b)	M	580

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-octanediol dinitrate $C_8H_{16}N_2O_6$ [121222-48-8] RLNKMZWMCSTIEM-UHFFFAOYSA-N	5.2×10^{-2}		Fischer and Ballschmiter (1998b)	M	580
1,8-octanediol dinitrate $C_8H_{16}N_2O_6$ [3457-95-2] BVIHOKFRPSZJEI-UHFFFAOYSA-N	7.8×10^{-1}		Fischer and Ballschmiter (1998b)	M	580
1,2-decanediol dinitrate $C_{10}H_{20}N_2O_6$ [60123-40-2] KKNGVXOJDIUADE-UHFFFAOYSA-N	2.0×10^{-2}		Fischer and Ballschmiter (1998b)	M	580
1,10-decanediol dinitrate $C_{10}H_{20}N_2O_6$ [3457-97-4] RHUZOYMELURURD-UHFFFAOYSA-N	4.3×10^{-1}		Fischer and Ballschmiter (1998b)	M	580
diethylene glycol dinitrate $C_4H_8N_2O_7$ [693-21-0] LYAGTVMJGHTIDH-UHFFFAOYSA-N	2.5×10^{1} 4.9×10^{1} 1.2×10^{2} 9.9×10^{2} 1.1×10^{2} 3.8		HSDB (2015) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Hilal et al. (2008) Modarresi et al. (2007)	V Q Q Q Q Q	 242, 243 244 245 67
ISOP1N2ONO2 $C_5H_8N_2O_6$ FQSKJUXVWIFNKX-UHFFFAOYSA-N	1.6	9400	Wieser et al. (2023)	Q	437
EPXISOPNONO2 $C_5H_8N_2O_7$ UAFKAIYDADHRMX-UHFFFAOYSA-N	5.3×10^{1}	13000	Wieser et al. (2023)	Q	437
ISOP1N23O4ONO2 $C_5H_8N_2O_7$ FSZUIXLMCRZJMS-UHFFFAOYSA-N	4.5×10^{1}	13000	Wieser et al. (2023)	Q	437
ISOP1N5ONO2 $C_5H_8N_2O_7$ WRGRJJOKHABEJT-UHFFFAOYSA-N	5.8×10^{4}	13000	Wieser et al. (2023)	Q	437
LIMAB15ONO22 $C_{10}H_{18}N_2O_8$ UNHNJOVXNACOSQ-UHFFFAOYSA-N	3.1×10^{7}	18000	Wieser et al. (2023)	Q	437

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
peroxyacetyl nitrate	2.8×10^{-2}	5700	Burkholder et al. (2019)	L	
$CH_3COOONO_2$	2.8×10^{-2}	5700	Burkholder et al. (2015)	L	
(PAN)	2.9×10^{-2}	5700	Warneck and Williams (2012)	L	
[2278-22-0]	2.8×10^{-2}	5700	Sander et al. (2011)	L	
VGQXTTSVLMQFHM-UHFFFAOYSA-N	2.8×10^{-2}	5700	Sander et al. (2006)	L	
	2.9×10^{-2}	5800	Leu and Zhang (1999)	L	
	3.0×10^{-2}	5600	Easterbrook et al. (2023)	M	
	2.3×10^{-2}	4800	Frenzel et al. (2000)	M	
	4.0×10^{-2}		Kames and Schurath (1995)	M	12
	2.8×10^{-2}	6500	Kames et al. (1991)	M	
	4.9×10^{-2}		Holdren et al. (1984)	M	373
	3.6×10^{-2}		Gaffney and Senum (1984)	X	389
	2.9×10^{-2}	5900	Pandis and Seinfeld (1989)	C	
	3.6×10^{-2}		Schwartz (1986)	C	87
	6.8×10^{-2}		Keshavarz et al. (2022)	Q	
	6.1×10^{-1}		Duchowicz et al. (2020)	Q	184
	4.9		Wang et al. (2017)	Q	80, 238
	1.0×10^{1}		Wang et al. (2017)	Q	80, 239
	7.4×10^{-4}		Wang et al. (2017)	Q	80, 240
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	4.9		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.2		Hilal et al. (2008)	Q	
	3.2		Modarresi et al. (2007)	Q	67
		4800	Kühne et al. (2005)	Q	
	3.6×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		6300	Kühne et al. (2005)	?	
			Warneck et al. (1996)	?	583
			Schurath et al. (1996)	W	584
peroxypropionyl nitrate	1.6×10^{-2}	6000	Easterbrook et al. (2023)	M	
$C_2H_5COOONO_2$	2.9×10^{-2}		Kames and Schurath (1995)	M	12
(PPN)	3.9		Wang et al. (2017)	Q	80, 238
[5796-89-4]	4.1		Wang et al. (2017)	Q	80, 239
TXINBPKSWKFMNB-UHFFFAOYSA-N	3.6×10^{-4}		Wang et al. (2017)	Q	80, 240
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
			Warneck et al. (1996)	?	583
			Schurath et al. (1996)	W	585
nitro butaneperoxoate	2.3×10^{-2}		Kames and Schurath (1995)	M	12
$C_3H_7COOONO_2$	3.2		Wang et al. (2017)	Q	80, 238
(PnBN)	2.2		Wang et al. (2017)	Q	80, 239
[27746-48-1]	2.6×10^{-4}		Wang et al. (2017)	Q	80, 240
HZUMMZVMNQSPFF-UHFFFAOYSA-N	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
			Warneck et al. (1996)	?	583
			Schurath et al. (1996)	W	586
peroxy-2-propenoyl nitrate	1.7×10^{-2}		Kames and Schurath (1995)	M	12
$CH_2C(CH_3)COOONO_2$	7.4		Wang et al. (2017)	Q	80, 238
(peroxymethacryloyl nitrate;	4.8		Wang et al. (2017)	Q	80, 239
MPAN)					
[88181-75-3]	2.4×10^{-4}		Wang et al. (2017)	Q	80, 240
LLZWPQFQEBKRLX-UHFFFAOYSA-N			Warneck et al. (1996)	W	583
			Schurath et al. (1996)	W	587
peroxy-isobutyryl nitrate	9.9×10^{-3}		Kames and Schurath (1995)	M	12
$C_3H_7COOONO_2$	3.6		Wang et al. (2017)	Q	80, 238
(PiBN)	2.3		Wang et al. (2017)	Q	80, 239
[65424-60-4]	1.8×10^{-4}		Wang et al. (2017)	Q	80, 240
BDNFHGUXBRZLRQ-UHFFFAOYSA-N	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	245
			Warneck et al. (1996)	?	583
			Schurath et al. (1996)	W	588
furoyl peroxynitrate	9.3×10^{-2}	8800	Roberts et al. (2022)	M	
$C_5H_3NO_6$	1.6×10^{-1}		Roberts et al. (2022)	Q	589
(fur-PAN)					
NMNZVYLGOWCHOD-UHFFFAOYSA-N					
MCM:CH3O2NO2	4.1×10^{-1}		Wang et al. (2017)	Q	80, 238
CH_3NO_4	1.5×10^{-1}		Wang et al. (2017)	Q	80, 239
LCFGXMPUQSXLCQ-UHFFFAOYSA-N	1.7×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:ETHO2HNO3	9.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_5NO_5$	2.8×10^{3}		Wang et al. (2017)	Q	80, 239
IYCQDYYQELIXMU-UHFFFAOYSA-N	3.1		Wang et al. (2017)	Q	80, 240
MCM:NO3CH2CO3H	1.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_2H_3NO_6$	2.3×10^{3}		Wang et al. (2017)	Q	80, 239
VLCOOHYMNNDETJ-UHFFFAOYSA-N	4.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:NO3CH2PAN	5.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_2N_2O_8$	1.9×10^{3}		Wang et al. (2017)	Q	80, 239
CSNUPQYBRZIENU-UHFFFAOYSA-N	3.0×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:ACRPAN	1.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_3H_3NO_5$	7.4		Wang et al. (2017)	Q	80, 239
[157258-66-7]	4.6×10^{-4}		Wang et al. (2017)	Q	80, 240
SFKRQQJZRXQGLC-UHFFFAOYSA-N	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	3.1		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	245

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PR1O2HNO3	8.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_3H_7NO_5$	1.0×10^{3}		Wang et al. (2017)	Q	80, 239
FROUFTMXOYPVCX-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	80, 240
MCM:PR2O2HNO3	8.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_3H_7NO_5$	1.1×10^{3}		Wang et al. (2017)	Q	80, 239
UHIVGIHVGRYUPL-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	80, 240
MCM:PRNO3CO3H	1.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_3H_5NO_6$	1.0×10^{3}		Wang et al. (2017)	Q	80, 239
FMRKJWQAPYMRJD-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	80, 240
MCM:PRNO3PAN	5.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_3H_4N_2O_8$	4.6×10^{2}		Wang et al. (2017)	Q	80, 239
ZLJYZUGEJFPONP-UHFFFAOYSA-N	1.6×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:BU1ENO3OOH	6.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_5$	5.5×10^{2}		Wang et al. (2017)	Q	80, 239
MFTWJXGCASCYHP-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	80, 240
MCM:C3DBPAN	1.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_5$	5.8		Wang et al. (2017)	Q	80, 239
YVSVRLGWMDVSPN-UHFFFAOYSA-N	1.2×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:C42NO33OOH	8.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_5$	5.1×10^{2}		Wang et al. (2017)	Q	80, 239
CGBCWMNQUOIZIB-UHFFFAOYSA-N	9.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C43NO34OOH	6.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_5$	5.5×10^{2}		Wang et al. (2017)	Q	80, 239
BQDGWSCZHPCGGT-UHFFFAOYSA-N	6.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C4PAN9	1.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_4N_2O_8$	2.3×10^{3}		Wang et al. (2017)	Q	80, 239
SHASFEZZYJNCIM-UHFFFAOYSA-N	5.4×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:MPRANO3OOH	4.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_5$	3.2×10^{2}		Wang et al. (2017)	Q	80, 239
DTPMQEMACNJTBJ-UHFFFAOYSA-N	9.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:MPRBNO3OOH	4.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_5$	3.5×10^{2}		Wang et al. (2017)	Q	80, 239
RCQWCNCMOFDCKD-UHFFFAOYSA-N	5.1		Wang et al. (2017)	Q	80, 240
MCM:MPRBNO3PAN	2.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_6N_2O_8$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
RAYRXKOIFAVDJK-UHFFFAOYSA-N	2.1×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:MPRNO3CO3H	6.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	2.2×10^{2}		Wang et al. (2017)	Q	80, 239
HDNCPEGDTKOFQI-UHFFFAOYSA-N	5.8×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NBUTDAOOH	2.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_5$	1.2×10^{3}		Wang et al. (2017)	Q	80, 239
ZIAMBHNGSMXNCM-UHFFFAOYSA-N	6.3		Wang et al. (2017)	Q	80, 240
MCM:NBUTDBNO3	4.1		Wang et al. (2017)	Q	80, 238
$C_4H_6N_2O_6$	3.6×10^{1}		Wang et al. (2017)	Q	80, 239
GCQJZAFTGYZGDG-UHFFFAOYSA-N	1.4×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:NBUTDBOOH	2.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_5$	4.0×10^{3}		Wang et al. (2017)	Q	80, 239
SSNXKZNERJCDKO-UHFFFAOYSA-N	5.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NC3CO3H	3.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_6$	5.0×10^{3}		Wang et al. (2017)	Q	80, 239
ZXNVOGOFZJSFAE-UHFFFAOYSA-N	3.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:TC4H9NO3	6.2×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_3$	9.1×10^{-3}		Wang et al. (2017)	Q	80, 239
[926-05-6]	1.0×10^{-3}		Wang et al. (2017)	Q	80, 240
AZAKMLHUDVIDFN-UHFFFAOYSA-N	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
MCM:C3ME3PAN	2.8		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	1.7		Wang et al. (2017)	Q	80, 239
OLNWAQLSTCXURT-UHFFFAOYSA-N	1.6×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:C3MNO3CO3H	9.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	3.2×10^{2}		Wang et al. (2017)	Q	80, 239
UNTXQXBLSROXLI-UHFFFAOYSA-N	2.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C3MNO3PAN	3.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_8$	1.6×10^{2}		Wang et al. (2017)	Q	80, 239
ULZBZSVLLIBTGC-UHFFFAOYSA-N	1.0×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:C43NO3CO3H	5.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	1.3×10^{2}		Wang et al. (2017)	Q	80, 239
KYFRJEXZVMOAMN-UHFFFAOYSA-N	1.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C43NO3PAN	2.2×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_8$	6.6×10^{1}		Wang et al. (2017)	Q	80, 239
WPFKHDFVFPXDFZ-UHFFFAOYSA-N	1.3×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:C4M2NO3OOH	4.5×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_5$	1.6×10^{2}		Wang et al. (2017)	Q	80, 239
BOAAVKBCMOPNIQ-UHFFFAOYSA-N	5.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C4MNO31OOH	6.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_5$	3.2×10^{2}		Wang et al. (2017)	Q	80, 239
LRRBWUKXCGVENZ-UHFFFAOYSA-N	7.3×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C4MNO32OOH	6.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_5$	3.2×10^{2}		Wang et al. (2017)	Q	80, 239
HXNZNKRZULBVRO-UHFFFAOYSA-N	4.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C4NO32MOOH	3.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_5$	1.7×10^{2}		Wang et al. (2017)	Q	80, 239
HCKTYRRBEFAEAC-UHFFFAOYSA-N	5.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C4NO3CO3H	8.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	3.0×10^{2}		Wang et al. (2017)	Q	80, 239
JPUVYTOGMBAUBQ-UHFFFAOYSA-N	1.7×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C4NO3M1OOH	3.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_5$	1.8×10^{2}		Wang et al. (2017)	Q	80, 239
MWSZSODDMCBKIX-UHFFFAOYSA-N	3.4		Wang et al. (2017)	Q	80, 240
MCM:C4NO3M2OOH	4.5×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_5$	1.5×10^{2}		Wang et al. (2017)	Q	80, 239
QXHHHGYKLMZJBA-UHFFFAOYSA-N	4.2		Wang et al. (2017)	Q	80, 240
MCM:C4NO3PAN	3.2×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_8$	1.6×10^{2}		Wang et al. (2017)	Q	80, 239
GGZFCBHNGNBLNW-UHFFFAOYSA-N	1.2×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:C51NO32OOH	6.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_5$	3.2×10^{2}		Wang et al. (2017)	Q	80, 239
YPLQKABNDDXYJG-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:C52NO31OOH	6.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_5$	3.2×10^{2}		Wang et al. (2017)	Q	80, 239
DCAGTGOPLFTTTQ-UHFFFAOYSA-N	4.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C52NO33OOH	6.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_5$	2.4×10^{2}		Wang et al. (2017)	Q	80, 239
FQGADFCNSPWVJM-UHFFFAOYSA-N	4.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C53NO32OOH	6.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_5$	2.6×10^{2}		Wang et al. (2017)	Q	80, 239
STNFTACLRXEYDM-UHFFFAOYSA-N	2.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C5PAN18	1.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_6N_2O_8$	2.2×10^{3}		Wang et al. (2017)	Q	80, 239
JYUXMKSXMIBDSN-UHFFFAOYSA-N	2.0×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:C5PAN4	2.8		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	1.5		Wang et al. (2017)	Q	80, 239
LGNOWHJLTKBAFC-UHFFFAOYSA-N	1.3×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:C5PAN6	2.0		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	1.4		Wang et al. (2017)	Q	80, 239
VQRIYOXAZWZCOV-UHFFFAOYSA-N	1.6×10^{-4}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:IPEANO3	8.3×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_3$	1.5×10^{-2}		Wang et al. (2017)	Q	80, 239
QSSWLPYLLKHHLB-UHFFFAOYSA-N	4.0×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:IPEBNO3	8.3×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_3$	1.4×10^{-2}		Wang et al. (2017)	Q	80, 239
OTVLXFGCWJFXJU-UHFFFAOYSA-N	4.2×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:IPECNO3	5.1×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_3$	6.6×10^{-3}		Wang et al. (2017)	Q	80, 239
UENFRVTUGZKXNH-UHFFFAOYSA-N	7.6×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:NC4CO3H	2.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_6$	4.6×10^{3}		Wang et al. (2017)	Q	80, 239
SLKHOLOIOGBFQB-UHFFFAOYSA-N	1.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:NEOPNO3	5.1×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_3$	1.2×10^{-2}		Wang et al. (2017)	Q	80, 239
YJGBGWFCCCQXIM-UHFFFAOYSA-N	4.1×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:NISOPNO3	2.6	9400	Wieser et al. (2023)	Q	437
$C_5H_8N_2O_6$	2.7		Wang et al. (2017)	Q	80, 238
JGJBVRGABXKDRR-UHFFFAOYSA-N	3.0×10^{1}		Wang et al. (2017)	Q	80, 239
	1.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:NISOPOOH	9.7×10^{2}	11000	Wieser et al. (2023)	Q	437
$C_5H_9NO_5$	1.8×10^{3}		Wang et al. (2017)	Q	80, 238
IRFXVIPRKCCSLU-UHFFFAOYSA-N	3.0×10^{3}		Wang et al. (2017)	Q	80, 239
	3.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PPEN	2.8		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	1.5		Wang et al. (2017)	Q	80, 239
UUYNBJNAIGBJAO-UHFFFAOYSA-N	2.2×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:C42MNO3OOH	2.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_5$	4.5×10^{1}		Wang et al. (2017)	Q	80, 239
KKTQLMUUOWWZBO-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	80, 240
MCM:C62NO33OOH	5.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_5$	1.5×10^{2}		Wang et al. (2017)	Q	80, 239
PJRWVMFJYMZPCW-UHFFFAOYSA-N	4.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C63NO32OOH	5.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_5$	1.9×10^{2}		Wang et al. (2017)	Q	80, 239
RLIDOIUHNSZVBK-UHFFFAOYSA-N	1.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C65NO36OOH	4.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_5$	2.2×10^{2}		Wang et al. (2017)	Q	80, 239
ZVRSMGCQHDCSBC-UHFFFAOYSA-N	2.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C65NO3CO3H	6.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	2.2×10^{2}		Wang et al. (2017)	Q	80, 239
RASQUKWKKRVIQJ-UHFFFAOYSA-N	1.4×10^{-2}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C65NO3PAN	3.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{10}N_2O_8$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
PNNYZMYYAAWSJH-UHFFFAOYSA-N	6.5×10^{-5}		Wang et al. (2017)	Q	80, 240
MCM:C66NO35OOH	4.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_5$	2.3×10^{2}		Wang et al. (2017)	Q	80, 239
YPVNGNKLOFDKIF-UHFFFAOYSA-N	9.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN10	2.6		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	1.3		Wang et al. (2017)	Q	80, 239
INNSDEOCGQAUTR-UHFFFAOYSA-N	1.8×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN15	1.6		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	9.8×10^{-1}		Wang et al. (2017)	Q	80, 239
GWYKJYISUPTXQD-UHFFFAOYSA-N	1.4×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN17	1.6		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	1.1		Wang et al. (2017)	Q	80, 239
CUMLTNLXWSMQLS-UHFFFAOYSA-N	1.7×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN18	3.0		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	1.4		Wang et al. (2017)	Q	80, 239
FPWBUKNMBKRQCI-UHFFFAOYSA-N	1.4×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN3	2.6		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	1.1		Wang et al. (2017)	Q	80, 239
BRVOFEXYGAZHOW-UHFFFAOYSA-N	1.5×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:CHEXNO3	2.0×10^{-2}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_3$	6.5×10^{-2}		Wang et al. (2017)	Q	80, 239
HLYOOCIMLHNMOG-UHFFFAOYSA-N	3.7×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:HEXBNO3	3.1×10^{-4}	6300	Wieser et al. (2023)	Q	437
$C_6H_{13}NO_3$	6.5×10^{-3}		Wang et al. (2017)	Q	80, 238
JLGBOJJVQLNMGV-UHFFFAOYSA-N	7.4×10^{-3}		Wang et al. (2017)	Q	80, 239
	4.3×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:HEXCNO3	6.5×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_3$	8.1×10^{-3}		Wang et al. (2017)	Q	80, 239
OJOZCOXRANAOPV-UHFFFAOYSA-N	3.2×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:M22C43NO3	4.8×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_3$	9.3×10^{-3}		Wang et al. (2017)	Q	80, 239
YUZOHIKIQPTSGJ-UHFFFAOYSA-N	3.7×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:M22C4NO3	4.6×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_3$	1.0×10^{-2}		Wang et al. (2017)	Q	80, 239
JOWPFKXUGRKJFA-UHFFFAOYSA-N	5.5×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:M23C43NO3	4.8×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_3$	7.4×10^{-3}		Wang et al. (2017)	Q	80, 239
PMABLOPIFVACLQ-UHFFFAOYSA-N	7.4×10^{-4}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:M23C4NO3	7.8×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_3$	1.5×10^{-2}		Wang et al. (2017)	Q	80, 239
HHRFTVZVEUIWEO-UHFFFAOYSA-N	4.4×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:M2PEANO3	6.5×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_3$	1.1×10^{-2}		Wang et al. (2017)	Q	80, 239
CETUNBADQVCCRS-UHFFFAOYSA-N	3.4×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:M2PEBNO3	7.8×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_3$	7.8×10^{-3}		Wang et al. (2017)	Q	80, 239
AYWPQHSAUPNICG-UHFFFAOYSA-N	3.6×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:M2PECNO3	7.8×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_3$	9.6×10^{-3}		Wang et al. (2017)	Q	80, 239
ZLERWGPAWILHHJ-UHFFFAOYSA-N	3.2×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:M2PEDNO3	4.6×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_3$	5.1×10^{-3}		Wang et al. (2017)	Q	80, 239
LFIPHSRTIDHJFT-UHFFFAOYSA-N	6.5×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:M33C4NO3	4.6×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_3$	9.8×10^{-3}		Wang et al. (2017)	Q	80, 239
DENSRMRCUIZNMK-UHFFFAOYSA-N	3.6×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:M3PEANO3	6.5×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_3$	1.3×10^{-2}		Wang et al. (2017)	Q	80, 239
HRVRJIMBNILCGN-UHFFFAOYSA-N	4.7×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:M3PEBNO3	7.8×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_3$	1.1×10^{-2}		Wang et al. (2017)	Q	80, 239
IEHIEWLLOPOHIZ-UHFFFAOYSA-N	4.1×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:M3PECNO3	4.6×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_3$	5.3×10^{-3}		Wang et al. (2017)	Q	80, 239
GFKONLNVJRACGN-UHFFFAOYSA-N	6.2×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:PHXN	2.2		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	1.1		Wang et al. (2017)	Q	80, 239
ITHMZXMFOKWUTQ-UHFFFAOYSA-N	1.8×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:HEPTNO3	5.4×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_7H_{15}NO_3$	6.3×10^{-3}		Wang et al. (2017)	Q	80, 239
RFSNRWONUSBTJN-UHFFFAOYSA-N	3.0×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:M2HEXANO3	6.2×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_7H_{15}NO_3$	5.9×10^{-3}		Wang et al. (2017)	Q	80, 239
YZGBSAOHUZMZSL-UHFFFAOYSA-N	4.0×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:M2HEXBNO3	3.7×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_7H_{15}NO_3$	3.9×10^{-3}		Wang et al. (2017)	Q	80, 239
CORAYZMLWQTCOE-UHFFFAOYSA-N	5.8×10^{-4}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:M3HEXANO3	6.2×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_7H_{15}NO_3$	6.6×10^{-3}		Wang et al. (2017)	Q	80, 239
ZIINVFVZOGZDQJ-UHFFFAOYSA-N	3.4×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:M3HEXBNO3	3.7×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_7H_{15}NO_3$	4.4×10^{-3}		Wang et al. (2017)	Q	80, 239
ADYNXMRWYWNUDX-UHFFFAOYSA-N	6.5×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:PHPTN	1.8		Wang et al. (2017)	Q	80, 238
$C_7H_{13}NO_5$	8.9×10^{-1}		Wang et al. (2017)	Q	80, 239
XCJVDRQLXVBBEC-UHFFFAOYSA-N	2.0×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:C8BCNO3	4.0×10^{-2}		Wang et al. (2017)	Q	80, 238
$C_8H_{13}NO_3$	3.2×10^{-2}		Wang et al. (2017)	Q	80, 239
OSNOKXIMBITXOJ-UHFFFAOYSA-N	3.6×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:OCTNO3	4.8×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_8H_{17}NO_3$	5.0×10^{-3}		Wang et al. (2017)	Q	80, 239
KDICWCURMCOQTP-UHFFFAOYSA-N	2.6×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:NONNO3	3.9×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_9H_{19}NO_3$	3.8×10^{-3}		Wang et al. (2017)	Q	80, 239
YXUXBXICIGKFLH-UHFFFAOYSA-N	2.5×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:DECNO3	3.0×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{21}NO_3$	3.0×10^{-3}		Wang et al. (2017)	Q	80, 239
VRGDYCVXNCXQKR-UHFFFAOYSA-N	2.8×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:NAPINAOOH	1.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_5$	2.3×10^{2}		Wang et al. (2017)	Q	80, 239
IKGBGFRUISEOBM-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NAPINBOOH	1.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_5$	2.5×10^{2}		Wang et al. (2017)	Q	80, 239
RUHGEBIMHPPSGQ-UHFFFAOYSA-N	6.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NBPINAOOH	1.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_5$	4.4×10^{2}		Wang et al. (2017)	Q	80, 239
VJCKFKSOBAWLFB-UHFFFAOYSA-N	3.5		Wang et al. (2017)	Q	80, 240
MCM:NBPINBOOH	1.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_5$	3.8×10^{2}		Wang et al. (2017)	Q	80, 239
AWECGRRBHMAEGP-UHFFFAOYSA-N	7.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NC91CO3H	1.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_6$	4.8×10^{2}		Wang et al. (2017)	Q	80, 239
TWWSFGIBZQJYPL-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	80, 240
MCM:NC91PAN	8.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{14}N_2O_8$	2.6×10^{2}		Wang et al. (2017)	Q	80, 239
LCMKIEFNSOTVJY-UHFFFAOYSA-N	9.8×10^{-4}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NLIMOOH	1.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_5$	6.9×10^{2}		Wang et al. (2017)	Q	80, 239
HSXYRSLOXSIYGP-UHFFFAOYSA-N	5.3		Wang et al. (2017)	Q	80, 240
MCM:UDECNO3	2.8×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{23}NO_3$	2.4×10^{-3}		Wang et al. (2017)	Q	80, 239
KGEKWWIIMVPQKA-UHFFFAOYSA-N	2.0×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:DDECNO3	2.2×10^{-3}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{25}NO_3$	1.9×10^{-3}		Wang et al. (2017)	Q	80, 239
BVAQOKLOUKLOJD-UHFFFAOYSA-N	1.9×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:NBCOOH	1.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{25}NO_5$	8.7×10^{2}		Wang et al. (2017)	Q	80, 239
BEFFZATUSVKAHP-UHFFFAOYSA-N	3.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C6H5CH2NO3	4.3×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_7H_7NO_3$	7.1×10^{-1}		Wang et al. (2017)	Q	80, 239
WOIVNLSVAKYSKX-UHFFFAOYSA-N	3.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:PBZN	1.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_7H_5NO_5$	2.6×10^{1}		Wang et al. (2017)	Q	80, 239
ONDCXZPWEKXYJE-UHFFFAOYSA-N	4.4×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:C6H5C2NO3	3.6×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_3$	5.6×10^{-1}		Wang et al. (2017)	Q	80, 239
REJUUAZLLYKBCW-UHFFFAOYSA-N	4.2×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C6H5CH2PAN	1.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_7NO_5$	4.7×10^{1}		Wang et al. (2017)	Q	80, 239
KKRIGRPRRNIVGL-UHFFFAOYSA-N	1.2×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:MXYLNO3	2.5×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_3$	6.5×10^{-1}		Wang et al. (2017)	Q	80, 239
OIEIRDPNAPXLBC-UHFFFAOYSA-N	3.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:MXYLPAN	8.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_8H_7NO_5$	2.3×10^{1}		Wang et al. (2017)	Q	80, 239
HJGURQOGPAEQPE-UHFFFAOYSA-N	4.1×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:NSTYRENOOH	3.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_5$	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
LKBHTMHNYICJQS-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:OXYLNO3	2.5×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_3$	7.1×10^{-1}		Wang et al. (2017)	Q	80, 239
WKRHODAGVPDBTG-UHFFFAOYSA-N	2.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:OXYLPAN	8.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_8H_7NO_5$	3.1×10^{1}		Wang et al. (2017)	Q	80, 239
TXXXSKKGTSQWKQ-UHFFFAOYSA-N	3.2×10^{-3}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:PXYLNO3	2.5×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_3$	7.8×10^{-1}		Wang et al. (2017)	Q	80, 239
SHZSDLPSACZYMH-UHFFFAOYSA-N	3.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:PXYLPAN	8.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_8H_7NO_5$	2.6×10^{1}		Wang et al. (2017)	Q	80, 239
ZGFUWGCXWYZODV-UHFFFAOYSA-N	6.5×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:ETOLNO3	2.3×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_3$	3.2×10^{-1}		Wang et al. (2017)	Q	80, 239
LYNFROWVHACAMO-UHFFFAOYSA-N	1.9×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:PHC3NO3	3.3×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_3$	2.2×10^{-1}		Wang et al. (2017)	Q	80, 239
IFDAHDBLKMQHMM-UHFFFAOYSA-N	1.8×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:PHIC3NO3	2.2×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_3$	1.5×10^{-1}		Wang et al. (2017)	Q	80, 239
YCCLKZYFPBVILU-UHFFFAOYSA-N	3.8×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:TM123BNO3	1.6×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_3$	9.8×10^{-1}		Wang et al. (2017)	Q	80, 239
GDXSVUXDQKEMHM-UHFFFAOYSA-N	3.0×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:TM123BPAN	5.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_9NO_5$	3.9×10^{1}		Wang et al. (2017)	Q	80, 239
VMALQUVLPIFIEM-UHFFFAOYSA-N	4.5×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:TM124BNO3	1.6×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_3$	9.3×10^{-1}		Wang et al. (2017)	Q	80, 239
VLXWVVSZKXVGNM-UHFFFAOYSA-N	3.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:TM124BPAN	5.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_9NO_5$	3.0×10^{1}		Wang et al. (2017)	Q	80, 239
SSMPYZHCWJGIJH-UHFFFAOYSA-N	7.4×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:TMBNO3	1.6×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_3$	5.5×10^{-1}		Wang et al. (2017)	Q	80, 239
CHDZRXQPKVNDRJ-UHFFFAOYSA-N	2.8×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:TMBPAN	5.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_9NO_5$	1.9×10^{1}		Wang et al. (2017)	Q	80, 239
QURBGWBLEPWFEF-UHFFFAOYSA-N	4.0×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:DM35EBNO3	1.4×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{13}NO_3$	2.4×10^{-1}		Wang et al. (2017)	Q	80, 239
CZPIEIXHJQQIGZ-UHFFFAOYSA-N	1.7×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:EMPHPAN	4.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{11}NO_5$	1.1×10^{1}		Wang et al. (2017)	Q	80, 239
DPRDWMVUHNTRQI-UHFFFAOYSA-N	3.2×10^{-3}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DE35TNO3	1.1×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{15}NO_3$	1.5×10^{-1}		Wang et al. (2017)	Q	80, 239
XLLLSPDIGUQFTC-UHFFFAOYSA-N	1.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:PHAN	6.2×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_3NO_6$	9.6×10^{3}		Wang et al. (2017)	Q	80, 239
KMDWHTZYVJXWAH-UHFFFAOYSA-N	6.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:A2PAN	7.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_3H_5NO_7$	2.3×10^{6}		Wang et al. (2017)	Q	80, 239
RQFAVCUBLOXLKI-UHFFFAOYSA-N	2.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C3PAN1	1.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_3H_5NO_6$	3.2×10^{4}		Wang et al. (2017)	Q	80, 239
ZDHDBTZUUXEIQG-UHFFFAOYSA-N	6.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:HO1C3NO3	2.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_3H_7NO_4$	1.2×10^{3}		Wang et al. (2017)	Q	80, 239
[100502-66-7]	6.3		Wang et al. (2017)	Q	80, 240
PTMLFFXFTRSBJW-UHFFFAOYSA-N	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	271, 243
	3.9×10^{2}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{2}		Raventos-Duran et al. (2010)	Q	245
MCM:IPROPOLPAN	5.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_3H_5NO_6$	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
VGQGEUUGHUVAJJ-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:BUTDANO3	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_4$	2.3×10^{3}		Wang et al. (2017)	Q	80, 239
JVISETCEJQRRQM-UHFFFAOYSA-N	3.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:BUTDBNO3	9.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_4$	2.5×10^{2}		Wang et al. (2017)	Q	80, 239
MVWTUBMDIKBQOB-UHFFFAOYSA-N	3.0		Wang et al. (2017)	Q	80, 240
MCM:C4PAN1	8.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	5.5×10^{4}		Wang et al. (2017)	Q	80, 239
ZAYFYZJEFHQRME-UHFFFAOYSA-N	2.1		Wang et al. (2017)	Q	80, 240
MCM:C4PAN2	1.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_7$	1.7×10^{7}		Wang et al. (2017)	Q	80, 239
KFPIYXZEKUAVMP-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C4PAN3	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	3.6×10^{4}		Wang et al. (2017)	Q	80, 239
PIBQEVCOTXTKAE-UHFFFAOYSA-N	4.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C4PAN4	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	2.0×10^{4}		Wang et al. (2017)	Q	80, 239
NXHSYZWHYBOEBH-UHFFFAOYSA-N	4.0×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C4PAN5	3.2×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	4.1×10^{3}		Wang et al. (2017)	Q	80, 239
BZGCEXLIVXRKKX-UHFFFAOYSA-N	5.5×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C4PAN7	3.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_6$	1.2×10^{5}		Wang et al. (2017)	Q	80, 239
YKQOPDHVAHDODD-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C4PAN8	1.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_6$	7.1×10^{3}		Wang et al. (2017)	Q	80, 239
QZCDOTFCQHJUGH-UHFFFAOYSA-N	6.5×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C56NO3	8.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_5$	9.1×10^{5}		Wang et al. (2017)	Q	80, 239
XYUWBXDQANMXIL-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:HMPAN	2.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_6$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
XPXMBKPWAOWOBP-UHFFFAOYSA-N	6.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:HO13C4NO3	8.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_5$	1.0×10^{6}		Wang et al. (2017)	Q	80, 239
IOYLZWMTXYBAPI-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO3C3PAN	5.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	6.2×10^{3}		Wang et al. (2017)	Q	80, 239
JGMDPJZYJFPSOE-UHFFFAOYSA-N	9.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:IBUTOLBNO3	2.2×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_4$	1.0×10^{2}		Wang et al. (2017)	Q	80, 239
ILMPSGIQBJFTRG-UHFFFAOYSA-N	6.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:IBUTOLCNO3	2.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_4$	6.9×10^{2}		Wang et al. (2017)	Q	80, 239
OARBGYKXUANYLR-UHFFFAOYSA-N	3.5		Wang et al. (2017)	Q	80, 240
MCM:MACRNBPAN	5.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_6N_2O_9$	7.6×10^{5}		Wang et al. (2017)	Q	80, 239
HHPQSZXZUAZGAQ-UHFFFAOYSA-N	1.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:MACRNCO3H	2.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_7$	2.3×10^{6}		Wang et al. (2017)	Q	80, 239
VCAMMMQHKHRNFT-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MACRNPAN	9.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_6N_2O_9$	2.8×10^{5}		Wang et al. (2017)	Q	80, 239
YVNHVFURNFQJQM-UHFFFAOYSA-N	1.2×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:NBUTDAOH	9.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_4$	2.9×10^{2}		Wang et al. (2017)	Q	80, 239
ZANUSWCYRLKDAN-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:TBUTOLNO3	2.2×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_4$	1.4×10^{2}		Wang et al. (2017)	Q	80, 239
SPXXYWSDFUWLEP-UHFFFAOYSA-N	9.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C3M3OH2PAN	4.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	4.9×10^{3}		Wang et al. (2017)	Q	80, 239
NSGPYXAFGPXNMV-UHFFFAOYSA-N	2.8×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C46PAN	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_6$	7.4×10^{4}		Wang et al. (2017)	Q	80, 239
WDMYRNZGJSFESH-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	80, 240
MCM:C4OH2CPAN	3.7×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_7$	3.5×10^{6}		Wang et al. (2017)	Q	80, 239
INCMEOVDRBCULR-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:C4OHPAN	4.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	3.7×10^{3}		Wang et al. (2017)	Q	80, 239
GAAOIPAQIRGTBI-UHFFFAOYSA-N	5.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C524NO3	1.7×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	2.6×10^{6}		Wang et al. (2017)	Q	80, 239
IRMGDWDXIVCKPE-UHFFFAOYSA-N	2.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C52NO3	2.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	5.0×10^{2}		Wang et al. (2017)	Q	80, 239
NBCYUKLMSBOGIC-UHFFFAOYSA-N	6.5		Wang et al. (2017)	Q	80, 240
MCM:C54NO3	4.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_5$	3.8×10^{5}		Wang et al. (2017)	Q	80, 239
OXSZOTYJVSIXIT-UHFFFAOYSA-N	9.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C57NO3CO3H	2.4×10^{10}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_8$	1.4×10^{9}		Wang et al. (2017)	Q	80, 239
BPRAPKBGVRGZEK-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C57NO3PAN	9.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_{10}$	2.7×10^{8}		Wang et al. (2017)	Q	80, 239
QHZGCLHPLOENFL-UHFFFAOYSA-N	2.5×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C58NO3CO3H	3.5×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_8$	5.8×10^{7}		Wang et al. (2017)	Q	80, 239
NFQMHUFQLLKQQS-UHFFFAOYSA-N	5.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C58NO3PAN	1.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_{10}$	4.2×10^{8}		Wang et al. (2017)	Q	80, 239
VIMTZSSJOGPGII-UHFFFAOYSA-N	8.5×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C5PAN10	1.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_7$	2.5×10^{7}		Wang et al. (2017)	Q	80, 239
YRCMXGZRWLAVBH-UHFFFAOYSA-N	9.6×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C5PAN11	5.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	2.4×10^{4}		Wang et al. (2017)	Q	80, 239
ISSHIIFFUOEHLT-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C5PAN12	7.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_7$	1.0×10^{7}		Wang et al. (2017)	Q	80, 239
VRGURBHINCFLEI-UHFFFAOYSA-N	9.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C5PAN13	1.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_7$	2.0×10^{7}		Wang et al. (2017)	Q	80, 239
GDYHQRWKNLRCBR-UHFFFAOYSA-N	5.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C5PAN14	9.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	2.2×10^{4}		Wang et al. (2017)	Q	80, 239
KAYGTWBSLGDXRV-UHFFFAOYSA-N	5.8×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C5PAN15	5.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	9.3×10^{3}		Wang et al. (2017)	Q	80, 239
DDVUSZKFLFMJLG-UHFFFAOYSA-N	5.0×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C5PAN17	2.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_6$	1.3×10^{5}		Wang et al. (2017)	Q	80, 239
WOHMTHRFBCBPEN-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C5PAN19	2.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_6$	1.0×10^{5}		Wang et al. (2017)	Q	80, 239
SXXBKHKGTQGHOF-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C5PAN1	8.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	4.0×10^{4}		Wang et al. (2017)	Q	80, 239
BXAPPDLQCWAVAO-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	80, 240
MCM:C5PAN3	8.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	3.3×10^{4}		Wang et al. (2017)	Q	80, 239
GANOVMQBFKDCJS-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	80, 240
MCM:C5PAN5	8.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	3.0×10^{4}		Wang et al. (2017)	Q	80, 239
SNADUXVVPGYKTN-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	80, 240
MCM:C5PAN8	8.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	1.9×10^{4}		Wang et al. (2017)	Q	80, 239
AVADEHRLOLZNNT-UHFFFAOYSA-N	7.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:H2M3C4NO3	2.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	5.0×10^{2}		Wang et al. (2017)	Q	80, 239
KRCHLCXLZXFPMO-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	80, 240
MCM:HM22C3NO3	1.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	3.2×10^{2}		Wang et al. (2017)	Q	80, 239
GJZIQWDDCYOUOR-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HM2C43NO3	2.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	4.1×10^{2}		Wang et al. (2017)	Q	80, 239
OLLXHFMQLUGEEM-UHFFFAOYSA-N	2.5		Wang et al. (2017)	Q	80, 240
MCM:HM33C3NO3	1.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	2.0×10^{2}		Wang et al. (2017)	Q	80, 239
LCUGTHWCLWAZIN-UHFFFAOYSA-N	5.3		Wang et al. (2017)	Q	80, 240
MCM:HO13C5NO3	8.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_5$	5.4×10^{5}		Wang et al. (2017)	Q	80, 239
HRXGEJHIRPMYKD-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO24C5NO3	8.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_5$	5.8×10^{5}		Wang et al. (2017)	Q	80, 239
GDKLMXJUXHUPHP-UHFFFAOYSA-N	1.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO2C54NO3	2.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	2.8×10^{2}		Wang et al. (2017)	Q	80, 239
BDOVYOMPHMUDCA-UHFFFAOYSA-N	1.8		Wang et al. (2017)	Q	80, 240
MCM:HO2M2C4NO3	1.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	3.6×10^{2}		Wang et al. (2017)	Q	80, 239
JLEBTGVTEJACMC-UHFFFAOYSA-N	1.6		Wang et al. (2017)	Q	80, 240
MCM:HO3C5NO3	2.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	3.8×10^{2}		Wang et al. (2017)	Q	80, 239
VSJMKXXNGJNYTF-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	80, 240
MCM:INAHCO3H	1.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_8$	4.9×10^{7}		Wang et al. (2017)	Q	80, 239
NANYPKIUOGNJFQ-UHFFFAOYSA-N	5.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:INAHPAN	5.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_{10}$	6.8×10^{8}		Wang et al. (2017)	Q	80, 239
ISRNXRSYOJKFEQ-UHFFFAOYSA-N	5.0		Wang et al. (2017)	Q	80, 240
MCM:INAHPCO3H	1.8×10^{12}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_9$	2.5×10^{9}		Wang et al. (2017)	Q	80, 239
ZYWYMWCOZFANRV-UHFFFAOYSA-N	3.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:INAHPPAN	8.0×10^{10}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_{11}$	1.1×10^{9}		Wang et al. (2017)	Q	80, 239
ZXVKOORKVQYPPA-UHFFFAOYSA-N	3.4		Wang et al. (2017)	Q	80, 240
MCM:INANCO3H	2.7×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_{10}$	2.6×10^{8}		Wang et al. (2017)	Q	80, 239
HKZKRKUNOXITIG-UHFFFAOYSA-N	3.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:INANO3	7.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}N_2O_8$	2.6×10^{7}		Wang et al. (2017)	Q	80, 239
VVVQXVVEBQASSQ-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:INANPAN	1.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_7N_3O_{12}$	3.7×10^{7}		Wang et al. (2017)	Q	80, 239
PTXQCTHWIXKTGJ-UHFFFAOYSA-N	4.7×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:INAOH	4.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_6$	2.9×10^{8}		Wang et al. (2017)	Q	80, 239
KOIOFJRFFFLZDV-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:INAOOH	5.3×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_7$	4.7×10^{8}		Wang et al. (2017)	Q	80, 239
JIJPRURLLPNXAY-UHFFFAOYSA-N	2.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:INB1HPCO3H	1.5×10^{12}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_9$	1.3×10^{9}		Wang et al. (2017)	Q	80, 239
UQVCIXBCKWUTPD-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:INB1HPPAN	6.9×10^{10}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_{11}$	5.3×10^{8}		Wang et al. (2017)	Q	80, 239
MXDOILKWVFGWCS-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:INB1NACO3H	2.6×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_{10}$	2.5×10^{8}		Wang et al. (2017)	Q	80, 239
IWCHPIGOQCZQCT-UHFFFAOYSA-N	8.3		Wang et al. (2017)	Q	80, 240
MCM:INB1NAPAN	1.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_7N_3O_{12}$	7.1×10^{7}		Wang et al. (2017)	Q	80, 239
NYNQOGZUUKXJDZ-UHFFFAOYSA-N	2.8×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:INB1NBCO3H	2.6×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_{10}$	2.0×10^{8}		Wang et al. (2017)	Q	80, 239
KPBUCMMBNBINOH-UHFFFAOYSA-N	3.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:INB1NBPAN	1.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_7N_3O_{12}$	5.8×10^{7}		Wang et al. (2017)	Q	80, 239
JLOMTJWSNAHKLK-UHFFFAOYSA-N	4.5×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:INB1NO3	7.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}N_2O_8$	1.4×10^{7}		Wang et al. (2017)	Q	80, 239
JJLGQNDDHJZYHP-UHFFFAOYSA-N	8.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:INB1OH	6.9×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_6$	1.7×10^{8}		Wang et al. (2017)	Q	80, 239
CMMIHJKAMSCCNX-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:INB1OOH	5.3×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_7$	1.1×10^{8}		Wang et al. (2017)	Q	80, 239
QLIFJAFKYUVUMD-UHFFFAOYSA-N	1.9×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:INB2OOH	5.3×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_7$	5.6×10^{8}		Wang et al. (2017)	Q	80, 239
KNHLEPZPJYMJKZ-UHFFFAOYSA-N	4.7×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:INCNCO3H	2.7×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_{10}$	3.0×10^{8}		Wang et al. (2017)	Q	80, 239
OBBLXUYPBVASEH-UHFFFAOYSA-N	8.0		Wang et al. (2017)	Q	80, 240
MCM:INCNO3	7.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}N_2O_8$	2.7×10^{7}		Wang et al. (2017)	Q	80, 239
YANCNBBJBURWKL-UHFFFAOYSA-N	2.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:INCNPAN	1.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_7N_3O_{12}$	5.4×10^{7}		Wang et al. (2017)	Q	80, 239
MINPDRSMAYIHHB-UHFFFAOYSA-N	2.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:INCOH	4.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_6$	2.8×10^{8}		Wang et al. (2017)	Q	80, 239
CLYWBEAWDTVRBE-UHFFFAOYSA-N	4.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:INCOOH	5.3×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_7$	6.9×10^{8}		Wang et al. (2017)	Q	80, 239
LZOWWVNBCGLMRZ-UHFFFAOYSA-N	2.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:INDHCO3H	3.5×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_8$	5.3×10^{7}		Wang et al. (2017)	Q	80, 239
QUYOEJZVAFIYRP-UHFFFAOYSA-N	5.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:INDHPAN	1.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_{10}$	6.3×10^{8}		Wang et al. (2017)	Q	80, 239
WUJYJPIJVADQSX-UHFFFAOYSA-N	3.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:INDHPCO3H	1.5×10^{12}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_9$	8.9×10^{8}		Wang et al. (2017)	Q	80, 239
XHWXDLVQLOECHL-UHFFFAOYSA-N	6.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:INDHPPAN	6.9×10^{10}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_{11}$	4.4×10^{8}		Wang et al. (2017)	Q	80, 239
MNXVJBKQIAYCJC-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	80, 240
MCM:INDOH	6.9×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_6$	1.7×10^{8}		Wang et al. (2017)	Q	80, 239
HMAKIHHEIIANEM-UHFFFAOYSA-N	3.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:INDOOH	5.3×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_7$	1.1×10^{8}		Wang et al. (2017)	Q	80, 239
MAYHMSJZSHQSOH-UHFFFAOYSA-N	7.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:ISOPANO3	6.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	1.9×10^{3}		Wang et al. (2017)	Q	80, 239
ISDFXKLTMWDHJL-UHFFFAOYSA-N	1.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ISOPBNO3	5.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
CIXVZPWFWFMUOH-UHFFFAOYSA-N	3.6×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:ISOPCNO3	6.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	1.9×10^{3}		Wang et al. (2017)	Q	80, 239
IDJHVSOIJITEQU-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ISOPDNO3	5.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	1.8×10^{2}		Wang et al. (2017)	Q	80, 239
PYTOMGVARIWPAT-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:M2BU2OLNO3	2.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	9.1×10^{1}		Wang et al. (2017)	Q	80, 239
AGMVBVSNQJHQAX-UHFFFAOYSA-N	5.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:M2BUOL2NO3	1.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	7.4×10^{1}		Wang et al. (2017)	Q	80, 239
RQINUHXDGZGUIX-UHFFFAOYSA-N	5.9×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:M3BU2OLNO3	3.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	1.4×10^{2}		Wang et al. (2017)	Q	80, 239
HJMHUJWXCZNPJL-UHFFFAOYSA-N	3.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:MBOANO3	6.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_5$	1.6×10^{5}		Wang et al. (2017)	Q	80, 239
SMFXIBRHTKUPLI-UHFFFAOYSA-N	5.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MBOBNO3	2.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_5$	1.6×10^{5}		Wang et al. (2017)	Q	80, 239
DYXSFFPMZZUQFC-UHFFFAOYSA-N	4.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:ME2BUOLNO3	2.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	8.1×10^{1}		Wang et al. (2017)	Q	80, 239
SBGDAJKUHMJEMT-UHFFFAOYSA-N	4.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:ME3BUOLNO3	3.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	1.4×10^{2}		Wang et al. (2017)	Q	80, 239
YWTWLHUMBHVVJS-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	80, 240
MCM:NC4OHCO3H	2.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_7$	1.6×10^{6}		Wang et al. (2017)	Q	80, 239
PAYOKBFCVVFNAB-UHFFFAOYSA-N	4.1		Wang et al. (2017)	Q	80, 240
MCM:NC4OHCPAN	9.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_9$	4.2×10^{5}		Wang et al. (2017)	Q	80, 239
JNBJPCXCCYUJJV-UHFFFAOYSA-N	2.8×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:NC524NO3	2.7×10^{10}		Wang et al. (2017)	Q	80, 238
$C_5H_{10}N_2O_9$	1.6×10^{10}		Wang et al. (2017)	Q	80, 239
NSZZUBPWOYNZJW-UHFFFAOYSA-N	1.0×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:NC524OH	1.1×10^{11}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_7$	1.4×10^{11}		Wang et al. (2017)	Q	80, 239
ZZGZKDXCMVGDSK-UHFFFAOYSA-N	5.4×10^{6}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NC524OOH	1.8×10^{13}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_8$	1.7×10^{11}		Wang et al. (2017)	Q	80, 239
IVLBZHUBMDVGDP-UHFFFAOYSA-N	9.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:NMBOAOOH	1.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_6$	9.8×10^{4}		Wang et al. (2017)	Q	80, 239
JWWMAKNKCQEFPZ-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NMBOBOOH	1.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_6$	4.3×10^{4}		Wang et al. (2017)	Q	80, 239
ZVOCBPRLBFFNTM-UHFFFAOYSA-N	3.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PE1ENEANO3	2.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
VVLSYMLJBKJHQI-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	80, 240
MCM:PE1ENEBNO3	2.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	1.3×10^{2}		Wang et al. (2017)	Q	80, 239
ZAYLQHAUCSLXCO-UHFFFAOYSA-N	6.5×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:PE2ENEANO3	3.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	1.2×10^{2}		Wang et al. (2017)	Q	80, 239
SNSYWPGYFWSVQC-UHFFFAOYSA-N	6.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:PE2ENEBNO3	3.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
FSHUAFNCTFMDNJ-UHFFFAOYSA-N	2.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:PROL11MNO3	1.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	8.5×10^{1}		Wang et al. (2017)	Q	80, 239
XLOGQOLFBMMDEL-UHFFFAOYSA-N	5.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:PROL1MPAN	3.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	2.5×10^{3}		Wang et al. (2017)	Q	80, 239
KGIFHBAEXLJKCU-UHFFFAOYSA-N	1.5×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:BZBIPERNO3	1.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_6$	8.7×10^{4}		Wang et al. (2017)	Q	80, 239
RBJPNJQUNYROJW-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C4ME2OHNO3	1.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	5.1×10^{1}		Wang et al. (2017)	Q	80, 239
KWGTWPROGIVFDL-UHFFFAOYSA-N	1.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C518PAN	1.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_6$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
SMGAVNKPBYTONP-UHFFFAOYSA-N	4.1×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C622NO3	3.5×10^{1}	11000	Wieser et al. (2023)	Q	437
$C_6H_{11}NO_4$	4.0×10^{1}		Wang et al. (2017)	Q	80, 238
UCAFMJJTBHTENA-UHFFFAOYSA-N	6.6×10^{2}		Wang et al. (2017)	Q	80, 239
	2.0		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C624NO3	4.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_4$	3.8×10^{2}		Wang et al. (2017)	Q	80, 239
NPRBCQJDIIBUMY-UHFFFAOYSA-N	5.4		Wang et al. (2017)	Q	80, 240
MCM:C64OH5NO3	2.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	7.8×10^{1}		Wang et al. (2017)	Q	80, 239
SZVWRLIYDKPIRS-UHFFFAOYSA-N	2.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C65OH4NO3	2.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	8.7×10^{1}		Wang et al. (2017)	Q	80, 239
ZZPOFDLVCBSRPC-UHFFFAOYSA-N	5.5×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C66NO35OH	2.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	8.9×10^{1}		Wang et al. (2017)	Q	80, 239
FGVUHVRIXFWTDQ-UHFFFAOYSA-N	5.9×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C6OH5NO3	2.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	8.1×10^{1}		Wang et al. (2017)	Q	80, 239
WNZDORMXFCCFFY-UHFFFAOYSA-N	8.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN11	7.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	2.8×10^{4}		Wang et al. (2017)	Q	80, 239
MMZOJEONIKVQSZ-UHFFFAOYSA-N	6.9×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN13	4.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	1.8×10^{4}		Wang et al. (2017)	Q	80, 239
UVFJOYDNGFNBNV-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	80, 240
MCM:C6PAN14	4.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	1.9×10^{4}		Wang et al. (2017)	Q	80, 239
OFISHWPBQMHPEB-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN19	7.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	2.6×10^{4}		Wang et al. (2017)	Q	80, 239
ZTVAXWHNQKLGPW-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	80, 240
MCM:C6PAN1	6.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	2.6×10^{4}		Wang et al. (2017)	Q	80, 239
INIWXNWKFGUMOJ-UHFFFAOYSA-N	6.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN20	7.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	1.5×10^{4}		Wang et al. (2017)	Q	80, 239
HBAXDJNNSYEITK-UHFFFAOYSA-N	4.8×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN21	4.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	1.6×10^{4}		Wang et al. (2017)	Q	80, 239
PXGXPDBWNDXFTJ-UHFFFAOYSA-N	3.0×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN22	6.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	1.3×10^{4}		Wang et al. (2017)	Q	80, 239
YIFZDOMLXOKIHL-UHFFFAOYSA-N	1.1×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C6PAN23	3.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	2.6×10^{3}		Wang et al. (2017)	Q	80, 239
OODNPGDDVDMKSB-UHFFFAOYSA-N	4.2×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN4	7.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	2.1×10^{4}		Wang et al. (2017)	Q	80, 239
ZWWUNLHZACGCEV-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:C6PAN8	4.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	2.8×10^{4}		Wang et al. (2017)	Q	80, 239
UOLRWSMDFSCHJH-UHFFFAOYSA-N	7.1×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:CYHXOLANO3	8.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_4$	4.6×10^{2}		Wang et al. (2017)	Q	80, 239
GVSCAKVHXWAQQJ-UHFFFAOYSA-N	4.7		Wang et al. (2017)	Q	80, 240
MCM:H13M3C5NO3	4.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_5$	2.8×10^{5}		Wang et al. (2017)	Q	80, 239
ZRQJKBICSYYJDC-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:H1MC5NO3	1.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	3.6×10^{2}		Wang et al. (2017)	Q	80, 239
YQESDLQNDPCVPT-UHFFFAOYSA-N	8.7		Wang et al. (2017)	Q	80, 240
MCM:H2MC5NO3	1.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	4.3×10^{2}		Wang et al. (2017)	Q	80, 239
OQOPDPWKHFKGPO-UHFFFAOYSA-N	4.7		Wang et al. (2017)	Q	80, 240
MCM:H3M3C5NO3	1.2×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	2.5×10^{2}		Wang et al. (2017)	Q	80, 239
KFPWVQORUDKTSF-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:HM22C4NO3	1.2×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	3.0×10^{2}		Wang et al. (2017)	Q	80, 239
VALJBIPPHZOXME-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:HM23C4NO3	1.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	4.8×10^{2}		Wang et al. (2017)	Q	80, 239
VYFSYIPQAVXJDI-UHFFFAOYSA-N	4.5		Wang et al. (2017)	Q	80, 240
MCM:HM33C4NO3	1.2×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	3.2×10^{2}		Wang et al. (2017)	Q	80, 239
HUEIARDLQBFSAX-UHFFFAOYSA-N	4.9		Wang et al. (2017)	Q	80, 240
MCM:HO1C6NO3	1.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	2.5×10^{2}		Wang et al. (2017)	Q	80, 239
ITCMBKDCMKPMFX-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	80, 240
MCM:HO1MC5NO3	1.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	2.4×10^{2}		Wang et al. (2017)	Q	80, 239
HKEZUADWXQLOIL-UHFFFAOYSA-N	4.9		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HO2C6NO3	1.6×10^{1}	10000	Wieser et al. (2023)	Q	437
$C_6H_{13}NO_4$	1.9×10^{1}		Wang et al. (2017)	Q	80, 238
PAWWQEMXBSLVJC-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	80, 239
	4.2		Wang et al. (2017)	Q	80, 240
MCM:HO2M2C5NO3	1.2×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	2.9×10^{2}		Wang et al. (2017)	Q	80, 239
VYPLOHRVLBPDEY-UHFFFAOYSA-N	5.0		Wang et al. (2017)	Q	80, 240
MCM:HO2MC5NO3	1.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	3.1×10^{2}		Wang et al. (2017)	Q	80, 239
HYCOTEZKEHIINQ-UHFFFAOYSA-N	3.5		Wang et al. (2017)	Q	80, 240
MCM:HO3C6NO3	1.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	3.0×10^{2}		Wang et al. (2017)	Q	80, 239
DLCRGHMYOOYQLW-UHFFFAOYSA-N	2.8		Wang et al. (2017)	Q	80, 240
MCM:NDNPHENOOH	1.2×10^{15}		Wang et al. (2017)	Q	80, 238
$C_6H_5N_3O_{12}$	3.2×10^{9}		Wang et al. (2017)	Q	80, 239
CXGWHQULUCBXTG-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NNCATECOOH	1.4×10^{16}		Wang et al. (2017)	Q	80, 238
$C_6H_6N_2O_{11}$	5.9×10^{8}		Wang et al. (2017)	Q	80, 239
SEZKEDQZGXKDIE-UHFFFAOYSA-N	1.0×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:NPHENOH	1.8×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_7$	8.5×10^{6}		Wang et al. (2017)	Q	80, 239
RMHIEAGXGVAIOV-UHFFFAOYSA-N	4.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:NPHENOOH	4.7×10^{10}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_8$	5.8×10^{6}		Wang et al. (2017)	Q	80, 239
AMKSGTJAMDYUMG-UHFFFAOYSA-N	4.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C622PAN	1.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{11}NO_6$	2.8×10^{4}		Wang et al. (2017)	Q	80, 239
YZCFVDKMDQZEJM-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:C624PAN	1.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{11}NO_6$	2.0×10^{4}		Wang et al. (2017)	Q	80, 239
GVGFFJILZZBAQC-UHFFFAOYSA-N	2.3		Wang et al. (2017)	Q	80, 240
MCM:C720NO3	1.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_7H_{11}NO_4$	1.7×10^{3}		Wang et al. (2017)	Q	80, 239
VRUSDNGIDALYSE-UHFFFAOYSA-N	3.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C7PAN1	3.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{13}NO_6$	2.1×10^{4}		Wang et al. (2017)	Q	80, 239
HWQKKNUBUUPBAM-UHFFFAOYSA-N	2.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C7PAN2	6.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{13}NO_6$	9.8×10^{3}		Wang et al. (2017)	Q	80, 239
LEPHBBVBSNQAKS-UHFFFAOYSA-N	6.9×10^{-2}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:H2M2C65NO3	1.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{15}NO_4$	1.4×10^{2}		Wang et al. (2017)	Q	80, 239
CAEJQFHLOCBFOE-UHFFFAOYSA-N	3.7		Wang et al. (2017)	Q	80, 240
MCM:H2M4C65NO3	1.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{15}NO_4$	2.1×10^{2}		Wang et al. (2017)	Q	80, 239
GNQNFXQMHRYYMA-UHFFFAOYSA-N	3.2		Wang et al. (2017)	Q	80, 240
MCM:H2M5C65NO3	1.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{15}NO_4$	9.6×10^{1}		Wang et al. (2017)	Q	80, 239
JWGQNCMAKPVWAL-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:H3M3C6NO3	1.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{15}NO_4$	2.3×10^{2}		Wang et al. (2017)	Q	80, 239
HWCRTHIHVAVLJX-UHFFFAOYSA-N	2.3		Wang et al. (2017)	Q	80, 240
MCM:HO3C76NO3	1.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{15}NO_4$	1.5×10^{2}		Wang et al. (2017)	Q	80, 239
FLDFLEPRHCTYNR-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	80, 240
MCM:MNNCATCOOH	1.0×10^{16}		Wang et al. (2017)	Q	80, 238
$C_7H_8N_2O_{11}$	5.5×10^{9}		Wang et al. (2017)	Q	80, 239
QARZHCGSBCBWKI-UHFFFAOYSA-N	1.2×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:NCRESOH	9.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_7$	3.4×10^{6}		Wang et al. (2017)	Q	80, 239
DNQMNVUMZARJRH-UHFFFAOYSA-N	7.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:NCRESOOH	2.6×10^{10}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_8$	2.1×10^{6}		Wang et al. (2017)	Q	80, 239
CBYLLFTZDVJCIH-UHFFFAOYSA-N	6.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NDNCRESOOH	7.1×10^{14}		Wang et al. (2017)	Q	80, 238
$C_7H_7N_3O_{12}$	1.4×10^{9}		Wang et al. (2017)	Q	80, 239
LRLYMWFOIDHJSH-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:TLBIPERNO3	5.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_6$	2.5×10^{4}		Wang et al. (2017)	Q	80, 239
BBVQCFWACDVWPL-UHFFFAOYSA-N	4.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C8PAN1	4.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{15}NO_6$	8.0×10^{3}		Wang et al. (2017)	Q	80, 239
JRARROZAJMGAPP-UHFFFAOYSA-N	7.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:EBZBPERNO3	5.4×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_6$	1.6×10^{4}		Wang et al. (2017)	Q	80, 239
GVVNXZZYBMLIBS-UHFFFAOYSA-N	1.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:ENNCATCOOH	8.7×10^{15}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}N_2O_{11}$	3.2×10^{9}		Wang et al. (2017)	Q	80, 239
SUCBZAKUUVBJMN-UHFFFAOYSA-N	5.8×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HO3C86NO3	1.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_8H_{17}NO_4$	1.2×10^{2}		Wang et al. (2017)	Q	80, 239
WNECKFLKAYSMQF-UHFFFAOYSA-N	1.8		Wang et al. (2017)	Q	80, 240
MCM:MXNNCATOOH	5.4×10^{15}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}N_2O_{11}$	2.0×10^{9}		Wang et al. (2017)	Q	80, 239
SNJAPGUPFXVMJK-UHFFFAOYSA-N	4.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:MXYBIPENO3	3.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_6$	8.9×10^{3}		Wang et al. (2017)	Q	80, 239
QFCKPTYGEYQVET-UHFFFAOYSA-N	1.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NDNEBZLOOH	6.3×10^{14}		Wang et al. (2017)	Q	80, 238
$C_8H_9N_3O_{12}$	8.5×10^{8}		Wang et al. (2017)	Q	80, 239
XZASAIPCUIAVQG-UHFFFAOYSA-N	4.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NDNMXYLOOH	4.6×10^{14}		Wang et al. (2017)	Q	80, 238
$C_8H_9N_3O_{12}$	8.0×10^{9}		Wang et al. (2017)	Q	80, 239
AAXPRTISYYDKLT-UHFFFAOYSA-N	1.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NDNOXYLOOH	8.5×10^{14}		Wang et al. (2017)	Q	80, 238
$C_8H_9N_3O_{12}$	2.3×10^{9}		Wang et al. (2017)	Q	80, 239
SEMBUWBKKSEFTL-UHFFFAOYSA-N	9.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NDNPXYLOOH	4.6×10^{14}		Wang et al. (2017)	Q	80, 238
$C_8H_9N_3O_{12}$	1.2×10^{9}		Wang et al. (2017)	Q	80, 239
YXONGYHUJBRFJO-UHFFFAOYSA-N	4.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NEBNZOLOH	7.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_7$	2.1×10^{6}		Wang et al. (2017)	Q	80, 239
GKEIZOZEJLMBMT-UHFFFAOYSA-N	2.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:NEBNZOLOOH	2.0×10^{10}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_8$	1.3×10^{6}		Wang et al. (2017)	Q	80, 239
DZFBJORWJYJOSR-UHFFFAOYSA-N	3.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NMXYOLOH	5.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_7$	1.4×10^{6}		Wang et al. (2017)	Q	80, 239
SFEIDLQIDXHPNL-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NMXYOLOOH	1.4×10^{10}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_8$	8.1×10^{5}		Wang et al. (2017)	Q	80, 239
ZTRVHLWFIBLUPT-UHFFFAOYSA-N	6.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NOXYOLOH	6.6×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_7$	2.3×10^{6}		Wang et al. (2017)	Q	80, 239
UBRWKHDWLQNZCI-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:NOXYOLOOH	1.7×10^{10}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_8$	1.5×10^{6}		Wang et al. (2017)	Q	80, 239
UHJNRWMXKFNWGQ-UHFFFAOYSA-N	2.0×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NPXYOLOH	6.6×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_7$	3.0×10^{6}		Wang et al. (2017)	Q	80, 239
DMOUSJNYQFTOEV-UHFFFAOYSA-N	2.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NPXYOLOOH	1.7×10^{10}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_8$	1.8×10^{6}		Wang et al. (2017)	Q	80, 239
XNVGITFEYRRJBZ-UHFFFAOYSA-N	3.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:OXNNCATOOH	1.0×10^{16}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}N_2O_{11}$	3.5×10^{8}		Wang et al. (2017)	Q	80, 239
GYUDSTHOULZHIU-UHFFFAOYSA-N	3.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:OXYBIPENO3	3.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_6$	9.1×10^{3}		Wang et al. (2017)	Q	80, 239
QQSYVIZUYAXYBZ-UHFFFAOYSA-N	2.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:PXNNCATOOH	5.4×10^{15}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}N_2O_{11}$	2.0×10^{8}		Wang et al. (2017)	Q	80, 239
PMLOPKQQVRFHBT-UHFFFAOYSA-N	4.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:PXYBIPENO3	3.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_6$	9.3×10^{3}		Wang et al. (2017)	Q	80, 239
DHJHBQWQGWNRCX-UHFFFAOYSA-N	2.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C9PAN1	3.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{17}NO_6$	6.8×10^{3}		Wang et al. (2017)	Q	80, 239
XXDOIRAKHRPRCF-UHFFFAOYSA-N	6.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:HO3C96NO3	1.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{19}NO_4$	9.3×10^{1}		Wang et al. (2017)	Q	80, 239
IBTJZAOBCFQTAU-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:IPBZBPRNO3	5.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_6$	1.5×10^{4}		Wang et al. (2017)	Q	80, 239
VLTHUNWGYHRCPS-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:IPNNCATOOH	8.1×10^{15}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}N_2O_{11}$	2.9×10^{9}		Wang et al. (2017)	Q	80, 239
QCQAPHFHFZPQHQ-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:METLBIPNO3	2.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_6$	5.9×10^{3}		Wang et al. (2017)	Q	80, 239
VQZACYIDHNLNBQ-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MTNNCATOOH	4.8×10^{15}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}N_2O_{11}$	1.2×10^{9}		Wang et al. (2017)	Q	80, 239
ILPSXJBNDMCAEH-UHFFFAOYSA-N	9.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NDNIPBLOOH	5.9×10^{14}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}N_3O_{12}$	8.0×10^{8}		Wang et al. (2017)	Q	80, 239
HEZPBZRCUHPAHJ-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NDNMETLOOH	3.8×10^{14}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}N_3O_{12}$	4.9×10^{9}		Wang et al. (2017)	Q	80, 239
GVOHWVMFRUNQQB-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NDNOETLOOH	6.9×10^{14}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}N_3O_{12}$	1.4×10^{9}		Wang et al. (2017)	Q	80, 239
DLTVFZDBANLVJD-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NDNPBZLOOH	5.1×10^{14}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}N_3O_{12}$	6.8×10^{8}		Wang et al. (2017)	Q	80, 239
JBFCRLZRPRJLGG-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NDNPETLOOH	3.8×10^{14}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}N_3O_{12}$	6.8×10^{8}		Wang et al. (2017)	Q	80, 239
HIQGLTMZAYSJOX-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NDNT123OOH	4.8×10^{14}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}N_3O_{12}$	1.1×10^{9}		Wang et al. (2017)	Q	80, 239
UGLBOUATFGGZQD-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NDNT124OOH	2.6×10^{14}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}N_3O_{12}$	5.5×10^{8}		Wang et al. (2017)	Q	80, 239
JFYUNHMAYFMSCF-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NIPBNZOLOH	7.3×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	2.1×10^{6}		Wang et al. (2017)	Q	80, 239
IAYADIRZIVDBNK-UHFFFAOYSA-N	6.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:NIPBZOLOOH	1.9×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_8$	1.2×10^{6}		Wang et al. (2017)	Q	80, 239
UJRLUYDBOZESDX-UHFFFAOYSA-N	2.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NMETOLOH	4.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	9.8×10^{5}		Wang et al. (2017)	Q	80, 239
JUUDFVZFULKTPV-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NMETOLOOH	1.1×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_8$	5.5×10^{5}		Wang et al. (2017)	Q	80, 239
CCCPQNSHVNXETJ-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NOETOLOH	6.5×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	2.9×10^{6}		Wang et al. (2017)	Q	80, 239
RRTVORKFFCXYCH-UHFFFAOYSA-N	4.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NOETOLOOH	1.7×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_8$	1.7×10^{6}		Wang et al. (2017)	Q	80, 239
CGRZNCSNBNPNBR-UHFFFAOYSA-N	2.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NPBNZOLOH	7.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	1.6×10^{6}		Wang et al. (2017)	Q	80, 239
PSGNFPQCVGIEDF-UHFFFAOYSA-N	2.9×10^{5}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NPBNZOLOOH	1.9×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_8$	9.8×10^{5}		Wang et al. (2017)	Q	80, 239
SNFHXCYEBCZPSO-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NPETOLOH	5.3×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	1.8×10^{6}		Wang et al. (2017)	Q	80, 239
ILVSHXKPUYWBMX-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NPETOLOOH	1.4×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_8$	8.9×10^{5}		Wang et al. (2017)	Q	80, 239
BKSLAYLCQMXSES-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NTM123LOOH	1.1×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_8$	9.1×10^{5}		Wang et al. (2017)	Q	80, 239
BTWUGVBELCWISQ-UHFFFAOYSA-N	5.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NTM123OLOH	4.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	1.6×10^{6}		Wang et al. (2017)	Q	80, 239
DXGFZPSQDYIOOU-UHFFFAOYSA-N	7.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NTM124LOOH	1.1×10^{10}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_8$	1.3×10^{6}		Wang et al. (2017)	Q	80, 239
JDMNMHRINWGUFB-UHFFFAOYSA-N	3.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NTM124OLOH	4.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	2.3×10^{6}		Wang et al. (2017)	Q	80, 239
RASHBSOBGFFOLP-UHFFFAOYSA-N	2.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NTM135LOOH	9.6×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_8$	5.1×10^{5}		Wang et al. (2017)	Q	80, 239
AUGMYCIDZMPUKI-UHFFFAOYSA-N	3.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NTM135OLOH	3.6×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
RAAKFDOLNJCXRG-UHFFFAOYSA-N	2.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:OETLBIPNO3	2.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_6$	6.2×10^{3}		Wang et al. (2017)	Q	80, 239
FQBYEMVYEQQXMF-UHFFFAOYSA-N	6.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:OTNNCATOOH	8.9×10^{15}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}N_2O_{11}$	2.1×10^{8}		Wang et al. (2017)	Q	80, 239
QVFSJCAPJVJPQJ-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:PBZBPERNO3	4.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_6$	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
XWXMYNZXCPDSAQ-UHFFFAOYSA-N	2.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PETLBIPNO3	2.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_6$	6.2×10^{3}		Wang et al. (2017)	Q	80, 239
SOIPWHDZHXSJJN-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:PNNCATCOOH	6.9×10^{15}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}N_2O_{11}$	2.5×10^{9}		Wang et al. (2017)	Q	80, 239
VZHROOMDTDJZFR-UHFFFAOYSA-N	4.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:PTNNCATOOH	4.8×10^{15}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}N_2O_{11}$	1.2×10^{8}		Wang et al. (2017)	Q	80, 239
DSPOEZNZVSBNSI-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:T123NCTOOH	9.3×10^{16}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_9$	3.4×10^{10}		Wang et al. (2017)	Q	80, 239
QTWHDHJHZAXHRP-UHFFFAOYSA-N	2.6×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:T123NNCOOH	3.0×10^{15}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}N_2O_{11}$	8.9×10^{8}		Wang et al. (2017)	Q	80, 239
DNVSLQYQQCSWFT-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:T124NCTOOH	1.7×10^{17}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_9$	3.4×10^{9}		Wang et al. (2017)	Q	80, 239
TXEYLBVXEVQRAA-UHFFFAOYSA-N	6.9×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:T124NNCOOH	3.0×10^{15}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}N_2O_{11}$	1.0×10^{8}		Wang et al. (2017)	Q	80, 239
ATYVZJLHFNLHKS-UHFFFAOYSA-N	7.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:TM123BPNO3	1.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_6$	4.9×10^{3}		Wang et al. (2017)	Q	80, 239
RQYOJMSOWIZBID-UHFFFAOYSA-N	2.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:TM124BPNO3	1.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_6$	3.8×10^{3}		Wang et al. (2017)	Q	80, 239
KUPKWWJOBRXSMW-UHFFFAOYSA-N	9.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:TM135BPNO3	2.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_6$	6.2×10^{3}		Wang et al. (2017)	Q	80, 239
VYQMVFHQGVVJTP-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:APINANO3	6.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_4$	7.3×10^{1}		Wang et al. (2017)	Q	80, 239
YITBNQHGOKCTCE-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	80, 240
MCM:APINBNO3	6.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_4$	9.3×10^{1}		Wang et al. (2017)	Q	80, 239
AFJBVFUZFQZZRG-UHFFFAOYSA-N	2.9		Wang et al. (2017)	Q	80, 240
MCM:APINCNO3	7.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_4$	9.3×10^{2}		Wang et al. (2017)	Q	80, 239
IHZLDCJLQGWYSD-UHFFFAOYSA-N	4.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:BPINANO3	6.2×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_4$	9.6×10^{1}		Wang et al. (2017)	Q	80, 239
LIKORQJDVXFFRR-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:BPINBNO3	6.2×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_4$	1.5×10^{2}		Wang et al. (2017)	Q	80, 239
PIICVRQEXAAMFO-UHFFFAOYSA-N	2.7		Wang et al. (2017)	Q	80, 240
MCM:BPINCNO3	6.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_4$	1.7×10^{3}		Wang et al. (2017)	Q	80, 239
IVSZOCZGKNSHLW-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C10PAN1	3.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{19}NO_6$	6.0×10^{3}		Wang et al. (2017)	Q	80, 239
PVQDOCOVRZVCAL-UHFFFAOYSA-N	6.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C918PAN	8.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_6$	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
GIWCNEZLGDWGNI-UHFFFAOYSA-N	6.5×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:DMEBIPNO3	1.7×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_6$	4.2×10^{3}		Wang et al. (2017)	Q	80, 239
LWYZBKFMLLCHQU-UHFFFAOYSA-N	7.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HO3C106NO3	1.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{21}NO_4$	7.6×10^{1}		Wang et al. (2017)	Q	80, 239
LRSOGLAVONYUMB-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	80, 240
MCM:LIMANO3	8.4×10^{1}	12000	Wieser et al. (2023)	Q	437
$C_{10}H_{17}NO_4$	6.5×10^{1}		Wang et al. (2017)	Q	80, 238
LZDKYYHMAURBIK-UHFFFAOYSA-N	1.8×10^{2}		Wang et al. (2017)	Q	80, 239
	2.8		Wang et al. (2017)	Q	80, 240
MCM:LIMBNO3	6.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_4$	2.3×10^{2}		Wang et al. (2017)	Q	80, 239
WIRXFNWUDJEZSG-UHFFFAOYSA-N	5.5		Wang et al. (2017)	Q	80, 240
MCM:LIMCNO3	8.6×10^{1}	19000	Wieser et al. (2023)	Q	437
$C_{10}H_{17}NO_4$	8.1×10^{1}		Wang et al. (2017)	Q	80, 238
ZELLOEPLERCREX-UHFFFAOYSA-N	6.2×10^{2}		Wang et al. (2017)	Q	80, 239
	8.1		Wang et al. (2017)	Q	80, 240
MCM:NDMEPHOLOH	3.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_7$	7.4×10^{5}		Wang et al. (2017)	Q	80, 239
XEZYIWLRTFENIO-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NDMEPLOOH	7.4×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_8$	3.4×10^{5}		Wang et al. (2017)	Q	80, 239
CUWVWZNCHDONFF-UHFFFAOYSA-N	7.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DETLBIPNO3	1.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{17}NO_6$	3.1×10^{3}		Wang et al. (2017)	Q	80, 239
HUKONYHKUULPQM-UHFFFAOYSA-N	4.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HO3C116NO3	8.0		Wang et al. (2017)	Q	80, 238
$C_{11}H_{23}NO_4$	6.2×10^{1}		Wang et al. (2017)	Q	80, 239
ZSRHOFPLHKNYIP-UHFFFAOYSA-N	9.6×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NDEMPHOLOH	2.6×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{17}NO_7$	4.7×10^{5}		Wang et al. (2017)	Q	80, 239
SFAWLNJVZQJDAW-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NDEMPLOOH	6.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{17}NO_8$	2.4×10^{5}		Wang et al. (2017)	Q	80, 239
KQXYYOILDOZYPH-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HO3C126NO3	6.5		Wang et al. (2017)	Q	80, 238
$C_{12}H_{25}NO_4$	4.8×10^{1}		Wang et al. (2017)	Q	80, 239
NBVYOETUGSGBPE-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:BCANO3	6.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{25}NO_4$	1.1×10^{3}		Wang et al. (2017)	Q	80, 239
DXJZLWPVAKABFC-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:BCBNO3	6.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{25}NO_4$	1.7×10^{3}		Wang et al. (2017)	Q	80, 239
GGDFBGYMWXIISJ-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:BCCNO3	8.5×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{25}NO_4$	2.0×10^{3}		Wang et al. (2017)	Q	80, 239
AJHNYRDSMBHFTD-UHFFFAOYSA-N	1.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:GLYPAN	4.5×10^{3}		Wang et al. (2017)	Q	80, 238
C_2HNO_6	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
WWNQODGUPABTBB-UHFFFAOYSA-N	4.2×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:NO3CH2CHO	1.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_2H_3NO_4$	9.3×10^{1}		Wang et al. (2017)	Q	80, 239
ABUBKAMLUVOXSP-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C3PAN2	3.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_3NO_6$	4.0×10^{3}		Wang et al. (2017)	Q	80, 239
JCWPFKBPQPIIIA-UHFFFAOYSA-N	5.9×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:CHOPRNO3	1.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_3H_5NO_4$	3.9×10^{1}		Wang et al. (2017)	Q	80, 239
IIFXHQMWCHWMFS-UHFFFAOYSA-N	3.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:BUTAL2NO3	8.1		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_4$	1.9×10^{1}		Wang et al. (2017)	Q	80, 239
JTMAFXAEAWTSPM-UHFFFAOYSA-N	1.9×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:BUTALNO3	8.1		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_4$	4.6×10^{1}		Wang et al. (2017)	Q	80, 239
YGQOBBYMNDZOFN-UHFFFAOYSA-N	1.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C4CONO3OOH	7.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	2.1×10^{5}		Wang et al. (2017)	Q	80, 239
OPYZRKWHBYWVFV-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C4NO3COOOH	7.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
LPNJZRUFCUXQKM-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	80, 240
MCM:CHOC2PAN	2.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_6$	9.3×10^{3}		Wang et al. (2017)	Q	80, 239
RNHARUXEGCOCNU-UHFFFAOYSA-N	2.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:CONM2CHO	5.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_5$	1.6×10^{3}		Wang et al. (2017)	Q	80, 239
UXLHNUQVUCPVFF-UHFFFAOYSA-N	4.5×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:CONM2CO3H	5.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_7$	1.0×10^{5}		Wang et al. (2017)	Q	80, 239
KDPSYMPAERQTCV-UHFFFAOYSA-N	1.6		Wang et al. (2017)	Q	80, 240
MCM:CONM2PAN	2.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_4N_2O_9$	4.5×10^{4}		Wang et al. (2017)	Q	80, 239
PRUSZGKEVUCSBM-UHFFFAOYSA-N	2.8×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:IBUALANO3	8.1		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_4$	6.0×10^{1}		Wang et al. (2017)	Q	80, 239
BBEYVRKCPRBWGK-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:IBUDIALPAN	3.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_6$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
ANKFJODHGNELSW-UHFFFAOYSA-N	6.0×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:MALDIALPAN	1.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_3NO_6$	2.3×10^{4}		Wang et al. (2017)	Q	80, 239
JVYQADFHFGBZRY-UHFFFAOYSA-N	2.2×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:MPRBNO3CHO	5.6		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_4$	7.8		Wang et al. (2017)	Q	80, 239
ZFRSNPXDNOXJAQ-UHFFFAOYSA-N	1.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:NC3CHO	3.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_4$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
IRCIUAVPVOGPAB-UHFFFAOYSA-N	3.7		Wang et al. (2017)	Q	80, 240
MCM:C3M3CHONO3	4.7		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	1.6×10^{1}		Wang et al. (2017)	Q	80, 239
FSONNVXXYIKSKL-UHFFFAOYSA-N	1.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C3MCODBPAN	7.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_5NO_6$	2.2×10^{4}		Wang et al. (2017)	Q	80, 239
ABUKHSDGKGHQTM-UHFFFAOYSA-N	6.8×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:C3MNO3CHO	7.6		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	1.4×10^{1}		Wang et al. (2017)	Q	80, 239
IIGIHDSEOSVDKL-UHFFFAOYSA-N	1.9×10^{-2}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C4CHOBNO3	6.8		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	2.5×10^{1}		Wang et al. (2017)	Q	80, 239
IRTPVYBICUATCF-UHFFFAOYSA-N	9.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C4NO3CHO	4.7		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	5.0		Wang et al. (2017)	Q	80, 239
WGTULXFSTHCAFV-UHFFFAOYSA-N	1.0×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C514NO3	6.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_5$	3.6×10^{4}		Wang et al. (2017)	Q	80, 239
CEGGSEAULUFJEH-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C52NO31CO	6.8		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	1.2×10^{1}		Wang et al. (2017)	Q	80, 239
OIPNOUWHATXHHM-UHFFFAOYSA-N	1.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:CO1M22PAN	1.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_6$	6.0×10^{2}		Wang et al. (2017)	Q	80, 239
JNBWLVYXFYINSW-UHFFFAOYSA-N	4.4×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:MC3CODBPAN	7.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_5NO_6$	1.9×10^{4}		Wang et al. (2017)	Q	80, 239
AENWJVOXGCGHKR-UHFFFAOYSA-N	4.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:NC4CHO	2.2×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_4$	9.8×10^{1}		Wang et al. (2017)	Q	80, 239
FHQODWHGFJXLCS-UHFFFAOYSA-N	6.3		Wang et al. (2017)	Q	80, 240
MCM:C522PAN	4.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_6$	4.6×10^{3}		Wang et al. (2017)	Q	80, 239
BLDVCFQHUDZGIY-UHFFFAOYSA-N	9.8×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C65NO36CHO	5.9		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_4$	8.9		Wang et al. (2017)	Q	80, 239
AWOTULOVYXZRSX-UHFFFAOYSA-N	1.4×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:CHOC4PAN	2.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_6$	3.6×10^{3}		Wang et al. (2017)	Q	80, 239
LKJHECXHBJSEQK-UHFFFAOYSA-N	3.1×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:CO1C6NO3	5.3		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_4$	2.9×10^{1}		Wang et al. (2017)	Q	80, 239
BSOUFWBHIRXMPX-UHFFFAOYSA-N	1.8		Wang et al. (2017)	Q	80, 240
MCM:C615PAN	1.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_7$	2.3×10^{5}		Wang et al. (2017)	Q	80, 239
QXDOZRAOCVERTF-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C729NO3	1.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_7H_{11}NO_4$	3.2×10^{1}		Wang et al. (2017)	Q	80, 239
IVMGVFSKIJXXOW-UHFFFAOYSA-N	4.7×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C729PAN	3.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_6$	1.6×10^{3}		Wang et al. (2017)	Q	80, 239
UQYKHYVNMQUYAN-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C810NO3	2.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{13}NO_5$	7.3×10^{3}		Wang et al. (2017)	Q	80, 239
CHBSGOHAWLCLGZ-UHFFFAOYSA-N	4.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C822NO3	2.9×10^{1}	10000	Wieser et al. (2023)	Q	437
$C_8H_{13}NO_4$	8.9		Wang et al. (2017)	Q	80, 238
JWAJNALJDDSHOA-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	80, 239
	1.1		Wang et al. (2017)	Q	80, 240
MCM:C830NO3	1.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_8H_{13}NO_4$	2.8×10^{1}		Wang et al. (2017)	Q	80, 239
FXBNRUYCAFEPCZ-UHFFFAOYSA-N	7.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C831NO3	2.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{13}NO_5$	9.3×10^{3}		Wang et al. (2017)	Q	80, 239
OVEOYJGENOZMLJ-UHFFFAOYSA-N	5.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C89NO3	1.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_8H_{13}NO_4$	2.8×10^{1}		Wang et al. (2017)	Q	80, 239
JVGNHSSLWSUTIF-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	80, 240
MCM:NC826OOH	1.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{13}NO_7$	5.1×10^{7}		Wang et al. (2017)	Q	80, 239
LIEZCAAIBRALIF-UHFFFAOYSA-N	3.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C822PAN	2.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_6$	1.1×10^{3}		Wang et al. (2017)	Q	80, 239
AEOJBADXVLGVNE-UHFFFAOYSA-N	3.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C830PAN	3.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_6$	2.4×10^{3}		Wang et al. (2017)	Q	80, 239
NSAJKAFLWKCEMC-UHFFFAOYSA-N	1.1×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C89PAN	3.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_6$	2.5×10^{3}		Wang et al. (2017)	Q	80, 239
MAIUDZACSGCMBD-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	80, 240
MCM:NC91CHO	1.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_4$	1.4×10^{1}		Wang et al. (2017)	Q	80, 239
AVQCYYCZMFYNOE-UHFFFAOYSA-N	8.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C126NO3	1.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{19}NO_4$	3.4×10^{1}		Wang et al. (2017)	Q	80, 239
LCRFSVKVQOPOBC-UHFFFAOYSA-N	7.3		Wang et al. (2017)	Q	80, 240
MCM:C126PAN	3.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{19}NO_6$	1.8×10^{3}		Wang et al. (2017)	Q	80, 239
TVUSLNPYCCAOKX-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C136NO3	8.7		Wang et al. (2017)	Q	80, 238
$C_{13}H_{21}NO_4$	3.0×10^{1}		Wang et al. (2017)	Q	80, 239
FAQBCXSJSFDOSN-UHFFFAOYSA-N	8.0		Wang et al. (2017)	Q	80, 240
MCM:NC1313OOH	2.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{21}NO_7$	9.1×10^{7}		Wang et al. (2017)	Q	80, 239
AIWUKZRYSUWIQN-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C136PAN	3.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{21}NO_6$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
HVYQJFOLIDVKQK-UHFFFAOYSA-N	4.1		Wang et al. (2017)	Q	80, 240
MCM:C42AOH	1.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_5NO_5$	1.6×10^{4}		Wang et al. (2017)	Q	80, 239
CQVFGUOZVNZZAM-UHFFFAOYSA-N	5.5		Wang et al. (2017)	Q	80, 240
MCM:HCOCOHPAN	1.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_3H_3NO_7$	5.4×10^{5}		Wang et al. (2017)	Q	80, 239
GGQYFRDCXKQQIA-UHFFFAOYSA-N	2.1×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C41NO3	5.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	1.4×10^{7}		Wang et al. (2017)	Q	80, 239
SGYMVPWBXCYWGY-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C42OH	1.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	1.6×10^{7}		Wang et al. (2017)	Q	80, 239
OIAGCOLJHCONRV-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C42OOH	1.3×10^{8}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_7$	1.4×10^{7}		Wang et al. (2017)	Q	80, 239
KUKJNXCETLVUQA-UHFFFAOYSA-N	1.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C4OCCOHNO3	1.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_5$	9.8×10^{3}		Wang et al. (2017)	Q	80, 239
NEHFOAWUQWHZTI-UHFFFAOYSA-N	1.6		Wang et al. (2017)	Q	80, 240
MCM:COCCOHNO3	3.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_5$	3.2×10^{4}		Wang et al. (2017)	Q	80, 239
HMCDHWALZVCNKO-UHFFFAOYSA-N	6.8		Wang et al. (2017)	Q	80, 240
MCM:COHM2PAN	6.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_7$	2.2×10^{5}		Wang et al. (2017)	Q	80, 239
UXUAXYPQPQSXRR-UHFFFAOYSA-N	5.0×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:MACRNB	1.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_5$	1.3×10^{4}		Wang et al. (2017)	Q	80, 239
DLZDCWJOERFHAS-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:MACRNO3	2.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_5$	7.1×10^{3}		Wang et al. (2017)	Q	80, 239
ALINXPRBVMXOGH-UHFFFAOYSA-N	3.2		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C4M2ALOHNO3	8.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_6$	1.4×10^{6}		Wang et al. (2017)	Q	80, 239
UOGOTHSJBRKVRR-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	80, 240
MCM:C510OH	1.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	1.2×10^{7}		Wang et al. (2017)	Q	80, 239
ZCOZZYNQPKXJEJ-UHFFFAOYSA-N	8.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C510OOH	7.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_7$	1.4×10^{7}		Wang et al. (2017)	Q	80, 239
GGBWELVRYZRQMP-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C57NO3	2.0×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	1.3×10^{7}		Wang et al. (2017)	Q	80, 239
KHAJTJUOMDNQGW-UHFFFAOYSA-N	6.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C58NO3	2.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	1.0×10^{7}		Wang et al. (2017)	Q	80, 239
UZUIBKBJXOKLGO-UHFFFAOYSA-N	5.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DNC524CO	7.1×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_9$	9.6×10^{8}		Wang et al. (2017)	Q	80, 239
WXHJTLSKHGDJHS-UHFFFAOYSA-N	1.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HNC524CO	2.9×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_7$	1.5×10^{10}		Wang et al. (2017)	Q	80, 239
UHQMTOKWUFCERL-UHFFFAOYSA-N	5.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:HPNC524CO	4.7×10^{12}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_8$	1.7×10^{10}		Wang et al. (2017)	Q	80, 239
QASKBBWYYSGCPQ-UHFFFAOYSA-N	1.9×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:INAHCHO	1.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	1.5×10^{7}		Wang et al. (2017)	Q	80, 239
GJDCYRXOLZPRRL-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:INAHPCHO	1.6×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_7$	2.6×10^{7}		Wang et al. (2017)	Q	80, 239
WOIAKHQAPCBXNP-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:INANCHO	2.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_8$	1.7×10^{6}		Wang et al. (2017)	Q	80, 239
AOWQROMNZIXQRL-UHFFFAOYSA-N	6.3		Wang et al. (2017)	Q	80, 240
MCM:INB1HPCHO	1.4×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_7$	1.9×10^{7}		Wang et al. (2017)	Q	80, 239
PPUPDRIHXISUBS-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:INB1NACHO	2.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_8$	7.4×10^{6}		Wang et al. (2017)	Q	80, 239
FPDRKJBIBBHIBW-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:INB1NBCHO	2.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_8$	5.4×10^{6}		Wang et al. (2017)	Q	80, 239
DIJODJNNHWDXRN-UHFFFAOYSA-N	2.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:INCNCHO	2.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_8$	3.4×10^{6}		Wang et al. (2017)	Q	80, 239
QYWHAZCEYLWYSZ-UHFFFAOYSA-N	3.1		Wang et al. (2017)	Q	80, 240
MCM:INDHCHO	2.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	1.6×10^{7}		Wang et al. (2017)	Q	80, 239
LXJORHVMGZGMRK-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:INDHPCHO	1.4×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_7$	1.3×10^{7}		Wang et al. (2017)	Q	80, 239
NKPKKBYOCYFEQQ-UHFFFAOYSA-N	4.0×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:MMALNACO3H	9.3×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_8$	2.0×10^{6}		Wang et al. (2017)	Q	80, 239
WWJYGONDDIBFHK-UHFFFAOYSA-N	8.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MMALNAPAN	4.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_6N_2O_{10}$	6.0×10^{7}		Wang et al. (2017)	Q	80, 239
JNHZFZYBXYVXPX-UHFFFAOYSA-N	2.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:MMALNBCO3H	9.3×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_8$	3.9×10^{7}		Wang et al. (2017)	Q	80, 239
ASZGKTQVJXPLHM-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MMALNBPAN	4.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_6N_2O_{10}$	1.3×10^{7}		Wang et al. (2017)	Q	80, 239
QNDDWZGVLTYMIK-UHFFFAOYSA-N	1.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:NMBOBCO	1.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	2.2×10^{4}		Wang et al. (2017)	Q	80, 239
ZWLCCOCHHFERQT-UHFFFAOYSA-N	1.6		Wang et al. (2017)	Q	80, 240
MCM:C1H4C5PAN	5.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_7$	2.5×10^{7}		Wang et al. (2017)	Q	80, 239
XKXYOEFJYDLELH-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C623NO3	4.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	6.0×10^{7}		Wang et al. (2017)	Q	80, 239
UTKYBRKMQKBGOV-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C67NO3	1.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	6.9×10^{4}		Wang et al. (2017)	Q	80, 239
MTROCBFSNOSSFX-UHFFFAOYSA-N	4.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C68NO3	1.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	6.8×10^{4}		Wang et al. (2017)	Q	80, 239
DFCRZDMTYDUCKH-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CO1H63NO3	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	6.0×10^{5}		Wang et al. (2017)	Q	80, 239
QWPYKWKOPQKYFO-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NC623OH	4.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	2.7×10^{8}		Wang et al. (2017)	Q	80, 239
LIALSLHETRNECK-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NC623OOH	1.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_7$	6.0×10^{7}		Wang et al. (2017)	Q	80, 239
LUCHFEJMQFYPEG-UHFFFAOYSA-N	6.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C728NO3	1.5×10^{8}	17000	Wieser et al. (2023)	Q	437
$C_7H_{13}NO_6$	3.2×10^{7}		Wang et al. (2017)	Q	80, 238
CDBHNFBQKSTCON-UHFFFAOYSA-N	2.0×10^{8}		Wang et al. (2017)	Q	80, 239
	3.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C730NO3	3.5×10^{9}	17000	Wieser et al. (2023)	Q	437
$C_7H_{13}NO_6$	3.2×10^{7}		Wang et al. (2017)	Q	80, 238
RVWIAVBELSCRER-UHFFFAOYSA-N	1.4×10^{9}		Wang et al. (2017)	Q	80, 239
	9.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NC728OH	3.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_{13}NO_6$	5.4×10^{8}		Wang et al. (2017)	Q	80, 239
RMGZPHZIJLBXBA-UHFFFAOYSA-N	9.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NC728OOH	7.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{13}NO_7$	2.0×10^{8}		Wang et al. (2017)	Q	80, 239
NMPAVXKBWDGSMK-UHFFFAOYSA-N	2.1×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:NC730OH	3.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_{13}NO_6$	2.4×10^{8}		Wang et al. (2017)	Q	80, 239
ZPFRZNAADTZJOS-UHFFFAOYSA-N	1.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NC730OOH	7.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{13}NO_7$	2.7×10^{9}		Wang et al. (2017)	Q	80, 239
LJYXGYOAXKBDIY-UHFFFAOYSA-N	6.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C826NO3	9.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{13}NO_6$	4.6×10^{7}		Wang et al. (2017)	Q	80, 239
HYUHCBAMOFNBPC-UHFFFAOYSA-N	5.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NC826OH	9.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{13}NO_6$	6.2×10^{7}		Wang et al. (2017)	Q	80, 239
UXZRCYKYQRKKOI-UHFFFAOYSA-N	3.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C127NO3	1.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{19}NO_5$	1.7×10^{5}		Wang et al. (2017)	Q	80, 239
RZJFRKYKWJUXLW-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C1311NO3	1.7×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{21}NO_5$	1.4×10^{5}		Wang et al. (2017)	Q	80, 239
HIIZKUNLVYOKLJ-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:C1313NO3	9.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{21}NO_6$	5.8×10^{7}		Wang et al. (2017)	Q	80, 239
SXMORIYKGFOKAB-UHFFFAOYSA-N	2.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NC1313OH	9.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{21}NO_6$	6.8×10^{7}		Wang et al. (2017)	Q	80, 239
RAUQQNONBFDDJB-UHFFFAOYSA-N	5.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C3NO3COOOH	5.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_3H_5NO_6$	4.0×10^{4}		Wang et al. (2017)	Q	80, 239
JXBSDKIVLYRFTK-UHFFFAOYSA-N	2.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CH3COPAN	2.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_3NO_6$	2.1×10^{3}		Wang et al. (2017)	Q	80, 239
BNYSUSDQQIWDSZ-UHFFFAOYSA-N	2.2×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:BUTONENO3	7.1		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_4$	3.5×10^{1}		Wang et al. (2017)	Q	80, 239
KFRUNLQRYXGRRS-UHFFFAOYSA-N	7.4×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:CO23C4NO3	3.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_5$	4.3×10^{3}		Wang et al. (2017)	Q	80, 239
RSORCZUYAJEINP-UHFFFAOYSA-N	7.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:CO2C3PAN	2.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_6$	4.0×10^{3}		Wang et al. (2017)	Q	80, 239
VXGDXYQGFKIYIJ-UHFFFAOYSA-N	1.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:CO2N3CO3H	6.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_7$	5.5×10^{5}		Wang et al. (2017)	Q	80, 239
PLOOSZKRSUJKKF-UHFFFAOYSA-N	4.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO2N3PAN	3.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_4N_2O_9$	2.3×10^{5}		Wang et al. (2017)	Q	80, 239
RXUYCSQEPKEYNB-UHFFFAOYSA-N	2.3×10^{-3}		Wang et al. (2017)	Q	80, 240
2-oxobutyl nitrate	5.9		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_4$	5.9×10^{1}		Wang et al. (2017)	Q	80, 239
[138779-12-1]	3.1×10^{-1}		Wang et al. (2017)	Q	80, 240
OVISQPFXRZOZFI-UHFFFAOYSA-N					
MCM:COC4NO3OOH	5.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	1.8×10^{4}		Wang et al. (2017)	Q	80, 239
AEHFBVVGPAXMNG-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MEKANO3	5.9		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_4$	1.3×10^{2}		Wang et al. (2017)	Q	80, 239
SQFMCLNZTZWUJY-UHFFFAOYSA-N	8.9×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:NMVK	1.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_4$	1.0×10^{2}		Wang et al. (2017)	Q	80, 239
YTEQPVIDLVIVHW-UHFFFAOYSA-N	3.4×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C4M2NO3ONE	3.8		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	7.3		Wang et al. (2017)	Q	80, 239
DIMIHFOKCQZMGY-UHFFFAOYSA-N	5.9×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C4M3NO3ONE	5.5		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	3.4×10^{1}		Wang et al. (2017)	Q	80, 239
SAHLZHFOPIFWKH-UHFFFAOYSA-N	1.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C4MCNO3OOH	2.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	8.3×10^{4}		Wang et al. (2017)	Q	80, 239
AOCDDMVLVLTZNT-UHFFFAOYSA-N	2.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C51NO324CO	3.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_5$	2.0×10^{4}		Wang et al. (2017)	Q	80, 239
KIDZPQUIRFWTHY-UHFFFAOYSA-N	8.0		Wang et al. (2017)	Q	80, 240
MCM:C51NO32CO	4.9		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	3.2×10^{1}		Wang et al. (2017)	Q	80, 239
TTZVKGPORDTQGG-UHFFFAOYSA-N	2.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C52NO33CO	5.5		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	1.6×10^{1}		Wang et al. (2017)	Q	80, 239
VOCQUTRGVIAJPG-UHFFFAOYSA-N	6.2×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C53NO324CO	3.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_5$	7.4×10^{3}		Wang et al. (2017)	Q	80, 239
QYJXVKSLJJQONK-UHFFFAOYSA-N	1.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C53NO32CO	5.5		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	1.7×10^{1}		Wang et al. (2017)	Q	80, 239
LVGYWFUEHRGRSS-UHFFFAOYSA-N	6.9×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C5CONO3OOH	2.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	3.7×10^{3}		Wang et al. (2017)	Q	80, 239
ZDTBCADGPXXLKE-UHFFFAOYSA-N	3.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C5COO2NO2	7.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_5NO_6$	3.9×10^{4}		Wang et al. (2017)	Q	80, 239
BZPLAICQOBBIOR-UHFFFAOYSA-N	4.7×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C5NO3O4OOH	4.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	4.6×10^{3}		Wang et al. (2017)	Q	80, 239
CASCWEIOXSCVGJ-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C5NO3OAOOH	4.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	5.3×10^{5}		Wang et al. (2017)	Q	80, 239
FLHIUJMTRYIPLY-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C5ONO34OOH	4.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	1.5×10^{5}		Wang et al. (2017)	Q	80, 239
LOZNRBAEPWQBFW-UHFFFAOYSA-N	2.9×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C5PAN16	1.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_6$	2.0×10^{3}		Wang et al. (2017)	Q	80, 239
IZEBTYZDWKBBFQ-UHFFFAOYSA-N	5.9×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C5PAN2	1.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_6$	9.6×10^{3}		Wang et al. (2017)	Q	80, 239
XMORPXKVSPHXDA-UHFFFAOYSA-N	5.1×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C5PAN7	2.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_6$	1.5×10^{3}		Wang et al. (2017)	Q	80, 239
VONRVKPFQAOOPX-UHFFFAOYSA-N	3.0×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C5PAN9	1.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_5NO_7$	2.5×10^{5}		Wang et al. (2017)	Q	80, 239
HJZPHZLLKGPYCO-UHFFFAOYSA-N	5.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:DIEKBNO3	4.9		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	5.5×10^{1}		Wang et al. (2017)	Q	80, 239
WKTFKAAKLZJYGP-UHFFFAOYSA-N	5.9×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:INANCOCO3H	4.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_6N_2O_{10}$	1.4×10^{7}		Wang et al. (2017)	Q	80, 239
OKQCOTADQFFQES-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	80, 240
MCM:INANCOPAN	1.9×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_5N_3O_{12}$	5.3×10^{6}		Wang et al. (2017)	Q	80, 239
OHHXWPYTKFCNFA-UHFFFAOYSA-N	8.0×10^{-5}		Wang et al. (2017)	Q	80, 240
MCM:MIPKBNO3	5.5		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	5.5×10^{1}		Wang et al. (2017)	Q	80, 239
PNKPSVUHDDVFRC-UHFFFAOYSA-N	6.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:MPRKNO3	5.5		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_4$	3.9×10^{1}		Wang et al. (2017)	Q	80, 239
GMHWHQCXUOCSQQ-UHFFFAOYSA-N	4.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C3COCPAN	1.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_6$	1.1×10^{3}		Wang et al. (2017)	Q	80, 239
QAGGXZNGFPYUOO-UHFFFAOYSA-N	4.9×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C4MCODBPAN	5.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_6$	3.3×10^{4}		Wang et al. (2017)	Q	80, 239
OBEVNDXPXGMJPT-UHFFFAOYSA-N	1.4×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C62NO335CO	3.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_5$	6.0×10^{3}		Wang et al. (2017)	Q	80, 239
ABDNFJAHWTWRFH-UHFFFAOYSA-N	3.9		Wang et al. (2017)	Q	80, 240
MCM:C62NO33CO	4.6		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_4$	9.8		Wang et al. (2017)	Q	80, 239
OBVLXHVNJQTRAU-UHFFFAOYSA-N	4.5×10^{-2}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C63NO32CO	4.6		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_4$	1.1×10^{1}		Wang et al. (2017)	Q	80, 239
QSKMGJAWRGUYGL-UHFFFAOYSA-N	5.5×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C64NO335CO	3.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_5$	4.2×10^{3}		Wang et al. (2017)	Q	80, 239
CHGSCHAFWLLPDM-UHFFFAOYSA-N	8.0×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C66NO35CO	4.3		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_4$	2.2×10^{1}		Wang et al. (2017)	Q	80, 239
NNYDFJRPKYRBEY-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C6CO134PAN	1.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_7$	1.4×10^{5}		Wang et al. (2017)	Q	80, 239
OIZONYBQGYIWDV-UHFFFAOYSA-N	2.2×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C6CONO3OOH	3.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	1.3×10^{5}		Wang et al. (2017)	Q	80, 239
JAMSWIXAFBYGGR-UHFFFAOYSA-N	3.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C6DCARBPAN	7.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_6$	1.8×10^{4}		Wang et al. (2017)	Q	80, 239
QTAROYORLXCHIO-UHFFFAOYSA-N	3.0×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C6NO324CO	2.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_5$	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
ZLHGCQIPJTVAEP-UHFFFAOYSA-N	4.4		Wang et al. (2017)	Q	80, 240
MCM:C6NO3COOOH	3.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	2.6×10^{5}		Wang et al. (2017)	Q	80, 239
HQTZSBFILMVSJZ-UHFFFAOYSA-N	5.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN12	1.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_6$	3.4×10^{3}		Wang et al. (2017)	Q	80, 239
LSIJQLAUAXHOJI-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN16	1.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_6$	5.3×10^{2}		Wang et al. (2017)	Q	80, 239
JDUNWYCOIXFXGK-UHFFFAOYSA-N	1.8×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN2	1.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_6$	4.9×10^{3}		Wang et al. (2017)	Q	80, 239
BSRDZZSTWMTZHH-UHFFFAOYSA-N	4.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN5	1.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_6$	3.4×10^{3}		Wang et al. (2017)	Q	80, 239
AYORGEAGFIRFHW-UHFFFAOYSA-N	4.1×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN6	1.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_6$	6.6×10^{2}		Wang et al. (2017)	Q	80, 239
STXATUQYWORJHN-UHFFFAOYSA-N	1.5×10^{-2}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C6PAN7	1.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_7$	1.0×10^{5}		Wang et al. (2017)	Q	80, 239
FEUNFERSGUKVTQ-UHFFFAOYSA-N	2.7×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:CONO3C6OOH	3.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	7.3×10^{4}		Wang et al. (2017)	Q	80, 239
BPHZXGKZHPQLPB-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CYHXONANO3	1.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_4$	3.6×10^{2}		Wang et al. (2017)	Q	80, 239
VLCBNIODXGFPBM-UHFFFAOYSA-N	9.8		Wang et al. (2017)	Q	80, 240
MCM:ECO3PAN	7.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_5NO_8$	4.0×10^{7}		Wang et al. (2017)	Q	80, 239
GLZSBLKUFXIYNN-UHFFFAOYSA-N	3.4×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:EIPKBNO3	4.6		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_4$	2.7×10^{1}		Wang et al. (2017)	Q	80, 239
QPLZWEVCYZLYTL-UHFFFAOYSA-N	2.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:HEX2ONANO3	4.6		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_4$	2.2×10^{1}		Wang et al. (2017)	Q	80, 239
OZSNHPHDGAJMHG-UHFFFAOYSA-N	2.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:HEX2ONBNO3	4.6		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_4$	3.0×10^{1}		Wang et al. (2017)	Q	80, 239
JYVFNKYOALTNTA-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	80, 240
MCM:HEX3ONANO3	4.6		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_4$	2.0×10^{1}		Wang et al. (2017)	Q	80, 239
KTYGBCIWLHIEKP-UHFFFAOYSA-N	4.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:HEX3ONDNO3	4.3		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_4$	3.6×10^{1}		Wang et al. (2017)	Q	80, 239
PRTKDFINSKNZSU-UHFFFAOYSA-N	6.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:M2BKANO3	5.1		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_4$	2.6×10^{1}		Wang et al. (2017)	Q	80, 239
NYAAKBDXIQFYDD-UHFFFAOYSA-N	3.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:MC4CODBPAN	5.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_6$	3.3×10^{4}		Wang et al. (2017)	Q	80, 239
WHFHKQLMYAOVSY-UHFFFAOYSA-N	2.2×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:MIBKANO3	3.0		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_4$	1.5×10^{1}		Wang et al. (2017)	Q	80, 239
PKJJSCYTBLHEMI-UHFFFAOYSA-N	1.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:MTBKNO3	3.0		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_4$	2.6×10^{1}		Wang et al. (2017)	Q	80, 239
OYSBYTCKEAIMOW-UHFFFAOYSA-N	5.4×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NBZQOOH	3.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_5NO_7$	5.6×10^{8}		Wang et al. (2017)	Q	80, 239
NXGPVQDYDGLWQQ-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C627PAN	9.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_7$	3.0×10^{6}		Wang et al. (2017)	Q	80, 239
FQVTWXYWQQSSRX-UHFFFAOYSA-N	2.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C7ADCPAN	3.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_6$	4.3×10^{4}		Wang et al. (2017)	Q	80, 239
OFKNKTFVVCSQBW-UHFFFAOYSA-N	8.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C7DCPAN	5.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_6$	9.6×10^{3}		Wang et al. (2017)	Q	80, 239
ZGBUEZLBCHGZPP-UHFFFAOYSA-N	1.4×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C7DDCPAN	4.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_6$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
WCHGYJHJZMHIAR-UHFFFAOYSA-N	5.5×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:C7PAN3	6.3×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_7NO_8$	1.7×10^{7}		Wang et al. (2017)	Q	80, 239
XMNXEIJPBOBVEP-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	80, 240
MCM:IC7DCPAN	6.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_6$	1.0×10^{4}		Wang et al. (2017)	Q	80, 239
NZLPHNCQTJFNGH-UHFFFAOYSA-N	8.1×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:NC71CO	3.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_7NO_6$	2.5×10^{7}		Wang et al. (2017)	Q	80, 239
CDHAVACRDDMHGZ-UHFFFAOYSA-N	1.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NC71OOH	4.5×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_7$	1.6×10^{9}		Wang et al. (2017)	Q	80, 239
CIJBWMVCSXGACJ-UHFFFAOYSA-N	5.6×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:NC72OOH	3.0×10^{11}		Wang et al. (2017)	Q	80, 238
$C_7H_7NO_8$	3.6×10^{10}		Wang et al. (2017)	Q	80, 239
RYHDNZNGTUJGAD-UHFFFAOYSA-N	5.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:NPTLQOOH	2.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_7H_7NO_7$	4.8×10^{8}		Wang et al. (2017)	Q	80, 239
WIZJVJIMHIROQF-UHFFFAOYSA-N	6.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C5DBEPAN	2.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_7$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
OYOZKJOWUFGKRQ-UHFFFAOYSA-N	9.6×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:C5EDBPAN	2.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_7$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
KNPMBKOCKIUXFV-UHFFFAOYSA-N	7.6×10^{-3}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:C727PAN	8.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_7$	6.9×10^{5}		Wang et al. (2017)	Q	80, 239
WBGZRMCIPBEEGH-UHFFFAOYSA-N	4.1		Wang et al. (2017)	Q	80, 240
MCM:C7CODBPAN	3.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_6$	7.6×10^{3}		Wang et al. (2017)	Q	80, 239
QVHZZCVTEAGIPK-UHFFFAOYSA-N	3.8×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:C817NO3	3.9×10^{4}	12000	Wieser et al. (2023)	Q	437
$C_8H_{13}NO_5$	2.2×10^{3}		Wang et al. (2017)	Q	80, 238
ZONZWPKPCIWKRN-UHFFFAOYSA-N	3.8×10^{4}		Wang et al. (2017)	Q	80, 239
	3.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NMXYQOOH	1.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_7$	9.6×10^{7}		Wang et al. (2017)	Q	80, 239
MDRQMTCFLWPCNU-UHFFFAOYSA-N	4.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NOXYQOOH	1.5×10^{9}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_7$	3.8×10^{8}		Wang et al. (2017)	Q	80, 239
SFYCEAPRSKIFCS-UHFFFAOYSA-N	4.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NPEBQOOH	2.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_7$	2.6×10^{8}		Wang et al. (2017)	Q	80, 239
HZFUWULOZSGVHH-UHFFFAOYSA-N	5.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NPXYQOOH	1.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_7$	9.3×10^{7}		Wang et al. (2017)	Q	80, 239
LMPSHWMXIGVDOI-UHFFFAOYSA-N	2.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C816PAN	2.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_6$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
JXXOSNUALVJMQL-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C817PAN	6.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	1.6×10^{6}		Wang et al. (2017)	Q	80, 239
AGDIJRUETYYZKI-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C827PAN	4.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	5.3×10^{5}		Wang et al. (2017)	Q	80, 239
QMDLSNSKOZAILD-UHFFFAOYSA-N	2.3		Wang et al. (2017)	Q	80, 240
MCM:C828PAN	3.6×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_8$	1.1×10^{7}		Wang et al. (2017)	Q	80, 239
LCFHBKSAGMTDCX-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:C88PAN	1.7×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_7$	1.4×10^{7}		Wang et al. (2017)	Q	80, 239
KLGKHKJTYFCRCN-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C917NO3	4.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_5$	2.5×10^{5}		Wang et al. (2017)	Q	80, 239
KVWUPUMJPKRVQS-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C923NO3	3.2×10^{1}	11000	Wieser et al. (2023)	Q	437
$C_9H_{15}NO_4$	6.0		Wang et al. (2017)	Q	80, 238
JEWJQSHMOKPQHI-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	80, 239
	4.1		Wang et al. (2017)	Q	80, 240
MCM:C928NO3	1.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{15}NO_5$	3.2×10^{4}		Wang et al. (2017)	Q	80, 239
HCHMIBGRYQMLLZ-UHFFFAOYSA-N	6.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C96NO3	6.6		Wang et al. (2017)	Q	80, 238
$C_9H_{15}NO_4$	5.0×10^{1}		Wang et al. (2017)	Q	80, 239
MMTOEOITRCIZDG-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	80, 240
MCM:C9DCNO3	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_5$	7.3×10^{5}		Wang et al. (2017)	Q	80, 239
TURIVFFHDFEFMU-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C9PAN2	2.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_6$	3.2×10^{3}		Wang et al. (2017)	Q	80, 239
VXDDXZNSSANCGN-UHFFFAOYSA-N	8.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:NIPRBQOOH	1.8×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_7$	1.8×10^{8}		Wang et al. (2017)	Q	80, 239
KGZDDJNUZZWZIJ-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NLMKAOOH	5.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{15}NO_6$	8.9×10^{5}		Wang et al. (2017)	Q	80, 239
ZOTFHCKOVMRARL-UHFFFAOYSA-N	5.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NMETLQOOH	1.1×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_7$	5.0×10^{7}		Wang et al. (2017)	Q	80, 239
FSVFAZAPMWXECG-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NOETLQOOH	1.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_7$	2.1×10^{8}		Wang et al. (2017)	Q	80, 239
GHGZYHLEQYQZHR-UHFFFAOYSA-N	3.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NOPINANO3	2.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_4$	2.3×10^{2}		Wang et al. (2017)	Q	80, 239
JEOFIBHUYPQAJL-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NOPINBNO3	2.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_4$	3.1×10^{2}		Wang et al. (2017)	Q	80, 239
QGVNTXJLRAHBMW-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NOPINCNO3	1.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_4$	8.1×10^{1}		Wang et al. (2017)	Q	80, 239
CLMUTFVSCXCGKI-UHFFFAOYSA-N	1.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NPETLQOOH	1.1×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_7$	4.8×10^{7}		Wang et al. (2017)	Q	80, 239
IMJMJNZTMWKOFO-UHFFFAOYSA-N	2.6×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NPPRBQOOH	1.6×10^{9}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_7$	1.8×10^{8}		Wang et al. (2017)	Q	80, 239
MMAZKJNYHBQGDL-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NTM124QOOH	8.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_7$	6.9×10^{7}		Wang et al. (2017)	Q	80, 239
ZMXXAPJGXNLYQU-UHFFFAOYSA-N	5.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C1011NO3	5.4		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_4$	2.5×10^{1}		Wang et al. (2017)	Q	80, 239
KLQCUGBDZZARMU-UHFFFAOYSA-N	1.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C10PAN2	2.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_6$	2.6×10^{3}		Wang et al. (2017)	Q	80, 239
XGWGKMXMXMPDAK-UHFFFAOYSA-N	4.7		Wang et al. (2017)	Q	80, 240
MCM:C923PAN	2.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_6$	1.0×10^{3}		Wang et al. (2017)	Q	80, 239
ZVYIPTRRRFMSSU-UHFFFAOYSA-N	2.3		Wang et al. (2017)	Q	80, 240
MCM:C928PAN	3.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_7$	1.5×10^{6}		Wang et al. (2017)	Q	80, 239
MIISGCVMOACDOR-UHFFFAOYSA-N	2.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NC101CO	1.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_4$	4.4×10^{1}		Wang et al. (2017)	Q	80, 239
BCIULZBFFUODJR-UHFFFAOYSA-N	4.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:NC101OOH	6.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_6$	3.4×10^{5}		Wang et al. (2017)	Q	80, 239
AQVSRLWLNUXIOL-UHFFFAOYSA-N	5.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NC102OOH	1.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_7$	4.0×10^{8}		Wang et al. (2017)	Q	80, 239
ZNOCONLMTXMLFU-UHFFFAOYSA-N	4.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C1011PAN	1.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{17}NO_6$	2.2×10^{3}		Wang et al. (2017)	Q	80, 239
PRDFPHJPDVZXHH-UHFFFAOYSA-N	2.9		Wang et al. (2017)	Q	80, 240
MCM:C131NO3	2.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{21}NO_5$	3.5×10^{4}		Wang et al. (2017)	Q	80, 239
HFRDBZMTZNPZMV-UHFFFAOYSA-N	2.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C131PAN	7.3×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{21}NO_7$	2.0×10^{6}		Wang et al. (2017)	Q	80, 239
YHMAABVAIQVHRP-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C141NO3	5.9		Wang et al. (2017)	Q	80, 238
$C_{14}H_{23}NO_4$	3.3×10^{1}		Wang et al. (2017)	Q	80, 239
JPXQKVXALDMDKF-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NBCKOOH	4.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{23}NO_6$	4.4×10^{5}		Wang et al. (2017)	Q	80, 239
IMGMBHKHHVQTQK-UHFFFAOYSA-N	1.5×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C141PAN	1.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{23}NO_6$	1.8×10^{3}		Wang et al. (2017)	Q	80, 239
PGNAVHCNSKAOHZ-UHFFFAOYSA-N	2.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C4PAN10	5.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_8$	1.9×10^{7}		Wang et al. (2017)	Q	80, 239
JOAGXXIRMSWAAZ-UHFFFAOYSA-N	2.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C4PAN6	8.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_7$	5.4×10^{5}		Wang et al. (2017)	Q	80, 239
QRAIBPAZBCTEOB-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:CO3C4NO3OH	8.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_5$	3.2×10^{4}		Wang et al. (2017)	Q	80, 239
HZFDSYFRCPAXEA-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:HMVKANO3	1.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_5$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
UFDPWCOBIOWDKA-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	80, 240
MCM:HMVKNO3	3.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	3.5×10^{7}		Wang et al. (2017)	Q	80, 239
NCLLRWDJHCXXDR-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HNBIACET	5.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_6$	1.4×10^{6}		Wang et al. (2017)	Q	80, 239
HPGBXXMJBUDRLY-UHFFFAOYSA-N	4.7		Wang et al. (2017)	Q	80, 240
MCM:HNMVKOH	1.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	6.8×10^{6}		Wang et al. (2017)	Q	80, 239
KPZZNRQGHDTQNJ-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HNMVKOOH	1.8×10^{9}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_7$	2.4×10^{7}		Wang et al. (2017)	Q	80, 239
CTKAFSDGNPEZFZ-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:MVKNO3	2.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_5$	2.0×10^{4}		Wang et al. (2017)	Q	80, 239
SCJOQBCZNBCTOQ-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MVKOHANO3	6.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	5.5×10^{5}		Wang et al. (2017)	Q	80, 239
DMSMZXCVKMBQGA-UHFFFAOYSA-N	1.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C4MCONO3OH	4.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	1.5×10^{4}		Wang et al. (2017)	Q	80, 239
VRAOJUVNSLNISW-UHFFFAOYSA-N	1.5×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:C517NO3	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	1.9×10^{5}		Wang et al. (2017)	Q	80, 239
DLLRFAPEEPVGBN-UHFFFAOYSA-N	7.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C51NO3	1.9×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	2.3×10^{5}		Wang et al. (2017)	Q	80, 239
OMTWKQRBUUWUQB-UHFFFAOYSA-N	2.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C5NO3CO4OH	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	3.1×10^{5}		Wang et al. (2017)	Q	80, 239
GEKIHWHZVPPEBT-UHFFFAOYSA-N	9.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CO2OH3MPAN	4.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_7$	1.6×10^{5}		Wang et al. (2017)	Q	80, 239
KOFNDQLSBTYFBZ-UHFFFAOYSA-N	6.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:CO3H4PAN	6.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_7$	2.8×10^{5}		Wang et al. (2017)	Q	80, 239
KVXLZPRANFUVNJ-UHFFFAOYSA-N	1.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:H1C23C4PAN	1.9×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_5NO_8$	7.4×10^{7}		Wang et al. (2017)	Q	80, 239
ZNIKVNWPMOTSJK-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	80, 240
MCM:H3C2C4PAN	2.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_7$	2.2×10^{6}		Wang et al. (2017)	Q	80, 239
UDPFGHOTTZCMEQ-UHFFFAOYSA-N	4.1		Wang et al. (2017)	Q	80, 240
MCM:HMVKBPAN	5.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_7$	3.6×10^{6}		Wang et al. (2017)	Q	80, 239
VVIGYLNPENSKGX-UHFFFAOYSA-N	3.0		Wang et al. (2017)	Q	80, 240
MCM:INANCO	1.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_8$	1.2×10^{6}		Wang et al. (2017)	Q	80, 239
IESHUNGXVKLDSS-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	80, 240
MCM:INB1CO	1.7×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	1.8×10^{7}		Wang et al. (2017)	Q	80, 239
ASROEBVFUUHBLI-UHFFFAOYSA-N	2.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:INCCO	3.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	2.9×10^{5}		Wang et al. (2017)	Q	80, 239
HXWBEXHMXOXGKY-UHFFFAOYSA-N	3.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C4COMOHPAN	2.8×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_8$	9.3×10^{6}		Wang et al. (2017)	Q	80, 239
KHOZKKAVCHSHMN-UHFFFAOYSA-N	3.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C4MOHOPAN	6.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_7$	1.9×10^{5}		Wang et al. (2017)	Q	80, 239
LVRCIQOIMYLYHB-UHFFFAOYSA-N	3.8×10^{-2}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C517PAN	4.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_7$	9.1×10^{6}		Wang et al. (2017)	Q	80, 239
BRUHFHISVNPPNB-UHFFFAOYSA-N	4.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C519PAN	4.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_7$	9.6×10^{6}		Wang et al. (2017)	Q	80, 239
QFUOUYQJXYVTOO-UHFFFAOYSA-N	3.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C5O45OHPAN	5.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_7$	1.7×10^{5}		Wang et al. (2017)	Q	80, 239
VCYALMFEDUSLKE-UHFFFAOYSA-N	5.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C610NO3	1.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	1.5×10^{5}		Wang et al. (2017)	Q	80, 239
KOUUCDJHLKRSEQ-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C614NO3	1.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_6$	8.9×10^{6}		Wang et al. (2017)	Q	80, 239
QPXWFZAVXNBNFW-UHFFFAOYSA-N	2.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C61NO3	1.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	1.4×10^{5}		Wang et al. (2017)	Q	80, 239
SYDWDJOZRNVKSU-UHFFFAOYSA-N	6.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C63NO3	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	9.8×10^{4}		Wang et al. (2017)	Q	80, 239
RHTCZESJRHZQFA-UHFFFAOYSA-N	3.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C64NO3	1.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	8.3×10^{4}		Wang et al. (2017)	Q	80, 239
IYYWGRLOLOMZAZ-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C6CONO34OH	1.8×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	1.6×10^{4}		Wang et al. (2017)	Q	80, 239
OLTUAQAPCXKDOJ-UHFFFAOYSA-N	2.7		Wang et al. (2017)	Q	80, 240
MCM:C6NO3CO4OH	1.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	1.8×10^{5}		Wang et al. (2017)	Q	80, 239
WWUUDQUMERSNEM-UHFFFAOYSA-N	4.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C6NO3CO5OH	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	8.1×10^{4}		Wang et al. (2017)	Q	80, 239
IZBQRALUURUKJG-UHFFFAOYSA-N	1.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C6PAN9	1.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_7$	5.1×10^{5}		Wang et al. (2017)	Q	80, 239
NJFFIXOWLQJQIZ-UHFFFAOYSA-N	6.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:MIBKAOHNO3	1.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	6.3×10^{4}		Wang et al. (2017)	Q	80, 239
YCHDRSSXCQCYSO-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C61CPAN	3.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_8$	1.2×10^{7}		Wang et al. (2017)	Q	80, 239
FWCVDVIZOKXUGJ-UHFFFAOYSA-N	1.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C62CPAN	3.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_8$	1.3×10^{7}		Wang et al. (2017)	Q	80, 239
LHOMRHYSYFWOPZ-UHFFFAOYSA-N	7.4×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C712NO3	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{13}NO_5$	5.4×10^{4}		Wang et al. (2017)	Q	80, 239
RPPGGLBPWJPSSV-UHFFFAOYSA-N	7.1		Wang et al. (2017)	Q	80, 240
MCM:C719NO3	1.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{11}NO_6$	4.8×10^{9}		Wang et al. (2017)	Q	80, 239
IXGSPJJVHFTXPK-UHFFFAOYSA-N	2.8×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C72NO3	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{13}NO_5$	6.5×10^{4}		Wang et al. (2017)	Q	80, 239
MWIGFUUCEWIWBB-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C77NO3	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_{13}NO_5$	5.0×10^{4}		Wang et al. (2017)	Q	80, 239
KZCKPUAVFWISTB-UHFFFAOYSA-N	7.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:H3C25C6PAN	1.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_8$	6.8×10^{8}		Wang et al. (2017)	Q	80, 239
GUUOCMMOMFUPSI-UHFFFAOYSA-N	1.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C6MOHCOPAN	9.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_8$	1.1×10^{9}		Wang et al. (2017)	Q	80, 239
PDGRPGJWHYLYKK-UHFFFAOYSA-N	6.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C7CO2OHPAN	9.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_8$	1.1×10^{9}		Wang et al. (2017)	Q	80, 239
MICPXOSCTLYWLE-UHFFFAOYSA-N	4.9×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C829NO3	4.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{13}NO_6$	1.3×10^{6}		Wang et al. (2017)	Q	80, 239
CDMYSTRAPZWSHD-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C82NO3	1.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_8H_{15}NO_5$	4.1×10^{4}		Wang et al. (2017)	Q	80, 239
HUKHBWOLGKLCRF-UHFFFAOYSA-N	7.4		Wang et al. (2017)	Q	80, 240
MCM:C6EO2OHPAN	7.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_8$	6.9×10^{8}		Wang et al. (2017)	Q	80, 239
YGQCKHJQVYPZEV-UHFFFAOYSA-N	3.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C7MJPPAN	7.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_8$	6.5×10^{8}		Wang et al. (2017)	Q	80, 239
XJDHGIQDEMCTOX-UHFFFAOYSA-N	8.9×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C7MOHCOPAN	5.5×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_8$	1.7×10^{9}		Wang et al. (2017)	Q	80, 239
SORJSZWEJQTGJA-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	80, 240
MCM:C927NO3	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{15}NO_5$	1.1×10^{5}		Wang et al. (2017)	Q	80, 239
RKOGSSYMWVPWJW-UHFFFAOYSA-N	2.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C93NO3	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{17}NO_5$	3.4×10^{4}		Wang et al. (2017)	Q	80, 239
OEEOAFFOONSSLD-UHFFFAOYSA-N	5.1		Wang et al. (2017)	Q	80, 240
MCM:C98NO3	4.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{15}NO_6$	5.6×10^{6}		Wang et al. (2017)	Q	80, 239
PQCIVFJRBSNULM-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:LMKANO3	2.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{15}NO_5$	2.2×10^{5}		Wang et al. (2017)	Q	80, 239
OCTKYXAOGSBZDD-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:LMKBNO3	2.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{15}NO_5$	2.6×10^{5}		Wang et al. (2017)	Q	80, 239
MVWAQQXSBOJSHS-UHFFFAOYSA-N	2.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C103NO3	8.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{19}NO_5$	3.0×10^{4}		Wang et al. (2017)	Q	80, 239
NTZGBOUJHFKYIP-UHFFFAOYSA-N	4.8		Wang et al. (2017)	Q	80, 240
MCM:C920PAN	3.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_7$	5.9×10^{5}		Wang et al. (2017)	Q	80, 239
JPFVAVYDZBUWDH-UHFFFAOYSA-N	1.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C113NO3	7.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{21}NO_5$	2.8×10^{4}		Wang et al. (2017)	Q	80, 239
XIMKJTRLGBXFHP-UHFFFAOYSA-N	9.3		Wang et al. (2017)	Q	80, 240
MCM:C123NO3	6.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{23}NO_5$	2.5×10^{4}		Wang et al. (2017)	Q	80, 239
MVMJPHZGIRWSLB-UHFFFAOYSA-N	3.4		Wang et al. (2017)	Q	80, 240
MCM:C133NO3	1.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{21}NO_7$	5.1×10^{8}		Wang et al. (2017)	Q	80, 239
ODJJFBKGWDLDSF-UHFFFAOYSA-N	1.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:BCKANO3	2.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{23}NO_5$	6.0×10^{5}		Wang et al. (2017)	Q	80, 239
YULYIMMPXZFYHU-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:BCKBNO3	2.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{23}NO_5$	1.0×10^{6}		Wang et al. (2017)	Q	80, 239
VHSFPWDPGIOBJY-UHFFFAOYSA-N	1.9×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C142NO3	1.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{23}NO_5$	1.9×10^{5}		Wang et al. (2017)	Q	80, 239
AZGAJOUTVTYWPD-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C143NO3	3.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{23}NO_6$	5.0×10^{7}		Wang et al. (2017)	Q	80, 239
NNHMCYUMVAAOGX-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:NMGLYOX	6.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_3NO_5$	4.1×10^{3}		Wang et al. (2017)	Q	80, 239
OPXOPVKLHYDIMX-UHFFFAOYSA-N	3.4×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C312COPAN	2.2×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_3NO_7$	2.8×10^{5}		Wang et al. (2017)	Q	80, 239
RRBQALAYWSLXKO-UHFFFAOYSA-N	3.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C4CONO3CO	6.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_5$	8.3×10^{3}		Wang et al. (2017)	Q	80, 239
RXLGSPGPVVHCFU-UHFFFAOYSA-N	2.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:NCO23CHO	3.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_3NO_6$	9.8×10^{5}		Wang et al. (2017)	Q	80, 239
VZDGBDWMYVQZKU-UHFFFAOYSA-N	1.1×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C4CO2DBPAN	6.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_3NO_7$	2.5×10^{6}		Wang et al. (2017)	Q	80, 239
BTFAHSUMXINULH-UHFFFAOYSA-N	4.9×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:C4M22CONO3	3.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_5$	1.6×10^{3}		Wang et al. (2017)	Q	80, 239
FQGALMJVSZOCNN-UHFFFAOYSA-N	5.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C512NO3	4.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_5$	2.0×10^{4}		Wang et al. (2017)	Q	80, 239
OAONLGDTCNNTSO-UHFFFAOYSA-N	8.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CHOC3COPAN	1.7×10^{6}		Wang et al. (2017)	Q	80, 238
$C_5H_5NO_7$	3.8×10^{5}		Wang et al. (2017)	Q	80, 239
MEMYBUIJIAQZMF-UHFFFAOYSA-N	9.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:INANCOCHO	4.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_6N_2O_8$	2.6×10^{5}		Wang et al. (2017)	Q	80, 239
ALBXLNVOOLMBSV-UHFFFAOYSA-N	1.5×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C511PAN	1.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_7$	8.9×10^{5}		Wang et al. (2017)	Q	80, 239
ADLPISUKTIUEBV-UHFFFAOYSA-N	8.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C5124COPAN	1.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_5NO_8$	1.3×10^{7}		Wang et al. (2017)	Q	80, 239
DHCQJQARWDKNBK-UHFFFAOYSA-N	2.1×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C512PAN	1.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_7$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
OLSCQSOEJBIJSE-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C515PAN	1.0×10^{9}		Wang et al. (2017)	Q	80, 238
$C_6H_5NO_8$	3.0×10^{7}		Wang et al. (2017)	Q	80, 239
QIUJGMPSWRWOQB-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	80, 240
MCM:C5CO2DBPAN	4.7×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_5NO_7$	2.1×10^{6}		Wang et al. (2017)	Q	80, 239
LCULQJDFGZNNJC-UHFFFAOYSA-N	2.8×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:C5DBCO2PAN	4.7×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_5NO_7$	2.1×10^{6}		Wang et al. (2017)	Q	80, 239
QMYFWHUFARKUQS-UHFFFAOYSA-N	3.6×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:C626NO3	4.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_5$	5.1×10^{4}		Wang et al. (2017)	Q	80, 239
OCVBVQJPDKPHST-UHFFFAOYSA-N	1.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C6COCHOPAN	1.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_7$	2.6×10^{6}		Wang et al. (2017)	Q	80, 239
YGLXJUWEIHLTAS-UHFFFAOYSA-N	8.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C4DBM2PAN	3.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_7NO_7$	3.0×10^{6}		Wang et al. (2017)	Q	80, 239
LSIPSXVETZQMNK-UHFFFAOYSA-N	5.4×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:C617PAN	8.7×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_7$	9.6×10^{4}		Wang et al. (2017)	Q	80, 239
PZZHENCPCXAAMZ-UHFFFAOYSA-N	6.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C618PAN	8.7×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_7$	7.8×10^{4}		Wang et al. (2017)	Q	80, 239
TUYXNXVHKYYCNT-UHFFFAOYSA-N	5.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C626PAN	1.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_7$	2.0×10^{6}		Wang et al. (2017)	Q	80, 239
JTOZIQOFBRFINW-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C717NO3	2.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_6$	8.0×10^{5}		Wang et al. (2017)	Q	80, 239
YBNFZHXBUOLIKA-UHFFFAOYSA-N	2.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C718NO3	2.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{11}NO_5$	3.5×10^{3}		Wang et al. (2017)	Q	80, 239
WMUFPKACUPNARK-UHFFFAOYSA-N	3.8		Wang et al. (2017)	Q	80, 240
MCM:C731NO3	3.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_7H_{11}NO_5$	4.5×10^{4}		Wang et al. (2017)	Q	80, 239
WJSMASANGLXUCK-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C7CO2DBPAN	3.7×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_7NO_7$	1.2×10^{6}		Wang et al. (2017)	Q	80, 239
FJSOTAPJABBDID-UHFFFAOYSA-N	2.6×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:NC61CO3H	1.7×10^{12}		Wang et al. (2017)	Q	80, 238
$C_7H_7NO_9$	6.2×10^{8}		Wang et al. (2017)	Q	80, 239
RCADYDMYBSYTRH-UHFFFAOYSA-N	6.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NC6PAN1	6.6×10^{10}		Wang et al. (2017)	Q	80, 238
$C_7H_6N_2O_{11}$	2.4×10^{8}		Wang et al. (2017)	Q	80, 239
LNWBMFOWVOYBBT-UHFFFAOYSA-N	2.0×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:C4DBMEPAN	2.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_7$	1.6×10^{6}		Wang et al. (2017)	Q	80, 239
JDCDQJWNYIFIQT-UHFFFAOYSA-N	3.5×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:C718PAN	7.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_7$	2.3×10^{5}		Wang et al. (2017)	Q	80, 239
IZJQRCOOVGKQNV-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	80, 240
MCM:C731PAN	1.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_7$	1.7×10^{6}		Wang et al. (2017)	Q	80, 239
BCDBCVPVNWUZKV-UHFFFAOYSA-N	4.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C8CO2DBPAN	3.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_7$	6.9×10^{5}		Wang et al. (2017)	Q	80, 239
IPAWZRQBQOFPJA-UHFFFAOYSA-N	1.4×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:C8DBCO2PAN	3.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_7$	8.0×10^{5}		Wang et al. (2017)	Q	80, 239
ZDCAPCKMKJMPHV-UHFFFAOYSA-N	1.0×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:C87PAN	6.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_8$	2.8×10^{7}		Wang et al. (2017)	Q	80, 239
KZPDHKTVZKNFJF-UHFFFAOYSA-N	7.8		Wang et al. (2017)	Q	80, 240
MCM:C915NO3	5.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_5$	3.2×10^{4}		Wang et al. (2017)	Q	80, 239
CFOCUCLSGKHNEG-UHFFFAOYSA-N	5.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C916NO3	1.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_6$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
VOXWFVUGDBUBCW-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C918NO3	5.9×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_5$	5.6×10^{3}		Wang et al. (2017)	Q	80, 239
AMOFMDWAGAYJCS-UHFFFAOYSA-N	5.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C919NO3	1.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_6$	1.0×10^{6}		Wang et al. (2017)	Q	80, 239
DCZHYWWXGROBKB-UHFFFAOYSA-N	8.0×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C930NO3	1.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_6$	5.6×10^{5}		Wang et al. (2017)	Q	80, 239
DDSHYSHFPVKRPI-UHFFFAOYSA-N	1.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C1010NO3	3.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_5$	8.5×10^{3}		Wang et al. (2017)	Q	80, 239
GVXIDPZAUKXFPR-UHFFFAOYSA-N	4.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C1012NO3	1.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_5$	8.1×10^{3}		Wang et al. (2017)	Q	80, 239
XKIZNDJDYSDNBL-UHFFFAOYSA-N	2.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C106NO3	1.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_6$	7.3×10^{5}		Wang et al. (2017)	Q	80, 239
DSEFLMWIAZKUSJ-UHFFFAOYSA-N	4.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C108NO3	1.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_6$	2.2×10^{5}		Wang et al. (2017)	Q	80, 239
MVSLQVXNIWKHQS-UHFFFAOYSA-N	6.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NLIMALOOH	1.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_7$	3.4×10^{7}		Wang et al. (2017)	Q	80, 239
NTLQQKIUYMIZPN-UHFFFAOYSA-N	2.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PINALNO3	3.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_5$	1.6×10^{4}		Wang et al. (2017)	Q	80, 239
FNTMCASBPWQXGD-UHFFFAOYSA-N	3.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C116NO3	4.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{17}NO_5$	3.7×10^{4}		Wang et al. (2017)	Q	80, 239
AWSJYNTZBDMUKU-UHFFFAOYSA-N	3.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C116PAN	1.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{17}NO_7$	2.3×10^{6}		Wang et al. (2017)	Q	80, 239
IHJLCJPVFFZKMO-UHFFFAOYSA-N	1.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C1210NO3	3.4×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{19}NO_5$	4.1×10^{4}		Wang et al. (2017)	Q	80, 239
IJHSXQWUSMROBJ-UHFFFAOYSA-N	7.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C1210PAN	1.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{19}NO_7$	2.0×10^{6}		Wang et al. (2017)	Q	80, 239
PWZZEUPXUFAYML-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NBCALOOH	1.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{25}NO_7$	8.5×10^{7}		Wang et al. (2017)	Q	80, 239
TUYLAULXHOKFAG-UHFFFAOYSA-N	7.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:H3NCO2CHO	1.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_6$	3.6×10^{6}		Wang et al. (2017)	Q	80, 239
VCTGKRYJUDQYFK-UHFFFAOYSA-N	3.4		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:HMVKNGLYOX	2.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_6$	9.3×10^{5}		Wang et al. (2017)	Q	80, 239
VDDXFUNTPSDTJP-UHFFFAOYSA-N	9.3		Wang et al. (2017)	Q	80, 240
MCM:INB1GLYOX	1.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_6$	3.1×10^{5}		Wang et al. (2017)	Q	80, 239
NAZCWKUVRXJZPX-UHFFFAOYSA-N	3.0		Wang et al. (2017)	Q	80, 240
MCM:INCGLYOX	6.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_6$	4.8×10^{5}		Wang et al. (2017)	Q	80, 239
DGCXGPGOOTUCCO-UHFFFAOYSA-N	3.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C5CO2OHPAN	2.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_5NO_8$	1.7×10^{9}		Wang et al. (2017)	Q	80, 239
MLSWEUDOYVEBFO-UHFFFAOYSA-N	7.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C6CO2OHPAN	1.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_7NO_8$	1.4×10^{9}		Wang et al. (2017)	Q	80, 239
GITGCCFTTYJWBT-UHFFFAOYSA-N	4.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C5M2OHOPAN	9.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_8$	2.0×10^{9}		Wang et al. (2017)	Q	80, 239
MJYXUWCXTAYXTN-UHFFFAOYSA-N	7.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C7OHCO2PAN	1.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_8$	8.3×10^{8}		Wang et al. (2017)	Q	80, 239
WKRTWLVIFYOGIB-UHFFFAOYSA-N	1.9×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C5MEJPAN	7.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_8$	1.2×10^{9}		Wang et al. (2017)	Q	80, 239
KTOTUVLJTIGMKC-UHFFFAOYSA-N	5.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C8CO2OHPAN	1.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_8$	6.6×10^{8}		Wang et al. (2017)	Q	80, 239
UEMVFSSSLHUULZ-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:C8OHCO2PAN	9.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_8$	5.8×10^{8}		Wang et al. (2017)	Q	80, 239
GUTUSTBTBKWXHL-UHFFFAOYSA-N	1.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:LIMALNO3	1.3×10^{8}	23000	Wieser et al. (2023)	Q	437
$C_{10}H_{17}NO_6$	5.3×10^{6}		Wang et al. (2017)	Q	80, 238
FDBNDHKWTKEDSC-UHFFFAOYSA-N	3.2×10^{7}		Wang et al. (2017)	Q	80, 239
	3.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NLIMALOH	5.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_6$	4.8×10^{7}		Wang et al. (2017)	Q	80, 239
NNOYMJCUDKQQLW-UHFFFAOYSA-N	2.7×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C117NO3	7.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{17}NO_6$	1.0×10^{7}		Wang et al. (2017)	Q	80, 239
VRGCJRKSASUXOA-UHFFFAOYSA-N	2.8×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C118NO3	2.2×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{17}NO_7$	6.5×10^{8}		Wang et al. (2017)	Q	80, 239
RHEKUCZWBZRVBN-UHFFFAOYSA-N	3.2×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C1215NO3	1.8×10^{9}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{19}NO_7$	1.1×10^{10}		Wang et al. (2017)	Q	80, 239
HIFZNEWSKKHKQF-UHFFFAOYSA-N	2.6×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C128NO3	6.5×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{19}NO_6$	5.3×10^{7}		Wang et al. (2017)	Q	80, 239
XVMHBNQZULJJQH-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C1312NO3	5.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{21}NO_6$	1.4×10^{8}		Wang et al. (2017)	Q	80, 239
LCWPKTPKZZROTF-UHFFFAOYSA-N	3.2×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:BCALNO3	4.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{25}NO_6$	5.3×10^{7}		Wang et al. (2017)	Q	80, 239
KJHBLMRUHUAACD-UHFFFAOYSA-N	8.7×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:NBCALOH	4.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{25}NO_6$	6.2×10^{7}		Wang et al. (2017)	Q	80, 239
YUOPYTDNMDNILJ-UHFFFAOYSA-N	6.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NO3CH2CO2H	1.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_2H_3NO_5$	8.3×10^{4}		Wang et al. (2017)	Q	80, 239
VHOVOPOBBVJMEP-UHFFFAOYSA-N	1.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:PRNO3CO2H	1.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_5NO_5$	9.1×10^{3}		Wang et al. (2017)	Q	80, 239
DVOPCQDTEPKYKW-UHFFFAOYSA-N	7.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MPRNO3CO2H	8.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_5$	3.3×10^{3}		Wang et al. (2017)	Q	80, 239
MSBKTJKUKRRTOZ-UHFFFAOYSA-N	3.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NC3CO2H	4.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_5$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
IYBHCPMQXJSPPT-UHFFFAOYSA-N	4.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C3MNO3CO2H	1.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	2.2×10^{3}		Wang et al. (2017)	Q	80, 239
CCKPHGGNTPAJHG-UHFFFAOYSA-N	2.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C43NO3CO2H	6.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
PAJLSJNKCRUQAA-UHFFFAOYSA-N	2.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C4NO3CO2H	9.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	2.0×10^{3}		Wang et al. (2017)	Q	80, 239
LHOHBJOUNVJDSQ-UHFFFAOYSA-N	2.7×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NC4CO2H	3.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_5$	9.6×10^{3}		Wang et al. (2017)	Q	80, 239
ZKTRJZJYWMAEEY-UHFFFAOYSA-N	7.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C65NO3CO2H	8.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	1.1×10^{3}		Wang et al. (2017)	Q	80, 239
JEDGAPUZBUOYQF-UHFFFAOYSA-N	2.5×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C721PAN	5.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_7$	4.3×10^{6}		Wang et al. (2017)	Q	80, 239
OMUZIQDFMVGNTC-UHFFFAOYSA-N	6.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C811NO3	1.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{13}NO_5$	1.7×10^{4}		Wang et al. (2017)	Q	80, 239
WYXUZPCNBFFDRO-UHFFFAOYSA-N	5.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C823NO3	1.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_{13}NO_5$	2.2×10^{4}		Wang et al. (2017)	Q	80, 239
QAJOXMTYFQHFPC-UHFFFAOYSA-N	4.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C811PAN	4.7×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	3.1×10^{6}		Wang et al. (2017)	Q	80, 239
BOYXRVFXWMBNIT-UHFFFAOYSA-N	3.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C823PAN	4.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	1.3×10^{6}		Wang et al. (2017)	Q	80, 239
GRHNTSHNCZZYLE-UHFFFAOYSA-N	2.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C137NO3	1.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{21}NO_5$	3.8×10^{4}		Wang et al. (2017)	Q	80, 239
CQGOUXQAADNZJX-UHFFFAOYSA-N	2.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C137PAN	4.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{14}H_{21}NO_7$	2.5×10^{6}		Wang et al. (2017)	Q	80, 239
KJDMPVAHMJBAAO-UHFFFAOYSA-N	9.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MACRNBCO2H	1.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	2.6×10^{6}		Wang et al. (2017)	Q	80, 239
WQOIEXBGIWRREH-UHFFFAOYSA-N	3.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:MACRNCO2H	3.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	8.5×10^{5}		Wang et al. (2017)	Q	80, 239
GPIMHHNLFCYMAO-UHFFFAOYSA-N	5.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C57NO3CO2H	2.8×10^{9}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_7$	1.6×10^{8}		Wang et al. (2017)	Q	80, 239
VNPCVOYEGJTTSH-UHFFFAOYSA-N	2.3×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C58NO3CO2H	4.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_7$	5.0×10^{8}		Wang et al. (2017)	Q	80, 239
QOEJXJLKIMUJIJ-UHFFFAOYSA-N	1.0×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:INAHCO2H	1.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_7$	1.7×10^{9}		Wang et al. (2017)	Q	80, 239
KDGUUBLLRPAORR-UHFFFAOYSA-N	5.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:INAHPCO2H	2.3×10^{11}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_8$	2.5×10^{9}		Wang et al. (2017)	Q	80, 239
CHIYBIMSWIBBRD-UHFFFAOYSA-N	1.6×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:INANCO2H	3.6×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_9$	3.6×10^{7}		Wang et al. (2017)	Q	80, 239
QEPBKMYMBRWSSY-UHFFFAOYSA-N	4.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:INB1HPCO2H	2.0×10^{11}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_8$	2.9×10^{8}		Wang et al. (2017)	Q	80, 239
XWZUZABUMCCUCE-UHFFFAOYSA-N	1.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:INB1NACO2H	3.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_9$	5.1×10^{6}		Wang et al. (2017)	Q	80, 239
FONBWUWRCYYCPB-UHFFFAOYSA-N	1.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:INB1NBCO2H	3.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_9$	7.3×10^{6}		Wang et al. (2017)	Q	80, 239
YGORAHXKOXOIMV-UHFFFAOYSA-N	2.9×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:INCNCO2H	3.6×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_8N_2O_9$	2.0×10^{7}		Wang et al. (2017)	Q	80, 239
LXTUVHDUSAOJOD-UHFFFAOYSA-N	1.6×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C139NO3	6.6×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{21}NO_7$	1.9×10^{8}		Wang et al. (2017)	Q	80, 239
UFNZJLDHNJULFY-UHFFFAOYSA-N	6.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:CONM2CO2H	7.4×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_6$	8.3×10^{4}		Wang et al. (2017)	Q	80, 239
LTGNKSWVEYSUMY-UHFFFAOYSA-N	3.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:MMALNACO2H	1.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_7$	4.5×10^{7}		Wang et al. (2017)	Q	80, 239
REHIBMNEJUPYOU-UHFFFAOYSA-N	6.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:MMALNBCO2H	1.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_7$	1.9×10^{7}		Wang et al. (2017)	Q	80, 239
RAMGTVAYJVLLRG-UHFFFAOYSA-N	5.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:INANCOCO2H	5.8×10^{7}		Wang et al. (2017)	Q	80, 238
$C_5H_6N_2O_9$	8.5×10^{6}		Wang et al. (2017)	Q	80, 239
XEVMEFHPLZUFAK-UHFFFAOYSA-N	6.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C732NO3	4.7×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_{11}NO_6$	3.7×10^{7}		Wang et al. (2017)	Q	80, 239
SXYZBZXZNRYERD-UHFFFAOYSA-N	4.9×10^{4}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C732PAN	1.7×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_8$	1.7×10^{9}		Wang et al. (2017)	Q	80, 239
WNUKRJOERGBBRT-UHFFFAOYSA-N	2.0×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C1211NO3	5.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{19}NO_6$	5.6×10^{7}		Wang et al. (2017)	Q	80, 239
DQVGSELEPUBBSS-UHFFFAOYSA-N	2.9×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C1211PAN	1.6×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{19}NO_8$	4.2×10^{9}		Wang et al. (2017)	Q	80, 239
IROGWMVYBREROI-UHFFFAOYSA-N	9.8×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:C813NO3	8.5×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{13}NO_7$	4.6×10^{7}		Wang et al. (2017)	Q	80, 239
GYZVFQOTJWTWBE-UHFFFAOYSA-N	7.1×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C1212NO3	2.3×10^{10}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{19}NO_8$	1.3×10^{10}		Wang et al. (2017)	Q	80, 239
NTNWJSADTNTFHH-UHFFFAOYSA-N	3.0×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C1213NO3	2.6×10^{11}		Wang et al. (2017)	Q	80, 238
$C_{12}H_{19}NO_8$	1.8×10^{11}		Wang et al. (2017)	Q	80, 239
FRAJAIDKFGOMCR-UHFFFAOYSA-N	3.6×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:C1310NO3	7.3×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{13}H_{21}NO_7$	1.4×10^{10}		Wang et al. (2017)	Q	80, 239
YNRLOWIUKIUEHR-UHFFFAOYSA-N	3.0×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:C151NO3	7.4×10^{8}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{25}NO_7$	2.6×10^{10}		Wang et al. (2017)	Q	80, 239
BHPYCCPMXIBJRO-UHFFFAOYSA-N	8.7×10^{8}		Wang et al. (2017)	Q	80, 240
MCM:CHOOCH2NO3	5.8		Wang et al. (2017)	Q	80, 238
$C_2H_3NO_5$	1.4×10^{1}		Wang et al. (2017)	Q	80, 239
OAQKKIQKQLJUJT-UHFFFAOYSA-N	2.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:CHOOMPAN	1.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_3NO_7$	1.6×10^{3}		Wang et al. (2017)	Q	80, 239
XZTQWYQUABOKPG-UHFFFAOYSA-N	1.9×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:ETHFORMNO3	5.4		Wang et al. (2017)	Q	80, 238
$C_3H_5NO_5$	3.5		Wang et al. (2017)	Q	80, 239
DOXRBPLNMOIQGP-UHFFFAOYSA-N	1.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:METACETNO3	3.9		Wang et al. (2017)	Q	80, 238
$C_3H_5NO_5$	1.9×10^{1}		Wang et al. (2017)	Q	80, 239
HRSAJZJMUADCNM-UHFFFAOYSA-N	3.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:MMCFNO3	1.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_3NO_7$	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
IFMSYUVMGRDEMV-UHFFFAOYSA-N	7.3×10^{-2}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:ACEC2H4NO3	3.2		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_5$	2.5×10^{1}		Wang et al. (2017)	Q	80, 239
QOXSFWPQUXLCPI-UHFFFAOYSA-N	9.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:ACETMEPAN	1.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_7$	1.8×10^{3}		Wang et al. (2017)	Q	80, 239
QMSGSFOWAUFKPL-UHFFFAOYSA-N	1.7×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:COO2C3PAN	1.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_7$	1.6×10^{3}		Wang et al. (2017)	Q	80, 239
YQMLKDOXYNVTNM-UHFFFAOYSA-N	7.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:ETACETNO3	3.6		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_5$	3.5		Wang et al. (2017)	Q	80, 239
KORDSAOMZNGUAL-UHFFFAOYSA-N	2.4×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:IPRFORMNO3	3.0		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_5$	6.9×10^{-1}		Wang et al. (2017)	Q	80, 239
DZSICYNSKFSRMV-UHFFFAOYSA-N	1.8×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:NBZFUOOH	2.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_4H_5NO_7$	3.0×10^{6}		Wang et al. (2017)	Q	80, 239
TXWHLSUKLWEERR-UHFFFAOYSA-N	2.5×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:ACCOMEPAN	5.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_5NO_8$	5.1×10^{5}		Wang et al. (2017)	Q	80, 239
ZQOVYYMCAFZVPL-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	80, 240
MCM:ACETC2PAN	1.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_7$	2.1×10^{3}		Wang et al. (2017)	Q	80, 239
VMVPPLVFXDAZML-UHFFFAOYSA-N	6.5×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:COO2C4PAN	1.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_7$	1.7×10^{3}		Wang et al. (2017)	Q	80, 239
GBAXNZCSCJEGAE-UHFFFAOYSA-N	1.6×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:IPRACBNO3	2.8		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	8.1		Wang et al. (2017)	Q	80, 239
ZEVCPCUWRCOHCL-UHFFFAOYSA-N	3.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:IPRACBPAN	1.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_7$	3.9×10^{2}		Wang et al. (2017)	Q	80, 239
UJCZQTHKWBYHPW-UHFFFAOYSA-N	2.2×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:IPRACNO3	2.0		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	8.0×10^{-1}		Wang et al. (2017)	Q	80, 239
JAQKAPGOMZJVBI-UHFFFAOYSA-N	2.2×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:MTBEAALNO3	2.7		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	2.5		Wang et al. (2017)	Q	80, 239
NIMOOIUOXYQIIM-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MTBEAALPAN	9.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_7$	6.5×10^{1}		Wang et al. (2017)	Q	80, 239
WKTKTTPKCZOXAQ-UHFFFAOYSA-N	1.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:NPRACANO3	2.8		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	8.1		Wang et al. (2017)	Q	80, 239
FPQZKAXTSOKJRB-UHFFFAOYSA-N	3.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:NPRACBNO3	2.8		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	1.9		Wang et al. (2017)	Q	80, 239
HTKMYQNNJMTEJQ-UHFFFAOYSA-N	1.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:NPRACCNO3	2.8		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_5$	1.5×10^{1}		Wang et al. (2017)	Q	80, 239
PSJLJILPBUYXRJ-UHFFFAOYSA-N	3.1		Wang et al. (2017)	Q	80, 240
MCM:NPXYFUOOH	1.2×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_7$	8.9×10^{5}		Wang et al. (2017)	Q	80, 239
ARRSNVVNYKGUFK-UHFFFAOYSA-N	5.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NTLFUOOH	2.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_7$	2.2×10^{6}		Wang et al. (2017)	Q	80, 239
OAXQEILKHMZHNV-UHFFFAOYSA-N	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:MCOOTBNO3	1.6		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	2.9		Wang et al. (2017)	Q	80, 239
BCWPDUXSEGSVPT-UHFFFAOYSA-N	1.2×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:NBUACANO3	2.6		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	6.9		Wang et al. (2017)	Q	80, 239
GNPRUWODPALWHJ-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	80, 240
MCM:NBUACBNO3	2.6		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	5.0		Wang et al. (2017)	Q	80, 239
UFOXFUDLAIUTHC-UHFFFAOYSA-N	4.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:NBUACCNO3	2.6		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	1.4		Wang et al. (2017)	Q	80, 239
PYXJHVBEHHCABK-UHFFFAOYSA-N	1.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:NDMMALYOOH	2.2×10^{11}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_8$	9.8×10^{7}		Wang et al. (2017)	Q	80, 239
RZSLUQVSVWAZFJ-UHFFFAOYSA-N	2.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NEBFUOOH	1.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_7$	1.4×10^{6}		Wang et al. (2017)	Q	80, 239
CZSCMTWZZQSKMX-UHFFFAOYSA-N	9.8×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NMXYFUOOH	1.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_7$	4.9×10^{5}		Wang et al. (2017)	Q	80, 239
URYSYTGABCBDCM-UHFFFAOYSA-N	6.3×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NOXYFUOOH	6.8×10^{7}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_7$	3.2×10^{5}		Wang et al. (2017)	Q	80, 239
CPPAIMSHWPDUBG-UHFFFAOYSA-N	2.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:NTMB1FUOOH	1.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_7$	1.7×10^{7}		Wang et al. (2017)	Q	80, 239
WRMOSOIHGVCRMO-UHFFFAOYSA-N	2.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:PRCOOMPAN	8.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_7$	5.6×10^{2}		Wang et al. (2017)	Q	80, 239
NSDDFRROKVQLRJ-UHFFFAOYSA-N	1.4×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:SBUACANO3	1.6		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	5.3×10^{-1}		Wang et al. (2017)	Q	80, 239
FWAMAOJLVLFAOA-UHFFFAOYSA-N	1.9×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:SBUACBNO3	3.0		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_5$	4.0		Wang et al. (2017)	Q	80, 239
FVMFJLQQOIKLHP-UHFFFAOYSA-N	2.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:TBUACPAN	6.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_7$	7.3×10^{1}		Wang et al. (2017)	Q	80, 239
WTCUHXTZKDYOTB-UHFFFAOYSA-N	2.6×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:NIPBFUOOH	1.7×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{11}NO_7$	1.3×10^{6}		Wang et al. (2017)	Q	80, 239
MJSJHBOZYWKETN-UHFFFAOYSA-N	5.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NMEBFUOOH	1.0×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{11}NO_7$	3.2×10^{5}		Wang et al. (2017)	Q	80, 239
LKMBYBKEMVMSAU-UHFFFAOYSA-N	3.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NPBFUOOH	1.5×10^{8}		Wang et al. (2017)	Q	80, 238
$C_7H_{11}NO_7$	1.1×10^{6}		Wang et al. (2017)	Q	80, 239
DGKCEZHRNXTHAZ-UHFFFAOYSA-N	4.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:NTMB2FUOOH	6.3×10^{7}		Wang et al. (2017)	Q	80, 238
$C_7H_{11}NO_7$	1.8×10^{5}		Wang et al. (2017)	Q	80, 239
IRLXCLTZUJZGMJ-UHFFFAOYSA-N	2.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C1013NO3	3.1		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_5$	5.4		Wang et al. (2017)	Q	80, 239
TWKDJCLTDHUPBZ-UHFFFAOYSA-N	3.2		Wang et al. (2017)	Q	80, 240
MCM:C1013PAN	9.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{17}NO_7$	4.8×10^{2}		Wang et al. (2017)	Q	80, 239
QVQKWVAIHQGLJY-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	80, 240
MCM:C1014NO3	7.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{17}NO_6$	1.9×10^{3}		Wang et al. (2017)	Q	80, 239
OQZDTLQTCPZSBL-UHFFFAOYSA-N	7.8×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C152NO3	3.0×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{25}NO_7$	1.3×10^{7}		Wang et al. (2017)	Q	80, 239
VUWXYQDBWQFZDF-UHFFFAOYSA-N	7.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:NBZFUONE	1.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_4H_3NO_6$	4.3×10^{6}		Wang et al. (2017)	Q	80, 239
LXADUFLCRLLGHU-UHFFFAOYSA-N	8.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C23O3CPAN	7.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_5NO_8$	2.8×10^{5}		Wang et al. (2017)	Q	80, 239
BCRDXKGRUUAZSU-UHFFFAOYSA-N	3.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:ACBUONANO3	1.7×10^{3}		Wang et al. (2017)	Q	80, 238
$C_6H_9NO_6$	2.2×10^{3}		Wang et al. (2017)	Q	80, 239
PDSBHIWVTCGSAN-UHFFFAOYSA-N	9.1		Wang et al. (2017)	Q	80, 240
MCM:C23O3MCPAN	7.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_8$	6.0×10^{4}		Wang et al. (2017)	Q	80, 239
MJYWDTPJLIMPPV-UHFFFAOYSA-N	2.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:NEBFUONE	1.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_6$	2.3×10^{6}		Wang et al. (2017)	Q	80, 239
LZGWKDALCOZNIJ-UHFFFAOYSA-N	8.1		Wang et al. (2017)	Q	80, 240
MCM:C23O3ECPAN	5.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_8$	3.2×10^{4}		Wang et al. (2017)	Q	80, 239
SOMJWLUSPZTMJM-UHFFFAOYSA-N	1.5×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:NIPBFUONE	1.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_6$	2.0×10^{6}		Wang et al. (2017)	Q	80, 239
OEYHEYBMUYSQHE-UHFFFAOYSA-N	4.8		Wang et al. (2017)	Q	80, 240
MCM:NPBFUONE	1.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_6$	1.7×10^{6}		Wang et al. (2017)	Q	80, 239
WTNUMEKWPLLNDJ-UHFFFAOYSA-N	6.6		Wang et al. (2017)	Q	80, 240
MCM:CH3OCH2NO3	3.4×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_2H_5NO_4$	3.4×10^{-1}		Wang et al. (2017)	Q	80, 239
VHAYDBAVTGOZLW-UHFFFAOYSA-N	4.5×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:DMMANO3	8.1		Wang et al. (2017)	Q	80, 238
$C_3H_7NO_5$	5.5		Wang et al. (2017)	Q	80, 239
ZKGVKOFAVUIIEY-UHFFFAOYSA-N	3.0×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:DMMBNO3	9.3		Wang et al. (2017)	Q	80, 238
$C_3H_7NO_5$	1.0×10^{-1}		Wang et al. (2017)	Q	80, 239
ADJOFNYUECRONI-UHFFFAOYSA-N	1.7×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:ETOMENO3	5.8×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_3H_7NO_3$	6.6×10^{-1}		Wang et al. (2017)	Q	80, 239
ZMUPMMOTQUHRHQ-UHFFFAOYSA-N	3.9×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MEMOXYPAN	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_3H_5NO_6$	2.2×10^{2}		Wang et al. (2017)	Q	80, 239
JBHGAGLULWBGCW-UHFFFAOYSA-N	1.0×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:DIETETNO3	2.8×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_4$	4.2×10^{-2}		Wang et al. (2017)	Q	80, 239
CAMRTYJYAQGENN-UHFFFAOYSA-N	7.3×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:ETOC2NO3	2.5×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_4$	2.5		Wang et al. (2017)	Q	80, 239
GDNQXPDYGNUKII-UHFFFAOYSA-N	4.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:ETOMEPAN	9.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_4H_7NO_6$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
CCYZAMBLJVQHMC-UHFFFAOYSA-N	1.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:IPROC21NO3	2.6×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	2.0×10^{-2}		Wang et al. (2017)	Q	80, 239
YQGFTPNVRZNXAP-UHFFFAOYSA-N	8.0×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:MTBEANO3	1.5×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	2.7×10^{-2}		Wang et al. (2017)	Q	80, 239
NXHUJDLNRCHXIE-UHFFFAOYSA-N	8.3×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:MTBEBNO3	1.5×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_5H_{11}NO_4$	6.2×10^{-1}		Wang et al. (2017)	Q	80, 239
HWZCMFJGZXOLOM-UHFFFAOYSA-N	4.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:MTBEBPAN	5.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_5H_9NO_6$	1.4×10^{1}		Wang et al. (2017)	Q	80, 239
PQCDPGWYIKXNFH-UHFFFAOYSA-N	5.5×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:BOXMPAN	6.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	5.1×10^{1}		Wang et al. (2017)	Q	80, 239
CPESEOWHBGRFRT-UHFFFAOYSA-N	3.2×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:DIIPRETNO3	1.4×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	4.9×10^{-3}		Wang et al. (2017)	Q	80, 239
RYKOUPKPIPKSCM-UHFFFAOYSA-N	1.5×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:ETBEANO3	1.2×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	3.2×10^{-1}		Wang et al. (2017)	Q	80, 239
WGHLTNOFPVNDHK-UHFFFAOYSA-N	4.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:ETBEAPAN	4.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	9.1		Wang et al. (2017)	Q	80, 239
ZFJPSAIQYMAFAB-UHFFFAOYSA-N	3.6×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:ETBEBNO3	1.4×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	7.1×10^{-3}		Wang et al. (2017)	Q	80, 239
BIDDBAQEKWTVIC-UHFFFAOYSA-N	1.1×10^{-2}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:ETBECNO3	1.2×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	4.0×10^{-1}		Wang et al. (2017)	Q	80, 239
MGOGEALWXAMIEO-UHFFFAOYSA-N	5.0×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:ETBECPAN	4.8×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	2.3×10^{1}		Wang et al. (2017)	Q	80, 239
JICVHVAZXJWJCM-UHFFFAOYSA-N	2.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:IPROMC2NO3	2.0×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_4$	4.6×10^{-1}		Wang et al. (2017)	Q	80, 239
XJQWDDGHWZGMDK-UHFFFAOYSA-N	2.9×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:IPROMCPAN	8.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_6H_{11}NO_6$	2.0×10^{1}		Wang et al. (2017)	Q	80, 239
SFYHCJJQTXJNNN-UHFFFAOYSA-N	3.9×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:MO2EOLANO3	1.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_7NO_5$	5.6×10^{2}		Wang et al. (2017)	Q	80, 239
FJVLHDUAJQRZPG-UHFFFAOYSA-N	3.2		Wang et al. (2017)	Q	80, 240
MCM:MO2EOLBNO3	1.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_7NO_5$	1.3×10^{3}		Wang et al. (2017)	Q	80, 239
QPXHYMSZINTGRC-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:EOX2OLANO3	1.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_5$	3.6×10^{2}		Wang et al. (2017)	Q	80, 239
UVLBVBPSPHSYND-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	80, 240
MCM:EOX2OLBNO3	9.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_5$	3.2×10^{2}		Wang et al. (2017)	Q	80, 239
DLOZDRFLLIHYBD-UHFFFAOYSA-N	8.9		Wang et al. (2017)	Q	80, 240
MCM:H2C3OCNO3	9.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_5$	9.1×10^{2}		Wang et al. (2017)	Q	80, 239
VJBSYBJCULHXOZ-UHFFFAOYSA-N	3.0		Wang et al. (2017)	Q	80, 240
MCM:PR2OHMONO3	1.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_4H_9NO_5$	3.8×10^{2}		Wang et al. (2017)	Q	80, 239
YOBYTHKQRGEURN-UHFFFAOYSA-N	8.5×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:IEAPAN	3.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_7$	2.3×10^{5}		Wang et al. (2017)	Q	80, 239
NFJKKZSQGXUZSI-UHFFFAOYSA-N	9.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:IECPAN	3.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_5H_7NO_7$	9.1×10^{4}		Wang et al. (2017)	Q	80, 239
UMKIAKGFUATPHT-UHFFFAOYSA-N	8.9×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:BOXEOHANO3	6.2×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_5$	1.4×10^{2}		Wang et al. (2017)	Q	80, 239
NBMGDPHUZJHVTA-UHFFFAOYSA-N	3.6		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:BOXEOHBNO3	6.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_6H_{13}NO_5$	1.4×10^{2}		Wang et al. (2017)	Q	80, 239
YIIBDLSBOAJITL-UHFFFAOYSA-N	3.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:BOXPOLANO3	5.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_7H_{15}NO_5$	8.3×10^{1}		Wang et al. (2017)	Q	80, 239
QDPFCROPCZKQGS-UHFFFAOYSA-N	1.6		Wang et al. (2017)	Q	80, 240
MCM:BOXPOLBNO3	6.5×10^{2}		Wang et al. (2017)	Q	80, 238
$C_7H_{15}NO_5$	9.1×10^{1}		Wang et al. (2017)	Q	80, 239
UNWFJVCQCSAFHA-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:BCSOZNO3	1.3×10^{6}		Wang et al. (2017)	Q	80, 238
$C_{15}H_{25}NO_7$	5.3×10^{3}		Wang et al. (2017)	Q	80, 239
HGUJSQZJFHDFKY-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:EPXDLPAN	3.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_4H_3NO_7$	1.2×10^{5}		Wang et al. (2017)	Q	80, 239
VASNFLPKLUXZKF-UHFFFAOYSA-N	8.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:EPXMDLPAN	1.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_5H_5NO_7$	2.3×10^{4}		Wang et al. (2017)	Q	80, 239
KZASOTCYMWAOFE-UHFFFAOYSA-N	3.5×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:BZEMUCPAN	9.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_5NO_7$	1.0×10^{5}		Wang et al. (2017)	Q	80, 239
RFFCGVCNFANFMQ-UHFFFAOYSA-N	7.1		Wang et al. (2017)	Q	80, 240
MCM:EPXM2DLPAN	9.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_7$	6.3×10^{3}		Wang et al. (2017)	Q	80, 239
KYBHJMDXHJGYTK-UHFFFAOYSA-N	4.2×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:EPXMEDLPAN	8.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_7$	3.5×10^{3}		Wang et al. (2017)	Q	80, 239
XUUSESMFYTYXHU-UHFFFAOYSA-N	4.4×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:OXYMUCPAN	2.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_7$	7.1×10^{3}		Wang et al. (2017)	Q	80, 239
VIRSPYOLFRMIKR-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:OETLMUCPAN	2.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_7$	4.3×10^{3}		Wang et al. (2017)	Q	80, 239
PYAKBDFKVOPHPS-UHFFFAOYSA-N	2.8		Wang et al. (2017)	Q	80, 240
MCM:BZEMUCNO3	1.1×10^{8}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_7$	1.7×10^{8}		Wang et al. (2017)	Q	80, 239
UGJSRYKPNYMSMJ-UHFFFAOYSA-N	1.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:OXYMUCNO3	7.8×10^{8}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_7$	3.2×10^{7}		Wang et al. (2017)	Q	80, 239
PMXJWIAVDRSVOJ-UHFFFAOYSA-N	2.6×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:OETLMUCNO3	6.3×10^{8}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	1.9×10^{7}		Wang et al. (2017)	Q	80, 239
KUQUSIKCNRTUGT-UHFFFAOYSA-N	7.6×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:EPXKTMPAN	1.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_7$	2.6×10^{4}		Wang et al. (2017)	Q	80, 239
DBXZZDVADSLSOS-UHFFFAOYSA-N	1.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:EPXMKTPAN	1.1×10^{5}		Wang et al. (2017)	Q	80, 238
$C_6H_7NO_7$	2.6×10^{4}		Wang et al. (2017)	Q	80, 239
UTKXQAWEMGMHOV-UHFFFAOYSA-N	4.9×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:BOXPROANO3	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_7H_{13}NO_5$	3.3×10^{1}		Wang et al. (2017)	Q	80, 239
FWQXAWHLSYKKGA-UHFFFAOYSA-N	1.1		Wang et al. (2017)	Q	80, 240
MCM:EPXEKTPAN	9.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_7$	1.6×10^{4}		Wang et al. (2017)	Q	80, 239
ZMAMXAXJQIDKIS-UHFFFAOYSA-N	3.1×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:TLEMUCPAN	5.5×10^{5}		Wang et al. (2017)	Q	80, 238
$C_7H_7NO_7$	2.0×10^{5}		Wang et al. (2017)	Q	80, 239
AUCFXVOKAUAJMN-UHFFFAOYSA-N	2.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:EBZMUCPAN	4.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_7$	1.0×10^{5}		Wang et al. (2017)	Q	80, 239
IJCUBYYAOSTAFY-UHFFFAOYSA-N	9.8		Wang et al. (2017)	Q	80, 240
MCM:MXYMUCPAN	3.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_7$	4.0×10^{4}		Wang et al. (2017)	Q	80, 239
FZEVZMXGRRYMCK-UHFFFAOYSA-N	1.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:PXYMUCPAN	3.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_7$	5.9×10^{4}		Wang et al. (2017)	Q	80, 239
JEHOQLADMHJYMP-UHFFFAOYSA-N	8.1		Wang et al. (2017)	Q	80, 240
MCM:IPBZMUCPAN	4.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_7$	6.2×10^{4}		Wang et al. (2017)	Q	80, 239
JAYKUYZEOSXCLM-UHFFFAOYSA-N	3.4		Wang et al. (2017)	Q	80, 240
MCM:METLMUCPAN	2.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_7$	1.9×10^{4}		Wang et al. (2017)	Q	80, 239
ZBESLNAUTTYMKY-UHFFFAOYSA-N	5.1		Wang et al. (2017)	Q	80, 240
MCM:PBZMUCPAN	4.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_7$	6.0×10^{4}		Wang et al. (2017)	Q	80, 239
BNKFVONIJIEPHK-UHFFFAOYSA-N	6.3		Wang et al. (2017)	Q	80, 240
MCM:PETLMUCPAN	2.8×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_7$	2.8×10^{4}		Wang et al. (2017)	Q	80, 239
ZDDBRQJYUBFFIJ-UHFFFAOYSA-N	8.1		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:TM124MUPAN	1.7×10^5		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_7$	1.3×10^4		Wang et al. (2017)	Q	80, 239
TXJRVENADFPPLH-UHFFFAOYSA-N	1.4×10^1		Wang et al. (2017)	Q	80, 240
MCM:TM135MUPAN	2.0×10^5		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_7$	3.7×10^4		Wang et al. (2017)	Q	80, 239
APWJKVMWYCHHEO-UHFFFAOYSA-N	2.9		Wang et al. (2017)	Q	80, 240
MCM:DMEBMUPAN	1.9×10^5		Wang et al. (2017)	Q	80, 238
$C_{10}H_{13}NO_7$	1.9×10^4		Wang et al. (2017)	Q	80, 239
OJIPANRKTQADST-UHFFFAOYSA-N	2.1		Wang et al. (2017)	Q	80, 240
MCM:DETLMUPAN	1.5×10^5		Wang et al. (2017)	Q	80, 238
$C_{11}H_{15}NO_7$	1.3×10^4		Wang et al. (2017)	Q	80, 239
WGGPAZKPQBFIGY-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	80, 240
MCM:TM123MUNO3	2.8×10^7		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	3.0×10^7		Wang et al. (2017)	Q	80, 239
CNKHLWZBBXJTJR-UHFFFAOYSA-N	5.0×10^2		Wang et al. (2017)	Q	80, 240
MCM:TLEMUCNO3	1.5×10^9		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_7$	3.5×10^8		Wang et al. (2017)	Q	80, 239
KLAQKLFQZHHGRD-UHFFFAOYSA-N	8.3×10^3		Wang et al. (2017)	Q	80, 240
MCM:EBZMUCNO3	1.4×10^9		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_7$	2.0×10^8		Wang et al. (2017)	Q	80, 239
ZZJNOSBMORNYPY-UHFFFAOYSA-N	1.7×10^4		Wang et al. (2017)	Q	80, 240
MCM:MXYMUCNO3	8.5×10^8		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_7$	7.8×10^7		Wang et al. (2017)	Q	80, 239
YZJRXCREGHPQLR-UHFFFAOYSA-N	6.5×10^3		Wang et al. (2017)	Q	80, 240
MCM:PXYMUCNO3	8.5×10^8		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_7$	9.3×10^7		Wang et al. (2017)	Q	80, 239
GICKPQRZPMBHKH-UHFFFAOYSA-N	1.6×10^3		Wang et al. (2017)	Q	80, 240
MCM:IPBZMUCNO3	1.3×10^9		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	1.5×10^8		Wang et al. (2017)	Q	80, 239
UHFJHZLCDDVXBJ-UHFFFAOYSA-N	1.1×10^4		Wang et al. (2017)	Q	80, 240
MCM:METLMUCNO3	7.6×10^8		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	4.6×10^7		Wang et al. (2017)	Q	80, 239
WWNOXWKNSLKIMY-UHFFFAOYSA-N	9.8×10^2		Wang et al. (2017)	Q	80, 240
MCM:PBZMUCNO3	1.1×10^9		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	1.4×10^8		Wang et al. (2017)	Q	80, 239
QLDJRFHCOXXYTH-UHFFFAOYSA-N	9.3×10^3		Wang et al. (2017)	Q	80, 240
MCM:PETLMUCNO3	7.6×10^8		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	5.8×10^7		Wang et al. (2017)	Q	80, 239
PIVPLJYVWKBKLM-UHFFFAOYSA-N	1.0×10^3		Wang et al. (2017)	Q	80, 240

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Table A4.6: Nitrates ($RONO_2$) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
MCM:TM124MUNO3	2.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	7.8×10^{6}		Wang et al. (2017)	Q	80, 239
NIRISDMZVMYRLC-UHFFFAOYSA-N	5.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:TM135MUNO3	2.2×10^{7}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_7$	1.4×10^{7}		Wang et al. (2017)	Q	80, 239
WYJKGTDXAIWZNI-UHFFFAOYSA-N	7.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DMEBMUNO3	1.9×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{10}H_{15}NO_7$	7.1×10^{6}		Wang et al. (2017)	Q	80, 239
KKQBKVQGVIRRAG-UHFFFAOYSA-N	2.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DETLMUNO3	1.4×10^{7}		Wang et al. (2017)	Q	80, 238
$C_{11}H_{17}NO_7$	4.6×10^{6}		Wang et al. (2017)	Q	80, 239
YPPYKYPDSBIFHG-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DMCNO3	2.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_3H_5NO_6$	3.6×10^{1}		Wang et al. (2017)	Q	80, 239
XNSIPMZBSRCICM-UHFFFAOYSA-N	5.4×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:MMFNO3	1.5×10^{2}		Wang et al. (2017)	Q	80, 238
$C_3H_5NO_6$	4.5		Wang et al. (2017)	Q	80, 239
KROMLYNKDFILIM-UHFFFAOYSA-N	4.5×10^{-2}		Wang et al. (2017)	Q	80, 240
ISOP1N5OOH	2.3×10^{7}	14000	Wieser et al. (2023)	Q	437
$C_5H_9NO_6$					
LLNBZHMZWYQLAS-UHFFFAOYSA-N					
C520ONO2	2.9×10^{9}	21000	Wieser et al. (2023)	Q	437
$C_5H_9NO_8$					
ZSADVAXZKGJKSG-UHFFFAOYSA-N					
ROO6R6ONO2	6.1×10^{5}	12000	Wieser et al. (2023)	Q	437
$C_6H_{11}NO_6$					
CRECMHNOVVIMCR-UHFFFAOYSA-N					
C624ONO2	2.0×10^{10}	19000	Wieser et al. (2023)	Q	437
$C_6H_{11}NO_7$					
XYBUKFJLXVIRLY-UHFFFAOYSA-N					
ROO6R5ONO2	1.7×10^{5}	15000	Wieser et al. (2023)	Q	437
$C_7H_{11}NO_7$					
LNWOWXJMUJHMJJ-UHFFFAOYSA-N					
ROO6R1ONO2	1.4×10^{2}	15000	Wieser et al. (2023)	Q	437
$C_{10}H_{17}NO_6$					
JOFCABYMPNXMIS-UHFFFAOYSA-N					
LIMAB15ONO2OOH	5.0×10^{9}	19000	Wieser et al. (2023)	Q	437
$C_{10}H_{19}NO_7$					
JBKULLYZCMWERK-UHFFFAOYSA-N					

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A4.7 Nitriles with oxygen (C, H, O, N)

Table A4.7: Nitriles with oxygen (C, H, O, N)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
isocyanic acid HNCO [75-13-8] OWIKHYCFFJSOEH-UHFFFAOYSA-N	2.3×10^{-1} 2.6×10^{-1} 2.1×10^{-1}	4700 4100	Roberts and Liu (2019) Borduas et al. (2016) Roberts et al. (2011) Burkholder et al. (2019)	M M M W	590 591 592
methyl isocyanate CH_3NCO [624-83-9] HAMGRBXTJNITHG-UHFFFAOYSA-N	1.3×10^{-2}		Roberts and Liu (2019)	M	
hydroxyacetonitrile C_2H_3NO (glycolonitrile) [107-16-4] LTYRAPJYLUPLCI-UHFFFAOYSA-N	1.3		HSDB (2015)	Q	99
2-hydroxypropanenitrile C_3H_5NO [78-97-7] WOFDVDFSGLBFAC-UHFFFAOYSA-N	1.0		HSDB (2015)	Q	99
3-hydroxypropanenitrile C_3H_5NO (ethylene cyanohydrin) [109-78-4] WSGYTJNNHPZFKR-UHFFFAOYSA-N	1.3×10^{3} 2.3×10^{4} 3.2×10^{2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
methyl cyanoacetate $C_4H_5NO_2$ [105-34-0] ANGDWNBGPBMQHW-UHFFFAOYSA-N	3.5×10^{1}		Ebert et al. (2023)	?	316
cyanoethanoic acid, ethyl ester $C_5H_7NO_2$ (ethyl cyanoacetate) [105-56-6] ZIUSEGSNTOUIPT-UHFFFAOYSA-N	3.4×10^{1} 3.4×10^{1} 1.3×10^{1} 7.7×10^{1} 4.9 7.7 3.5×10^{1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Yao et al. (2002) Yaws (1999)	V V Q Q Q Q ?	186 67 229 21
2-hydroxybenzoic acid nitrile C_7H_5NO (2-cyanophenol) [611-20-1] CHZCERSEMVWNHL-UHFFFAOYSA-N	2.8×10^{1}		Hilal et al. (2008)	Q	

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Table A4.7: Nitriles with oxygen (C, H, O, N) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-hydroxybenzoic acid nitrile	4.0×10^{4}		Hilal et al. (2008)	Q	
C_7H_5NO	1.6×10^{3}		Modarresi et al. (2007)	Q	67
(3-cyanophenol)	3.6×10^{3}		English and Carroll (2001)	Q	230, 231
[873-62-1]	3.3×10^{5}		Nirmalakhandan et al. (1997)	Q	
SGHBRHKBCLLVCI-UHFFFAOYSA-N	3.8×10^{3}		Abraham et al. (1990)	?	
4-hydroxybenzoic acid nitrile	1.4×10^{4}		Hilal et al. (2008)	Q	
C_7H_5NO	2.0×10^{3}		Modarresi et al. (2007)	Q	67
(4-cyanophenol)	3.3×10^{5}		Nirmalakhandan et al. (1997)	Q	
[767-00-0]	1.2×10^{4}		Abraham et al. (1990)	?	
CVNOWLNNPYYEOH-UHFFFAOYSA-N					
phenyl isocyanate	2.5×10^{-5}		Yaws (2003)	X	237, 12
C_7H_5NO	2.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
[103-71-9]	1.8×10^{-5}		Yaws (1999)	?	21, 12
DGTNSSLYPYDJGL-UHFFFAOYSA-N					
1,1',1"-nitrilotris-2-propanol	1.0×10^{6}		HSDB (2015)	Q	447
$C_9H_{21}NO_3$					
(triisopropanolamine)					
[122-20-3]					
SLINHMUFWFWBMU-UHFFFAOYSA-N					
cyometrinil	1.1×10^{4}		MacBean (2012a)	?	
$C_{10}H_7N_3O$					
[78370-21-5]					
PYKLUAIDKVVEOS-JLHYYAGUSA-N					
fenpropathrin	5.5×10^{-2}		HSDB (2015)	V	
$C_{22}H_{23}NO_3$	1.7×10^{1}		Siebers and Mattusch (1996)	V	12
[39515-41-8]					
XQUXKZZNEFRCAW-UHFFFAOYSA-N					

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A4.8 Nitro compounds (RNO_2)

Table A4.8: Nitro compounds (RNO_2)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
nitromethane	3.4×10^{-1}	4000	Burkholder et al. (2019)	L	
CH_3NO_2	3.4×10^{-1}	4000	Burkholder et al. (2015)	L	
[75-52-5]	3.6×10^{-1}	3900	Brockbank (2013)	L	1
LYGJENNIWJXYER-UHFFFAOYSA-N	3.4×10^{-1}	4000	Sander et al. (2011)	L	
	3.4×10^{-1}	4000	Sander et al. (2006)	L	
	3.5×10^{-1}	4000	Beneš and Dohnal (1999)	M	
	3.6×10^{-1}		Park et al. (1987)	M	
	4.5×10^{-1}		Rohrschneider (1973)	M	
	3.4×10^{-2}		Yaws (2003)	X	237
	3.5×10^{-1}		Gaffney and Senum (1984)	X	389
	4.4×10^{-1}		Hayer et al. (2022)	Q	20
	2.5×10^{-1}		Keshavarz et al. (2022)	Q	
	6.2×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
	3.4×10^{-1}		Hilal et al. (2008)	Q	
	3.3×10^{-2}		Modarresi et al. (2007)	Q	67
		3700	Kühne et al. (2005)	Q	
	2.3×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	6.2×10^{-1}		English and Carroll (2001)	Q	230, 231
	2.8×10^{-2}		Katritzky et al. (1998)	Q	
	7.3×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	3.5×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		3500	Kühne et al. (2005)	?	
	3.4×10^{-2}		Yaws (1999)	?	21
	1.8×10^{-1}		Abraham and Weathersby (1994)	?	21
	3.6×10^{-2}		Yaws and Yang (1992)	?	21
	3.6×10^{-1}		Abraham et al. (1990)	?	
nitromethane-13C CH_3NO_2 [32480-00-5] LYGJENNIWJXYER-OUBTZVSYSA-N	4.8×10^{-1}	5000	Hiatt (2013)	M	
nitroethane	2.1×10^{-1}	4400	Burkholder et al. (2019)	L	
$C_2H_5NO_2$	2.1×10^{-1}	4400	Burkholder et al. (2015)	L	
[79-24-3]	2.1×10^{-1}	4700	Brockbank (2013)	L	1
MCSAJNNLRCFZED-UHFFFAOYSA-N	2.1×10^{-1}	4400	Sander et al. (2011)	L	
	2.1×10^{-1}	4400	Sander et al. (2006)	L	
	2.2×10^{-1}	4400	Beneš and Dohnal (1999)	M	
	1.4×10^{-1}		Friant and Suffet (1979)	M	38, 593
	1.9×10^{-1}		Hwang et al. (1992)	V	
	2.1×10^{-1}		Hine and Mookerjee (1975)	V	
	2.1×10^{-1}		Gaffney and Senum (1984)	X	389

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	3.4×10^{-1}		Keshavarz et al. (2022)	Q	
	3.7×10^{-1}		Duchowicz et al. (2020)	Q	184
	2.1×10^{-1}		Li et al. (2014)	Q	241
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	3.0×10^{-2}		Modarresi et al. (2007)	Q	67
		4100	Kühne et al. (2005)	Q	
	2.3×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	3.1×10^{-1}		English and Carroll (2001)	Q	230, 260
	2.6×10^{-2}		Katritzky et al. (1998)	Q	
	6.1×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	1.5×10^{-1}		Suzuki et al. (1992)	Q	232
	2.1×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		4200	Kühne et al. (2005)	?	
	2.5×10^{-1}		Yaws (1999)	?	21
	2.1×10^{-1}		Abraham et al. (1990)	?	
1-nitropropane $C_3H_7NO_2$ [108-03-2] JSZOAYXJRCEYSX-UHFFFAOYSA-N	1.3×10^{-1}	4700	Burkholder et al. (2019)	L	
	1.3×10^{-1}	4700	Burkholder et al. (2015)	L	
	1.4×10^{-1}	5100	Brockbank (2013)	L	1
	1.3×10^{-1}	4700	Sander et al. (2011)	L	
	1.3×10^{-1}	4700	Sander et al. (2006)	L	
	1.3×10^{-1}	4700	Beneš and Dohnal (1999)	M	
	1.6×10^{-1}		Welke et al. (1998)	M	
	1.1×10^{-1}		Hine and Mookerjee (1975)	V	
	9.2×10^{-2}		Keshavarz et al. (2022)	Q	
	4.8×10^{-1}		Duchowicz et al. (2020)	Q	299
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	1.5×10^{-1}		Hilal et al. (2008)	Q	
	2.3×10^{-2}		Modarresi et al. (2007)	Q	67
		4400	Kühne et al. (2005)	Q	
	1.2×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	1.2×10^{-1}		English and Carroll (2001)	Q	230, 231
	3.1×10^{-2}		Katritzky et al. (1998)	Q	
	4.7×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	7.2×10^{-3}		Suzuki et al. (1992)	Q	232
	1.1×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		4400	Kühne et al. (2005)	?	
	1.2×10^{-1}		Yaws (1999)	?	21, 12
	1.6×10^{-1}		Yaws and Yang (1992)	?	21, 12
	1.1×10^{-1}		Abraham et al. (1990)	?	

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
2-nitropropane	8.3×10^{-2}	4500	Burkholder et al. (2019)	L	
$CH_3CH(NO_2)CH_3$	8.3×10^{-2}	4500	Burkholder et al. (2015)	L	
[79-46-9]	8.6×10^{-2}	4800	Brockbank (2013)	L	1
FGLBSLMDCBOPQK-UHFFFAOYSA-N	8.3×10^{-2}	4500	Sander et al. (2011)	L	
	8.3×10^{-2}	4500	Sander et al. (2006)	L	
	8.4×10^{-2}	4500	Beneš and Dohnal (1999)	M	
	8.3×10^{-2}		Duchowicz et al. (2020)	V	186
	8.3×10^{-2}		HSDB (2015)	V	
	8.0×10^{-2}		Hine and Mookerjee (1975)	V	
	2.2×10^{-1}		Duchowicz et al. (2020)	Q	
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	7.2×10^{-2}		Hilal et al. (2008)	Q	
	2.7×10^{-2}		Modarresi et al. (2007)	Q	67
		4400	Kühne et al. (2005)	Q	
	8.6×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	7.2×10^{-2}		English and Carroll (2001)	Q	230, 274
	2.1×10^{-2}		Katritzky et al. (1998)	Q	
	4.1×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	8.4×10^{-3}		Suzuki et al. (1992)	Q	232
		4400	Kühne et al. (2005)	?	
	8.2×10^{-2}		Yaws (1999)	?	21, 12
	1.1×10^{-1}		Yaws and Yang (1992)	?	21, 12
	8.0×10^{-2}		Abraham et al. (1990)	?	
1-nitrobutane	7.6×10^{-2}		Brockbank (2013)	L	
$C_4H_9NO_2$	8.3×10^{-2}		Duchowicz et al. (2020)	V	186
[627-05-4]	5.6×10^{-1}		Duchowicz et al. (2020)	Q	
NALZTFARIYUCBY-UHFFFAOYSA-N	9.7×10^{-2}		Hilal et al. (2008)	Q	
	1.8×10^{-2}		Modarresi et al. (2007)	Q	67
	3.7×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	7.5×10^{-2}		Abraham et al. (1990)	?	
tert-butylnitrite	7.9×10^{-3}		Hilal et al. (2008)	Q	
C_4H_9ONO					
[540-80-7]					
IOGXOCVLYRDXLW-UHFFFAOYSA-N					
1-nitropentane	4.7×10^{-2}		Amoore and Buttery (1978)	V	
$C_5H_{11}NO_2$	6.0×10^{-2}		Hilal et al. (2008)	Q	
[628-05-7]	1.4×10^{-2}		Modarresi et al. (2007)	Q	67
BVALZCVRLDMXOQ-UHFFFAOYSA-N	2.9×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	4.7×10^{-2}		Abraham et al. (1990)	?	

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tris(hydroxymethyl)ethane trinitrate	2.2×10^{3}		Zhang et al. (2010)	Q	287, 288
$C_5H_9N_3O_9$	1.4×10^{2}		Zhang et al. (2010)	Q	287, 289
[3032-55-1]	2.4×10^{3}		Zhang et al. (2010)	Q	287, 290
IPPYBNCEPZCLNI-UHFFFAOYSA-N	3.4×10^{1}		Zhang et al. (2010)	Q	287, 291
1-nitrohexane	4.5×10^{-2}		Hilal et al. (2008)	Q	
$C_6H_{13}NO_2$					
[646-14-0]					
FEYJIFXFOHFGCC-UHFFFAOYSA-N					
nitrocyclohexane	2.4×10^{-1}		Hilal et al. (2008)	Q	
$C_6H_{11}NO_2$					
[1122-60-7]					
NJNQUTDUIPVROZ-UHFFFAOYSA-N					
2-nitroethanol	2.0×10^{2}		Raventos-Duran et al. (2010)	Q	242, 243
$C_2H_5NO_3$	3.1×10^{2}		Raventos-Duran et al. (2010)	Q	244
[625-48-9]	4.9×10^{3}		Raventos-Duran et al. (2010)	Q	245
KIPMDPDAFINLIV-UHFFFAOYSA-N	1.6×10^{2}		Hilal et al. (2008)	Q	
1-nitro-2-propanol	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	242, 243
$C_3H_7NO_3$	2.5×10^{2}		Raventos-Duran et al. (2010)	Q	244
[3156-73-8]	3.9×10^{3}		Raventos-Duran et al. (2010)	Q	245
PFNCKQIYLAVYJF-UHFFFAOYSA-N	7.9×10^{1}		Hilal et al. (2008)	Q	
2-nitro-1-propanol	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	242, 243
$C_3H_7NO_3$	2.5×10^{2}		Raventos-Duran et al. (2010)	Q	244
[2902-96-7]	3.9×10^{3}		Raventos-Duran et al. (2010)	Q	245
PCNWBUOSTLGPMI-UHFFFAOYSA-N	9.9×10^{1}		Hilal et al. (2008)	Q	
1-nitro-2-butanol	7.3×10^{1}		Hilal et al. (2008)	Q	
$C_4H_9NO_3$					
[3156-74-9]					
FMEFHKJRIGHSLB-UHFFFAOYSA-N					
2-nitro-1-butanol	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	271, 243
$C_4H_9NO_3$	2.0×10^{2}		Raventos-Duran et al. (2010)	Q	244
[609-31-4]	2.5×10^{3}		Raventos-Duran et al. (2010)	Q	245
MHIHRIPETCJEMQ-UHFFFAOYSA-N	7.5×10^{1}		Hilal et al. (2008)	Q	
3-nitro-2-butanol	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
$C_4H_9NO_3$	2.0×10^{2}		Raventos-Duran et al. (2010)	Q	244
[6270-16-2]	2.5×10^{3}		Raventos-Duran et al. (2010)	Q	245
OJVOGABFNZDOOZ-UHFFFAOYSA-N	5.7×10^{1}		Hilal et al. (2008)	Q	
nitroguanidine	2.2×10^{10}		HSDB (2015)	V	
$CH_4N_4O_2$					
[556-88-7]					
IDCPFAYURAQKDZ-UHFFFAOYSA-N					

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tetranitromethane CN_4O_8 [509-14-8] NYTOUQBROMCLBJ-UHFFFAOYSA-N	4.1×10^{-3}		HSDB (2015)	V	
N-methyl-N'-nitro-N-nitrosoguanidine $C_2H_5N_5O_3$ [70-25-7] VZUNGTLZRAYYDE-UHFFFAOYSA-N	8.2×10^{6}		HSDB (2015)	Q	99
2-(hydroxymethyl)-2-nitro-1,3-propanediol $C_4H_9NO_5$ [126-11-4] OLQJQHSAWMFDJE-UHFFFAOYSA-N	2.1×10^{6}		HSDB (2015)	Q	99
MCM:NC4DCO2H $C_4H_3NO_5$ ODFCIXRXNCCVGH-UHFFFAOYSA-N	6.9×10^{6} 3.5×10^{6} 2.3×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:NC4MDCO2H $C_5H_5NO_5$ LXEJKNKBIPISQO-UHFFFAOYSA-N	4.2×10^{6} 4.7×10^{6} 6.5×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:NC4EDCO2H $C_6H_7NO_5$ GVSLZEQKUBDLJE-UHFFFAOYSA-N	3.6×10^{6} 6.9×10^{6} 3.9×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:DNPHENOOH $C_6H_6N_2O_{10}$ AKJGOKAIBHUAAE-UHFFFAOYSA-N	7.3×10^{16} 8.0×10^{10} 5.4×10^{7}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:NCATECOOH $C_6H_7NO_9$ UERHMILVGXASDJ-UHFFFAOYSA-N	8.1×10^{17} 1.6×10^{10} 4.4×10^{9}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:NC5MDCO2H $C_6H_7NO_5$ VRGZGZRSZACGSZ-UHFFFAOYSA-N	2.8×10^{6} 1.1×10^{7} 2.5×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:NC4IPDCO2H $C_7H_9NO_5$ VOBLVGUNJWYRHD-UHFFFAOYSA-N	3.5×10^{6} 3.5×10^{6} 1.8×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:NC4PDCO2H $C_7H_9NO_5$ MSTRQTMGALLSFO-UHFFFAOYSA-N	3.0×10^{6} 4.2×10^{6} 2.2×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:DNCRESOOH $C_7H_8N_2O_{10}$ FHWDGQSKNURQKZ-UHFFFAOYSA-N	4.0×10^{16} 3.6×10^{10} 1.4×10^{6}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MNCATECOOH	3.0×10^{17}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_9$	1.7×10^{11}		Wang et al. (2017)	Q	80, 239
OCHAAZKMUDWIOE-UHFFFAOYSA-N	4.4×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:TL4ONO2OOH	1.4×10^{14}		Wang et al. (2017)	Q	80, 238
$C_7H_9NO_8$	2.8×10^{9}		Wang et al. (2017)	Q	80, 239
MEXRHSIIQRTIBR-UHFFFAOYSA-N	3.5×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:DNEBNZLOOH	3.6×10^{16}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}N_2O_{10}$	2.3×10^{10}		Wang et al. (2017)	Q	80, 239
FNCRENCSRXRIPJ-UHFFFAOYSA-N	3.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:DNMXYOLOOH	2.7×10^{16}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}N_2O_{10}$	2.2×10^{11}		Wang et al. (2017)	Q	80, 239
KSAVSEUSLRIGAB-UHFFFAOYSA-N	5.9×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:DNOXYOLOOH	3.2×10^{16}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}N_2O_{10}$	5.9×10^{10}		Wang et al. (2017)	Q	80, 239
PBZRLTNSSYSOGL-UHFFFAOYSA-N	7.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:DNPXYOLOOH	2.7×10^{16}		Wang et al. (2017)	Q	80, 238
$C_8H_{10}N_2O_{10}$	3.1×10^{10}		Wang et al. (2017)	Q	80, 239
AYHFAKIJCOHXBG-UHFFFAOYSA-N	1.5×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:ENCATECOOH	2.6×10^{17}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_9$	8.9×10^{10}		Wang et al. (2017)	Q	80, 239
QJBJEZDKVLRDGQ-UHFFFAOYSA-N	1.8×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:MXNCATCOOH	1.6×10^{17}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_9$	6.2×10^{10}		Wang et al. (2017)	Q	80, 239
QYJOURKZCRGVGB-UHFFFAOYSA-N	3.4×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:MXOHNO2OOH	1.8×10^{14}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_8$	1.2×10^{9}		Wang et al. (2017)	Q	80, 239
RRWTXIWIABDEOZ-UHFFFAOYSA-N	1.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:OXNCATCOOH	3.9×10^{17}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_9$	1.2×10^{10}		Wang et al. (2017)	Q	80, 239
GWPIPVPJLOZVKC-UHFFFAOYSA-N	3.7×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PXNCATCOOH	3.0×10^{17}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_9$	5.5×10^{9}		Wang et al. (2017)	Q	80, 239
RMUFWTRDQQMPCD-UHFFFAOYSA-N	1.4×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:TM124NOOH	1.8×10^{14}		Wang et al. (2017)	Q	80, 238
$C_8H_{11}NO_8$	1.3×10^{9}		Wang et al. (2017)	Q	80, 239
LGMZUZOZZXWRQX-UHFFFAOYSA-N	5.1×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:DNIPBZLOOH	3.2×10^{16}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}N_2O_{10}$	2.3×10^{10}		Wang et al. (2017)	Q	80, 239
YKBFACRSJWRBHR-UHFFFAOYSA-N	3.7×10^{6}		Wang et al. (2017)	Q	80, 240

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DNMETOLOOH	2.1×10^{16}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}N_2O_{10}$	1.4×10^{11}		Wang et al. (2017)	Q	80, 239
LAMZNFDUTXWEFA-UHFFFAOYSA-N	1.5×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:DNOETOLOOH	2.5×10^{16}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}N_2O_{10}$	3.9×10^{10}		Wang et al. (2017)	Q	80, 239
KMVIJWGCTFHDMC-UHFFFAOYSA-N	7.6×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:DNPBNZLOOH	2.9×10^{16}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}N_2O_{10}$	1.9×10^{10}		Wang et al. (2017)	Q	80, 239
YOHJWFCUZUQBMA-UHFFFAOYSA-N	2.8×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:DNPETOLOOH	2.1×10^{16}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}N_2O_{10}$	1.9×10^{10}		Wang et al. (2017)	Q	80, 239
IOZSITWJVFMIBH-UHFFFAOYSA-N	2.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:DNT123LOOH	1.7×10^{16}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}N_2O_{10}$	3.9×10^{10}		Wang et al. (2017)	Q	80, 239
GBPJMJLXQYJDMC-UHFFFAOYSA-N	4.5×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:DNT124LOOH	1.4×10^{16}		Wang et al. (2017)	Q	80, 238
$C_9H_{12}N_2O_{10}$	2.0×10^{10}		Wang et al. (2017)	Q	80, 239
INCIWBVFUFSSNB-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:EMPONO2OOH	1.4×10^{14}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_8$	1.5×10^{9}		Wang et al. (2017)	Q	80, 239
FZXCIHOWKZKJRK-UHFFFAOYSA-N	6.3×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:IPNCATCOOH	2.5×10^{17}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_9$	8.3×10^{10}		Wang et al. (2017)	Q	80, 239
NYRKVILWQFQUNU-UHFFFAOYSA-N	9.3×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:MTNCATCOOH	1.5×10^{17}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_9$	3.6×10^{10}		Wang et al. (2017)	Q	80, 239
MCLPDHQAEZEULP-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:OTNCATCOOH	3.6×10^{17}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_9$	7.1×10^{9}		Wang et al. (2017)	Q	80, 239
MVMRAYXEOTUUSG-UHFFFAOYSA-N	2.5×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:PNCATECOOH	2.1×10^{17}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_9$	6.6×10^{10}		Wang et al. (2017)	Q	80, 239
AWPUGBPLGLTYEJ-UHFFFAOYSA-N	5.9×10^{7}		Wang et al. (2017)	Q	80, 240
MCM:PTNCATCOOH	2.8×10^{17}		Wang et al. (2017)	Q	80, 238
$C_9H_{13}NO_9$	3.5×10^{9}		Wang et al. (2017)	Q	80, 239
IJEUJFHQTRRKRP-UHFFFAOYSA-N	9.6×10^{6}		Wang et al. (2017)	Q	80, 240

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
nitrobenzene	4.7×10^{-1}	6100	Brockbank (2013)	L	1
$C_6H_5NO_2$	6.7×10^{-1}		Chao et al. (2017)	M	
[98-95-3]	6.4×10^{-1}	7500	Hiatt (2013)	M	
LQNUZADURLCDLV-UHFFFAOYSA-N	1.4×10^{-1}		Zhang et al. (2013)	M	325
	2.3×10^{-2}	11000	Dewulf et al. (1999)	M	594
	1.2		Altschuh et al. (1999)	M	
	1.4×10^{-1}		Hellmann (1987)	M	87
	4.1×10^{-1}		Warner et al. (1980)	M	
	4.7×10^{-1}		Chao et al. (2017)	V	
	4.8×10^{-1}	6400	Bernauer et al. (2006)	V	1
	7.7×10^{-1}		Mackay et al. (2006d)	V	
	4.2×10^{-1}		Lide and Frederikse (1995)	V	
	7.7×10^{-1}		Mackay et al. (1995)	V	
	4.6×10^{-1}		Hwang et al. (1992)	V	
	7.8×10^{-1}		Yoshida et al. (1983)	V	
	4.3×10^{-1}		Warner et al. (1980)	V	
	4.2×10^{-1}		Hine and Mookerjee (1975)	V	
	4.7×10^{-1}	4500	Goldstein (1982)	X	298
	4.2×10^{-1}		Hilal et al. (2008)	C	
	4.1×10^{-1}		Schüürmann (2000)	C	21
	7.5×10^{-1}		Mackay et al. (1995)	C	
	7.5×10^{-1}		Ryan et al. (1988)	C	
	4.1×10^{-1}		Shen (1982)	C	
	1.1		Keshavarz et al. (2022)	Q	
	2.1		Duchowicz et al. (2020)	Q	299
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	2.7×10^{-1}		Modarresi et al. (2007)	Q	67
		4600	Kühne et al. (2005)	Q	
	4.2×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	5.1×10^{-1}		Yao et al. (2002)	Q	229
	2.9×10^{-1}		Katritzky et al. (1998)	Q	
	3.3		Nirmalakhandan et al. (1997)	Q	
	2.0×10^{-1}		Russell et al. (1992)	Q	279
	7.0×10^{-1}		Suzuki et al. (1992)	Q	232
	4.1×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		5600	Kühne et al. (2005)	?	
	4.7×10^{-1}		Yaws (1999)	?	21
	4.2×10^{-1}		Abraham et al. (1990)	?	
nitrobenzene-d5	8.5×10^{-1}	7500	Hiatt (2013)	M	
$C_6D_5NO_2$					
[4165-60-0]					
LQNUZADURLCDLV-RALIUCGRSA-N					

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
2-nitrotoluene	2.4×10^{-1}	5800	Brockbank (2013)	L	1
$C_6H_4(NO_2)CH_3$	9.6×10^{-1}		Chao et al. (2017)	M	
[88-72-2]	7.9×10^{-1}		Altschuh et al. (1999)	M	
PLAZTCDQAHEYBI-UHFFFAOYSA-N	2.7×10^{-1}		Mackay et al. (2006d)	V	
	1.9×10^{-1}		Schüürmann (2000)	V	
	1.8×10^{-1}		Lide and Frederikse (1995)	V	
	2.7×10^{-1}		Mackay et al. (1995)	V	
	1.7×10^{-1}		Hine and Mookerjee (1975)	V	
	7.7×10^{-2}	2900	Goldstein (1982)	X	298
	1.5		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	299
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	4.2×10^{-1}		Zhang et al. (2010)	Q	287, 288
	2.4×10^{-1}		Zhang et al. (2010)	Q	287, 289
	2.5×10^{-1}		Zhang et al. (2010)	Q	287, 290
	1.8×10^{-1}		Zhang et al. (2010)	Q	287, 291
	4.2×10^{-1}		Zhang et al. (2010)	Q	287, 288
	2.4×10^{-1}		Zhang et al. (2010)	Q	287, 289
	2.2×10^{-1}		Zhang et al. (2010)	Q	287, 290
	1.8×10^{-1}		Zhang et al. (2010)	Q	287, 291
	1.4×10^{-1}		Hilal et al. (2008)	Q	
	2.3×10^{-1}		Modarresi et al. (2007)	Q	67
		4900	Kühne et al. (2005)	Q	
	1.4×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	2.3		Nirmalakhandan et al. (1997)	Q	
	5.7×10^{-1}		Suzuki et al. (1992)	Q	232
	7.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		5900	Kühne et al. (2005)	?	
	1.7×10^{-1}		Abraham et al. (1990)	?	
3-nitrotoluene	2.7×10^{-1}	7000	Brockbank (2013)	L	1
$C_6H_4(NO_2)CH_3$	1.3		Chao et al. (2017)	M	
[99-08-1]	1.1		Altschuh et al. (1999)	M	
QZYHIOPPLUPUJF-UHFFFAOYSA-N	2.8×10^{-1}		Li and Carr (1993)	M	
	1.3×10^{-1}		Mackay et al. (2006d)	V	
	1.3×10^{-1}		Mackay et al. (1995)	V	
	1.4×10^{-1}		Hine and Mookerjee (1975)	V	
	1.4×10^{-1}	3200	Goldstein (1982)	X	298
	1.5		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	299
	4.2×10^{-1}		Zhang et al. (2010)	Q	287, 288
	2.5×10^{-1}		Zhang et al. (2010)	Q	287, 289
	4.1×10^{-1}		Zhang et al. (2010)	Q	287, 290
	1.8×10^{-1}		Zhang et al. (2010)	Q	287, 291
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Modarresi et al. (2007)	Q	67

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
		4900	Kühne et al. (2005)	Q	
	1.4×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.3		Nirmalakhandan et al. (1997)	Q	
	5.7×10^{-1}		Suzuki et al. (1992)	Q	232
	1.1		Duchowicz et al. (2020)	?	185, 21
		4900	Kühne et al. (2005)	?	
	1.3×10^{-1}		Yaws (1999)	?	21, 38
	1.4×10^{-1}		Abraham et al. (1990)	?	
4-nitrotoluene	8.9×10^{-1}	7100	Brockbank (2013)	L	1
$C_6H_4(NO_2)CH_3$	1.8		Altschuh et al. (1999)	M	
[99-99-0]	2.8		Mackay et al. (2006d)	V	
ZPTVNYMJQHSSEA-UHFFFAOYSA-N	2.0×10^{-1}		Lide and Frederikse (1995)	V	
	2.8		Mackay et al. (1995)	V	
	1.6×10^{-1}	3100	Goldstein (1982)	X	298
	1.5		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	184
	1.4×10^{-1}		Li et al. (2014)	Q	241
	4.2×10^{-1}		Zhang et al. (2010)	Q	287, 288
	2.8×10^{-1}		Zhang et al. (2010)	Q	287, 289
	9.0×10^{-1}		Zhang et al. (2010)	Q	287, 290
	1.8×10^{-1}		Zhang et al. (2010)	Q	287, 291
	2.0×10^{-1}		Hilal et al. (2008)	Q	
	2.4×10^{-1}		Modarresi et al. (2007)	Q	67
		4900	Kühne et al. (2005)	Q	
	1.8		Duchowicz et al. (2020)	?	185, 21
		3800	Kühne et al. (2005)	?	
1,2-dinitrobenzene	1.9×10^{2}		Duchowicz et al. (2020)	V	186
$C_6H_4N_2O_4$	1.9×10^{2}		HSDB (2015)	V	
[528-29-0]	3.5×10^{2}		Duchowicz et al. (2020)	Q	
IZUKQUVSCNEFMJ-UHFFFAOYSA-N	1.2×10^{2}		Zhang et al. (2010)	Q	287, 288
	3.2×10^{1}		Zhang et al. (2010)	Q	287, 289
	2.6×10^{1}		Zhang et al. (2010)	Q	287, 290
	2.7×10^{1}		Zhang et al. (2010)	Q	287, 291
1,3-dinitrobenzene	1.8×10^{2}		Chao et al. (2017)	M	
$C_6H_4N_2O_4$	2.0×10^{2}		Altschuh et al. (1999)	M	
[99-65-0]			Mackay et al. (2006d)	V	558
WDCYWAQPCXBPJA-UHFFFAOYSA-N	5.0×10^{2}		Mackay et al. (1995)	V	
	3.9×10^{1}		Smith et al. (1981a)	V	
	2.5×10^{2}		Keshavarz et al. (2022)	Q	
	2.1×10^{2}		Duchowicz et al. (2020)	Q	
	2.0×10^{2}		Gharagheizi et al. (2012)	Q	
	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{2}		Duchowicz et al. (2020)	?	185, 21

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1,4-dinitrobenzene	2.0×10^{-1}		Mackay et al. (2006d)	V	
$C_6H_4N_2O_4$	2.0×10^{-1}		Mackay et al. (1995)	V	
[100-25-4]	1.2×10^{2}		HSDB (2015)	Q	99
FYFDQJRXFWGIBS-UHFFFAOYSA-N					
1,3,5-trinitrobenzene	1.5×10^{3}		HSDB (2015)	V	
$C_6H_3N_3O_6$	2.7×10^{2}		Yaws (2003)	X	237, 80
[99-35-4]	2.8×10^{2}		Gharagheizi et al. (2010)	Q	246
UATJOMSPNYCXIX-UHFFFAOYSA-N					
2,4,6-trinitrophenol	3.0×10^{5}		Ebert et al. (2023)	?	316
$C_6H_3N_3O_7$					
(picric acid)					
[88-89-1]					
OXNIZHLAWKMVMX-UHFFFAOYSA-N					
2-nitrobenzenamine	7.1×10^{1}	6800	Brockbank (2013)	L	1
$C_6H_6N_2O_2$	1.7×10^{2}		Altschuh et al. (1999)	M	
(2-nitroaniline)	1.0×10^{2}		Abraham et al. (1994a)	R	
[88-74-4]	2.0×10^{2}		Keshavarz et al. (2022)	Q	
DPJCXCZTLWNFOH-UHFFFAOYSA-N	2.5×10^{2}		Duchowicz et al. (2020)	Q	184
	3.1×10^{1}		Hilal et al. (2008)	Q	
	2.1×10^{2}		Modarresi et al. (2007)	Q	67
	4.5×10^{2}		Nirmalakhandan et al. (1997)	Q	
	1.7×10^{2}		Duchowicz et al. (2020)	?	185, 21
3-nitrobenzenamine	6.9×10^{2}		Meylan and Howard (1991)	V	
$C_6H_6N_2O_2$	1.2×10^{3}		Abraham et al. (1994a)	R	
(3-nitroaniline)	4.2×10^{3}		Keshavarz et al. (2022)	Q	
[99-09-2]	1.5×10^{3}		Duchowicz et al. (2020)	Q	
XJCVRTZCHMZPBD-UHFFFAOYSA-N	2.7×10^{3}		Hilal et al. (2008)	Q	
	4.0×10^{2}		Modarresi et al. (2007)	Q	67
	6.0×10^{2}		English and Carroll (2001)	Q	230, 231
	4.4×10^{2}		Nirmalakhandan et al. (1997)	Q	
	1.3×10^{3}		Meylan and Howard (1991)	Q	
	1.2×10^{3}		Duchowicz et al. (2020)	?	185, 21
	1.2×10^{3}		HSDB (2015)	?	419
4-nitrobenzenamine	8.7×10^{3}	8200	Brockbank (2013)	L	1
$C_6H_6N_2O_2$	8.6×10^{3}		Altschuh et al. (1999)	M	
(4-nitroaniline)	1.4×10^{4}		Abraham et al. (1994a)	R	
[100-01-6]	1.8×10^{2}		Yaws (2003)	X	237
TYMLOMAKGOJONV-UHFFFAOYSA-N	4.2×10^{3}		Keshavarz et al. (2022)	Q	
	1.5×10^{3}		Duchowicz et al. (2020)	Q	
	8.5×10^{2}		Gharagheizi et al. (2012)	Q	
	1.7×10^{2}		Gharagheizi et al. (2010)	Q	246
	2.2×10^{3}		Hilal et al. (2008)	Q	
	1.5×10^{2}		Modarresi et al. (2007)	Q	67
	4.4×10^{2}		Nirmalakhandan et al. (1997)	Q	
	7.8×10^{3}		Duchowicz et al. (2020)	?	185, 21

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4-dinitrobenzenamine $C_6H_5N_3O_4$ [97-02-9] LXQOQPGNCGEELI-UHFFFAOYSA-N	6.5×10^{4}		HSDB (2015)	Q	545
2-methyl-6-nitroaniline $C_7H_8N_2O_2$ [570-24-1] FCMRHMPITHLLLA-UHFFFAOYSA-N	4.6×10^{1}		Abraham et al. (2019)	Q	
1-methyl-2,3-dinitrobenzene $C_7H_6N_2O_4$ (2,3-dinitrotoluene; 2,3-DNT) [602-01-7] DYSXLQBUUOPLBB-UHFFFAOYSA-N	1.1×10^{2}		HSDB (2015)	Q	447
	1.1×10^{2}		Zhang et al. (2010)	Q	287, 288
	2.2×10^{1}		Zhang et al. (2010)	Q	287, 289
	9.5		Zhang et al. (2010)	Q	287, 290
	1.5×10^{1}		Zhang et al. (2010)	Q	287, 291
	1.1×10^{2}		Zhang et al. (2010)	Q	287, 288
	2.3×10^{1}		Zhang et al. (2010)	Q	287, 289
	1.1×10^{1}		Zhang et al. (2010)	Q	287, 290
	1.5×10^{1}		Zhang et al. (2010)	Q	287, 291
1-methyl-2,4-dinitrobenzene $C_7H_6N_2O_4$ (2,4-dinitrotoluene; 2,4-DNT) [121-14-2] RMBFBMJGBANMMK-UHFFFAOYSA-N	4.0×10^{1}	7900	Brockbank (2013)	L	1
	1.8×10^{2}		Altschuh et al. (1999)	M	
	1.1×10^{1}		Mackay et al. (2006d)	V	
	1.0×10^{2}		Schüürmann (2000)	V	
	1.1×10^{1}		Mackay et al. (1995)	V	
	6.3×10^{1}		Smith et al. (1981a)	V	
	2.1×10^{-1}	2900	Goldstein (1982)	X	298
	2.2		Mackay et al. (1995)	C	
	3.1×10^{-2}		Ryan et al. (1988)	C	
	3.4×10^{2}		Keshavarz et al. (2022)	Q	
	1.6×10^{2}		Duchowicz et al. (2020)	Q	
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	1.1×10^{2}		Zhang et al. (2010)	Q	287, 288
	1.6×10^{1}		Zhang et al. (2010)	Q	287, 289
	5.0		Zhang et al. (2010)	Q	287, 290
	1.5×10^{1}		Zhang et al. (2010)	Q	287, 291
	1.8×10^{2}		Duchowicz et al. (2020)	?	185, 21
2-methyl-1,4-dinitrobenzene $C_7H_6N_2O_4$ (2,5-dinitrotoluene; 2,5-DNT) [619-15-8] KZBOXYKTSUUBTO-UHFFFAOYSA-N	1.8×10^{1}		HSDB (2015)	V	
	1.1×10^{2}		Zhang et al. (2010)	Q	287, 288
	1.8×10^{1}		Zhang et al. (2010)	Q	287, 289
	1.4		Zhang et al. (2010)	Q	287, 290
	1.5×10^{1}		Zhang et al. (2010)	Q	287, 291

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
2-methyl-1,3-dinitrobenzene	4.8	7600	Brockbank (2013)	L	1
$C_7H_6N_2O_4$	1.3×10^{1}		Duchowicz et al. (2020)	V	186
(2,6-dinitrotoluene; 2,6-DNT)	1.5×10^{1}		HSDB (2015)	V	
[606-20-2]	1.4×10^{1}		Mackay et al. (2006d)	V	
XTRDKALNCIHHNI-UHFFFAOYSA-N	1.4×10^{1}		Mackay et al. (1995)	V	
	1.2		Mackay et al. (1995)	C	
	3.1×10^{-2}		Ryan et al. (1988)	C	
	1.6×10^{2}		Duchowicz et al. (2020)	Q	
	1.6		Li et al. (2014)	Q	241
	1.1×10^{2}		Zhang et al. (2010)	Q	287, 288
	2.1×10^{1}		Zhang et al. (2010)	Q	287, 289
	4.3		Zhang et al. (2010)	Q	287, 290
	1.5×10^{1}		Zhang et al. (2010)	Q	287, 291
4-methyl-1,2-dinitrobenzene	3.3×10^{1}	9600	Brockbank (2013)	L	1
$C_7H_6N_2O_4$	1.1×10^{2}		HSDB (2015)	Q	447
(3,4-dinitrotoluene; 3,4-DNT)	1.1×10^{2}		Zhang et al. (2010)	Q	287, 288
[610-39-9]	3.9×10^{1}		Zhang et al. (2010)	Q	287, 289
INYDMNPNDHRJQJ-UHFFFAOYSA-N	3.1×10^{1}		Zhang et al. (2010)	Q	287, 290
	1.5×10^{1}		Zhang et al. (2010)	Q	287, 291
1-methyl-2,4,6-trinitrobenzene	4.7×10^{2}	7700	Brockbank (2013)	L	1
$C_7H_5N_3O_6$	4.7×10^{2}		HSDB (2015)	V	
(2,4,6-trinitrotoluene; TNT)	5.4×10^{2}		Schüürmann (2000)	V	
[118-96-7]		6200	Kühne et al. (2005)	Q	
SPSSULHKWOKEEL-UHFFFAOYSA-N		6400	Kühne et al. (2005)	?	
2,4,6-trinitro-1,3-dimethyl-5-*tert*-butylbenzene	3.2×10^{-1}		Lee et al. (2012)	M	
$C_{12}H_{15}N_3O_6$	1.7×10^{-2}		Amoore and Buttery (1978)	V	
(musk xylene)	1.3×10^{3}		HSDB (2015)	Q	99
[81-15-2]	9.5×10^{3}		Zhang et al. (2010)	Q	287, 288
XMWRWTSZNLOZFN-UHFFFAOYSA-N	5.6		Zhang et al. (2010)	Q	287, 289
	4.8×10^{-2}		Zhang et al. (2010)	Q	287, 290
	1.5×10^{2}		Zhang et al. (2010)	Q	287, 291
2-nitrophenol	9.9		Chao et al. (2017)	M	
$HOC_6H_4(NO_2)$	1.4	5700	Guo and Brimblecombe (2007)	M	
[88-75-5]	8.3×10^{-1}	6300	Harrison et al. (2002)	M	
IQUPABOKLQSFBK-UHFFFAOYSA-N	8.9×10^{-1}	6300	Müller and Heal (2001)	M	
	7.7×10^{-1}		Tremp et al. (1993)	M	12
	6.1×10^{-1}		Mackay et al. (2006c)	V	
	2.9		Lide and Frederikse (1995)	V	
	7.9×10^{-1}		Riederer (1990)	V	
	7.3×10^{-1}		Schwarzenbach et al. (1988)	V	12
	2.8		Leuenberger et al. (1985)	V	416
	9.2×10^{-1}		Abraham et al. (1994a)	R	
	6.9×10^{-1}	4600	Goldstein (1982)	X	298
	1.3		Ryan et al. (1988)	C	

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	1.1		Abraham et al. (2019)	Q	
	6.6		Wang et al. (2017)	Q	80, 238
	2.0		Wang et al. (2017)	Q	80, 239
	2.1×10^{-1}		Wang et al. (2017)	Q	80, 240
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	1.6		Raventos-Duran et al. (2010)	Q	245
	5.3		Hilal et al. (2008)	Q	
		4400	Kühne et al. (2005)	Q	
	3.5×10^{1}		Katritzky et al. (1998)	Q	
	1.5×10^{4}		Nirmalakhandan et al. (1997)	Q	
		6300	Kühne et al. (2005)	?	
	7.0×10^{-1}		Abraham et al. (1990)	?	
3-nitrophenol $HOC_6H_4(NO_2)$ [554-84-7] RTZZCYNQPHTPPL-UHFFFAOYSA-N	1.6×10^{2}		Guo and Brimblecombe (2007)	M	555
	1.0		Lide and Frederikse (1995)	V	
	4.9×10^{3}		Gaffney and Senum (1984)	X	389
	2.1×10^{4}		Keshavarz et al. (2022)	Q	
	1.4×10^{4}		Duchowicz et al. (2020)	Q	299
	2.2×10^{3}		Abraham et al. (2019)	Q	
	2.0×10^{3}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{4}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{3}		Raventos-Duran et al. (2010)	Q	245
	9.5×10^{3}		Hilal et al. (2008)	Q	
	2.1×10^{2}		Modarresi et al. (2007)	Q	67
	4.8×10^{3}		English and Carroll (2001)	Q	230, 231
	1.5×10^{4}		Nirmalakhandan et al. (1997)	Q	
	4.9×10^{3}		Duchowicz et al. (2020)	?	185, 21
	4.6×10^{3}		Abraham et al. (1990)	?	
4-nitrophenol $HOC_6H_4(NO_2)$ [100-02-7] BTJIUGUIPKRLHP-UHFFFAOYSA-N	1.4×10^{1}		Chao et al. (2017)	M	
	2.1×10^{2}		Guo and Brimblecombe (2007)	M	555
	7.7×10^{2}		Tremp et al. (1993)	M	12
	3.0×10^{2}		Lide and Frederikse (1995)	V	
	2.0×10^{4}		Riederer (1990)	V	
	3.0×10^{2}		Schwarzenbach et al. (1988)	V	12
	9.4×10^{4}		Yoshida et al. (1983)	V	
	2.6×10^{4}	9100	Parsons et al. (1971)	T	417
	9.8	6000	Goldstein (1982)	X	298
	1.6		Ryan et al. (1988)	C	
	2.1×10^{4}		Keshavarz et al. (2022)	Q	
	2.2×10^{4}		Duchowicz et al. (2020)	Q	184
	1.4×10^{4}		Abraham et al. (2019)	Q	
	2.4×10^{4}		Li et al. (2014)	Q	241
	2.0×10^{3}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{3}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{3}		Raventos-Duran et al. (2010)	Q	245
	6.1×10^{3}		Hilal et al. (2008)	Q	

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	2.3×10^2		Modarresi et al. (2007)	Q	67
	1.5×10^4		Nirmalakhandan et al. (1997)	Q	
	2.4×10^4		Duchowicz et al. (2020)	?	185, 21
	2.6×10^4		Abraham et al. (1990)	?	
4-nitroanisole $C_7H_7NO_3$ [100-17-4] BNUHAJGCKIQFGE-UHFFFAOYSA-N	5.0		Ebert et al. (2023)	?	365
3-methyl-2-nitrophenol $C_7H_7NO_3$ [4920-77-8] QIORDSKCCHRSSD-UHFFFAOYSA-N	3.2		Tremp et al. (1993)	M	12
	2.4		Schwarzenbach et al. (1988)	V	12
	1.9×10^2		Modarresi et al. (2007)	Q	67
		4700	Kühne et al. (2005)	Q	
		4200	Kühne et al. (2005)	?	
4-methyl-2-nitrophenol $C_7H_7NO_3$ [119-33-5] SYDNSSSQVSOXTN-UHFFFAOYSA-N	6.7×10^{-1}		Tremp et al. (1993)	M	12
	6.1×10^{-1}		Schwarzenbach et al. (1988)	V	12
	3.9		Wang et al. (2017)	Q	80, 238
	1.9		Wang et al. (2017)	Q	80, 239
	2.5×10^{-1}		Wang et al. (2017)	Q	80, 240
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	1.2		Raventos-Duran et al. (2010)	Q	245
		4700	Kühne et al. (2005)	Q	
		6800	Kühne et al. (2005)	?	
5-methyl-2-nitrophenol $C_7H_7NO_3$ [700-38-9] NQXUSSVLFOBRSE-UHFFFAOYSA-N	7.7×10^{-1}		Tremp et al. (1993)	M	12
	6.7×10^{-1}		Schwarzenbach et al. (1988)	V	12
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	271, 243
	7.8×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	1.2		Raventos-Duran et al. (2010)	Q	245
		4700	Kühne et al. (2005)	Q	
		5600	Kühne et al. (2005)	?	
6-methyl-2-nitrophenol $C_7H_7NO_3$ [13073-29-5] AQDKZPFDOWHRDZ-UHFFFAOYSA-N	2.9×10^{-1}		Tremp et al. (1993)	M	12
	3.9		Wang et al. (2017)	Q	80, 238
	2.0×10^1		Wang et al. (2017)	Q	80, 239
	1.2×10^{-1}		Wang et al. (2017)	Q	80, 240
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9		Raventos-Duran et al. (2010)	Q	244
	1.2		Raventos-Duran et al. (2010)	Q	245
		4700	Kühne et al. (2005)	Q	
		5200	Kühne et al. (2005)	?	
3-methyl-4-nitrophenol $C_7H_7NO_3$ [2581-34-2] PIIZYNQECPTVEO-UHFFFAOYSA-N	6.2×10^2		Tremp et al. (1993)	M	12
	1.6×10^3		Raventos-Duran et al. (2010)	Q	271, 243
	3.9×10^3		Raventos-Duran et al. (2010)	Q	244
	3.9×10^3		Raventos-Duran et al. (2010)	Q	245
	2.1×10^2		Modarresi et al. (2007)	Q	67

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
4-methoxy-2-nitrophenol	5.3		Tremp et al. (1993)	M	12
$C_7H_7NO_4$	2.3×10^{-1}		Schwarzenbach et al. (1988)	V	12
[1568-70-3]	6.2		Raventos-Duran et al. (2010)	Q	242, 243
YBUGOACXDPDUIR-UHFFFAOYSA-N	1.2×10^{2}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	245
	9.4×10^{1}		Modarresi et al. (2007)	Q	67
		4900	Kühne et al. (2005)	Q	
		6600	Kühne et al. (2005)	?	
4-amino-2,6-dinitrotoluene	7.3×10^{3}		Ebert et al. (2023)	?	365
$C_7H_7N_3O_4$					
[19406-51-0]					
KQRJATLINVYHEZ-UHFFFAOYSA-N					
4-hydroxy-3-nitro-benzaldehyde	9.4		Schwarzenbach et al. (1988)	V	12
$C_7H_5NO_4$	3.9×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
[3011-34-5]	2.0×10^{2}		Raventos-Duran et al. (2010)	Q	244
YTHJCZRFJGXPTL-UHFFFAOYSA-N	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	245
2,4-dinitrophenol	9.7×10^{2}		Chao et al. (2017)	M	
$C_6H_4N_2O_5$	1.1×10^{2}		Tremp et al. (1993)	M	12
[51-28-5]	3.5×10^{1}		Schwarzenbach et al. (1988)	V	12
UFBJCMHMOXMLKC-UHFFFAOYSA-N	1.5×10^{4}		Ryan et al. (1988)	C	
	2.0×10^{2}		Abraham et al. (2019)	Q	
	2.6×10^{3}		Wang et al. (2017)	Q	80, 238
	2.1×10^{3}		Wang et al. (2017)	Q	80, 239
	3.0		Wang et al. (2017)	Q	80, 240
	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{2}		Raventos-Duran et al. (2010)	Q	245
	3.6×10^{2}		Zhang et al. (2010)	Q	287, 288
	6.2×10^{2}		Zhang et al. (2010)	Q	287, 289
	4.7		Zhang et al. (2010)	Q	287, 290
	1.3×10^{3}		Zhang et al. (2010)	Q	287, 291
	4.7×10^{1}		Modarresi et al. (2007)	Q	67
		5000	Kühne et al. (2005)	Q	
		3300	Kühne et al. (2005)	?	
2,5-dinitrophenol	1.5×10^{1}		Schwarzenbach et al. (1988)	V	12
$C_6H_4N_2O_5$	1.1×10^{2}		Abraham et al. (2019)	Q	
[329-71-5]	7.8×10^{1}		Raventos-Duran et al. (2010)	Q	271, 243
UWEZBKLLMKVIPI-UHFFFAOYSA-N	4.9×10^{2}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{2}		Raventos-Duran et al. (2010)	Q	245
picramic acid	1.0×10^{6}		HSDB (2015)	Q	99
$C_6H_5N_3O_5$					
(4,6-dinitro-2-aminophenol)					
[96-91-3]					
QXYMVUZOGFVPGH-UHFFFAOYSA-N					

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-amino-2-nitrophenol $C_6H_6N_2O_3$ [119-34-6] WHODQVWERNSQEO-UHFFFAOYSA-N	4.5×10^{6}		HSDB (2015)	Q	99
2-amino-5-nitrophenol $C_6H_6N_2O_3$ [121-88-0] DOPJTDJKZNWLRB-UHFFFAOYSA-N	1.3×10^{7}		HSDB (2015)	Q	99
2-amino-4-nitrophenol $C_6H_6N_2O_3$ [99-57-0] VLZVIIYRNMWPSN-UHFFFAOYSA-N	4.5×10^{6}		HSDB (2015)	Q	99
4-nitro-*o*-phenylenediamine $C_6H_7N_3O_2$ (4-nitro-1,2-diaminobenzene) [99-56-9] RAUWPNXIALNKQM-UHFFFAOYSA-N	1.3×10^{6}		HSDB (2015)	Q	99
4-nitrobenzene-1,3-diamine $C_6H_7N_3O_2$ [5131-58-8] DPIZKMGPXNXSGL-UHFFFAOYSA-N	1.7×10^{5}		HSDB (2015)	Q	99
2-nitro-1,4-benzenediamine $C_6H_7N_3O_2$ [5307-14-2] HVHNMNGARPCGGD-UHFFFAOYSA-N	1.7×10^{5}		HSDB (2015)	Q	99
4-methyl-2,6-dinitrophenol $C_7H_6N_2O_5$ (2,6-dinitro-*p*-cresol) [609-93-8] HOYRZHJJAHRMLL-UHFFFAOYSA-N	1.9×10^{2} 3.2×10^{2} 3.4×10^{3} 8.8×10^{1} 8.0 4.0×10^{1}	 3000 3400	Tremp et al. (1993) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Modarresi et al. (2007) Kühne et al. (2005) Kühne et al. (2005)	M Q Q Q Q Q Q ?	12 287, 288 287, 289 287, 290 287, 291 67
2-methyl-4,6-dinitrophenol $C_7H_6N_2O_5$ (6-methyl-2,4-dinitrophenol; 4,6-dinitro-*o*-cresol; DNOC) [534-52-1] ZXVONLUNISGICL-UHFFFAOYSA-N	4.3×10^{1} 7.0 9.2×10^{1} 2.3×10^{1} 9.1×10^{1} 9.0×10^{-1} 7.0 1.7 1.3×10^{3} 1.5×10^{3}		Tremp et al. (1993) Warner et al. (1980) Mackay et al. (2006d) Schwarzenbach et al. (1988) Suntio et al. (1988) Barcelo and Hennion (1997) Shen (1982) Keshavarz et al. (2022) Duchowicz et al. (2020) Wang et al. (2017)	M M V V V X C Q Q Q	12 12 12 567 80, 238

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	1.7×10^4		Wang et al. (2017)	Q	80, 239
	3.4		Wang et al. (2017)	Q	80, 240
	3.2×10^2		Zhang et al. (2010)	Q	287, 288
	2.3×10^3		Zhang et al. (2010)	Q	287, 289
	1.9×10^1		Zhang et al. (2010)	Q	287, 290
	7.2×10^2		Zhang et al. (2010)	Q	287, 291
	4.1		Goodarzi et al. (2010)	Q	568
	3.4×10^1		Modarresi et al. (2007)	Q	67
		5400	Kühne et al. (2005)	Q	
	7.0		Duchowicz et al. (2020)	?	185, 21
		4200	Kühne et al. (2005)	?	
5-nitrobenzimidazole $C_7H_5N_3O_2$ [94-52-0] XPAZGLFMMUODDK-UHFFFAOYSA-N	2.7×10^1		HSDB (2015)	Q	99
3-nitrobenzoic acid $C_7H_5NO_4$ [121-92-6] AFPHTEQTJZKQAQ-UHFFFAOYSA-N	3.4×10^3		Abraham et al. (2019)	Q	
4-nitrobenzoic acid $C_7H_5NO_4$ [62-23-7] OTLNPYWUJOZPPA-UHFFFAOYSA-N	3.2×10^3 2.6×10^4		Abraham et al. (2019) HSDB (2015)	Q Q	 99
3,5-dinitrobenzoic acid $C_7H_4N_2O_6$ [99-34-3] VYWYYJYRVSBHJQ-UHFFFAOYSA-N	8.0×10^4		Abraham et al. (2019)	Q	
2,4,6-trinitrobenzoic acid $C_7H_3N_3O_8$ [129-66-8] KAQBNBSMMVTKRN-UHFFFAOYSA-N	3.8×10^8		HSDB (2015)	Q	99
dinitrotoluene $C_7H_6N_2O_4$ [25321-14-6] MOSFIJXAXDLOML-UHFFFAOYSA-N	1.1×10^2		HSDB (2015)	Q	447
1-methyl-3,5-dinitrobenzene $C_7H_6N_2O_4$ [618-85-9] RUIFULUFLANOCI-UHFFFAOYSA-N	1.1×10^2		HSDB (2015)	Q	447

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d \ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1-methoxy-2-nitrobenzene	2.3×10^{1}		Duchowicz et al. (2020)	V	186
$C_7H_7NO_3$	2.3×10^{1}		HSDB (2015)	V	
[91-23-6]	3.3×10^{1}		Duchowicz et al. (2020)	Q	
CFBYEGUGFPZCNF-UHFFFAOYSA-N	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	7.8		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{2}		Katritzky et al. (1998)	Q	
2-methyl-5-nitrobenzenamine	1.2×10^{3}		HSDB (2015)	Q	99
$C_7H_8N_2O_2$					
(5-nitro-*o*-toluidine)					
[99-55-8]					
DSBIJCMXAIKKKI-UHFFFAOYSA-N					
2-methoxy-5-nitrobenzenamine	7.6×10^{2}		HSDB (2015)	Q	545
$C_7H_8N_2O_3$					
(5-nitro-*o*-anisidine)					
[99-59-2]					
NIPDVSLAMPAWTP-UHFFFAOYSA-N					
(2-nitroethenyl)benzene	2.8		HSDB (2015)	Q	447
$C_8H_7NO_2$					
[102-96-5]					
PIAOLBVUVDXHHL-UHFFFAOYSA-N					
1,2-dimethyl-3-nitrobenzene	1.9×10^{-1}		HSDB (2015)	Q	447
$C_8H_9NO_2$	3.9×10^{-1}		Zhang et al. (2010)	Q	287, 288
[83-41-0]	2.9×10^{-1}		Zhang et al. (2010)	Q	287, 289
FVHAWXWFPBPFOS-UHFFFAOYSA-N	2.6×10^{-1}		Zhang et al. (2010)	Q	287, 290
	1.0×10^{-1}		Zhang et al. (2010)	Q	287, 291
1,2-dimethyl-4-nitrobenzene	3.9×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_8H_9NO_2$	3.1×10^{-1}		Zhang et al. (2010)	Q	287, 289
[99-51-4]	8.0×10^{-1}		Zhang et al. (2010)	Q	287, 290
HFZKOYWDLDYELC-UHFFFAOYSA-N	1.0×10^{-1}		Zhang et al. (2010)	Q	287, 291
1,4-dimethyl-2-nitrobenzene	3.9×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_8H_9NO_2$	2.5×10^{-1}		Zhang et al. (2010)	Q	287, 289
[89-58-7]	2.2×10^{-1}		Zhang et al. (2010)	Q	287, 290
BSFHJMGROOFSRA-UHFFFAOYSA-N	1.0×10^{-1}		Zhang et al. (2010)	Q	287, 291
2,4-dimethyl-1-nitrobenzene	3.9×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_8H_9NO_2$	3.1×10^{-1}		Zhang et al. (2010)	Q	287, 289
[89-87-2]	4.3×10^{-1}		Zhang et al. (2010)	Q	287, 290
BBUPBICWUURTNP-UHFFFAOYSA-N	1.0×10^{-1}		Zhang et al. (2010)	Q	287, 291
4-methyl-2-nitroanisole	7.2		Zhang et al. (2010)	Q	287, 288
$C_8H_9NO_3$	1.6		Zhang et al. (2010)	Q	287, 289
[119-10-8]	6.0×10^{1}		Zhang et al. (2010)	Q	287, 290
LGNMURXRPLMVJI-UHFFFAOYSA-N	2.7		Zhang et al. (2010)	Q	287, 291

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
2-methyl-3-nitrobenzoic acid $C_8H_7NO_4$ [1975-50-4] YPQAFWHSMWWPLX-UHFFFAOYSA-N	2.2×10^{3}		Abraham et al. (2019)	Q	
3-methyl-4-nitrobenzoic acid $C_8H_7NO_4$ [3113-71-1] XDTTUTIFWDAMIX-UHFFFAOYSA-N	9.2×10^{2}		Abraham et al. (2019)	Q	
2-methyl-3,5-dinitrobenzoic acid $C_8H_6N_2O_6$ [28169-46-2] CDVNZMKTJIBBBV-UHFFFAOYSA-N	3.7×10^{6}		Abraham et al. (2019)	Q	
1-(1-methylethyl)-4-nitrobenzene $C_9H_{11}NO_2$ [1817-47-6] JXMYUMNAEKRMIP-UHFFFAOYSA-N	2.4×10^{-1} 1.3×10^{-1} 3.9×10^{-1} 1.4×10^{-1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
5-nitro-8-hydroxyquinoline $C_9H_6N_2O_3$ (nitroxoline) [4008-48-4] RJIWZDNTCBHXAL-UHFFFAOYSA-N	2.7×10^{3}		Abraham et al. (2019)	Q	
2-(1-methylpropyl)-4,6-dinitrophenol $C_{10}H_{12}N_2O_5$ (dinoseb) [88-85-7] OWZPCEFYPSAJFR-UHFFFAOYSA-N	2.2 2.0×10^{-2} 1.9×10^{-4} 1.4×10^{2} 5.2×10^{2} 1.3×10^{2} 4.3×10^{2} 6.2×10^{-3} 1.7×10^{3} 	 6400 7200 	Tremp et al. (1993) Suntio et al. (1988) Barcelo and Hennion (1997) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Goodarzi et al. (2010) Kühne et al. (2005) MacBean (2012a) Kühne et al. (2005) Mackay et al. (2006d)	M V X Q Q Q Q Q Q ? ? W	12 12 567 287, 288 287, 289 287, 290 287, 291 568, 571 12 595
1-nitronaphthalene $C_{10}H_7NO_2$ [86-57-7] RJKGJBPXVHTNJL-UHFFFAOYSA-N	4.6 5.6 2.9×10^{-1} 3.8 9.8 6.4 3.5 4.7 4.2		Chao et al. (2017) Altschuh et al. (1999) Mackay et al. (2006d) Mackay et al. (1995) Keshavarz et al. (2022) Duchowicz et al. (2020) Abraham et al. (2019) Parnis et al. (2015) Zhang et al. (2010) Zhang et al. (2010)	M M V V Q Q Q Q Q Q	 558 369 287, 288 287, 289

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
	1.6		Zhang et al. (2010)	Q	287, 290
	4.7		Zhang et al. (2010)	Q	287, 291
	2.1		Modarresi et al. (2007)	Q	67
	5.6		Duchowicz et al. (2020)	?	185, 21
2-nitronaphthalene $C_{10}H_7NO_2$ [581-89-5] ZJYJZEAJZXVAMF-UHFFFAOYSA-N	6.8		Parnis et al. (2015)	Q	369
1,3-dinitronaphthalene $C_{10}H_6N_2O_4$ [606-37-1] ULALSFRIGPMWRS-UHFFFAOYSA-N	1.2×10^2		Parnis et al. (2015)	Q	369
1,5-dinitronaphthalene $C_{10}H_6N_2O_4$ [605-71-0] ZUTCJXFCHHDFJS-UHFFFAOYSA-N	1.1×10^2		Parnis et al. (2015)	Q	369
1,8-dinitronaphthalene $C_{10}H_6N_2O_4$ [602-38-0] AVCSMMMOCOTIHF-UHFFFAOYSA-N	5.2×10^3		Parnis et al. (2015)	Q	369
dinoterb $C_{10}H_{12}N_2O_5$ [1420-07-1] IIPZYDQGBIWLBU-UHFFFAOYSA-N	1.7 9.1×10^{-1} 9.3×10^{-1}		Barcelo and Hennion (1997) Goodarzi et al. (2010) MacBean (2012a)	X Q ?	567 568, 569
4-(1-methylpropyl)-2-nitrophenol $C_{10}H_{13}NO_3$ (4-*sec*-butyl-2-nitrophenol) [3555-18-8] GCDCKEORRIGZKI-UHFFFAOYSA-N	1.0×10^{-1} 2.4×10^{-1} 1.2×10^{-1} 3.9×10^{-1} 4.9×10^{-1}		Tremp et al. (1993) Schwarzenbach et al. (1988) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010)	M V Q Q Q	12 12 242, 243 244 245
		5800 4300	Kühne et al. (2005) Kühne et al. (2005)	Q ?	
1-methyl-4-nitronaphthalene $C_{11}H_9NO_2$ [880-93-3] FRLVKAJKOYFHKQ-UHFFFAOYSA-N	7.7		Parnis et al. (2015)	Q	369
1-methyl-5-nitronaphthalene $C_{11}H_9NO_2$ [91137-27-8] AOSRALZFDNFXFZ-UHFFFAOYSA-N	5.0		Parnis et al. (2015)	Q	369

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
1-methyl-6-nitronaphthalene $C_{11}H_9NO_2$ [105752-67-8] SOXBGESONWKYDX-UHFFFAOYSA-N	5.0		Parnis et al. (2015)	Q	369
2-methyl-1-nitronaphthalene $C_{11}H_9NO_2$ [881-03-8] IZNWACYOILBFEG-UHFFFAOYSA-N	1.5		Parnis et al. (2015)	Q	369
3-methyl-1-nitronaphthalene $C_{11}H_9NO_2$ [13615-38-8] HKMFJWNUOWBRGF-UHFFFAOYSA-N	3.9		Parnis et al. (2015)	Q	369
3-nitrodibenzofuran $C_{12}H_7NO_3$ [5410-97-9] UVFAHDAUVZRVCC-UHFFFAOYSA-N	2.6×10^{1}		Parnis et al. (2015)	Q	369
musk ambrette (artificial) $C_{12}H_{16}N_2O_5$ [83-66-9] SUAUILGSCPYJCS-UHFFFAOYSA-N	1.4×10^{1} 7.0×10^{2} 2.4 2.2×10^{-1} 4.6×10^{1}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	99 287, 288 287, 289 287, 290 287, 291
bis(*p*-nitrophenyl) ether $C_{12}H_8N_2O_5$ [101-63-3] MWAGUKZCDDRDCS-UHFFFAOYSA-N	5.4×10^{3} 2.3×10^{2} 3.0×10^{3} 1.1×10^{4}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
4-nitroazobenzene $C_{12}H_9N_3O_2$ [2491-52-3] TZTDJBMGPQLSLI-UHFFFAOYSA-N	1.8×10^{1}		Ebert et al. (2023)	?	316
4-nitro-N-phenylbenzenamine $C_{12}H_{10}N_2O_2$ [836-30-6] XXYMSQQCBUKFHE-UHFFFAOYSA-N	2.4×10^{3} 1.7×10^{2} 2.9×10^{4} 2.5×10^{3}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
2-cyclohexyl-4,6-dinitrophenol $C_{12}H_{14}N_2O_5$ [131-89-5] QJYHUJAGJUHXJN-UHFFFAOYSA-N	1.8×10^{2}		HSDB (2015)	Q	99
dinoseb acetate $C_{12}H_{14}N_2O_6$ [2813-95-8] RDJTWDKSYLLHRW-UHFFFAOYSA-N	1.5×10^{3}		Ebert et al. (2023)	?	316

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dipicrylamine $C_{12}H_5N_7O_{12}$ (2,2',4,4',6,6'- hexanitrodiphenylamine) [131-73-7] CBCIHIVRDWLAME-UHFFFAOYSA-N	4.3×10^{11}		HSDB (2015)	Q	99
1,2-dihydro-5-nitroacenaphthylene $C_{12}H_9NO_2$ (5-nitroacenaphthene) [602-87-9] CUARLQDWYSRQDF-UHFFFAOYSA-N	9.0 9.2		HSDB (2015) Parnis et al. (2015)	Q Q	99 369
2-nitro-1,1'-biphenyl $C_{12}H_9NO_2$ [86-00-0] YOJKKXRJMXIKSR-UHFFFAOYSA-N	1.6×10^{1}		Parnis et al. (2015)	Q	369
3-nitro-1,1'-biphenyl $C_{12}H_9NO_2$ [2113-58-8] FYRPEHRWMVMHQM-UHFFFAOYSA-N	9.9		Parnis et al. (2015)	Q	369
4-nitro-1,1'-biphenyl $C_{12}H_9NO_2$ [92-93-3] BAJQRLZAPXASRD-UHFFFAOYSA-N	2.8 2.5×10^{1}		HSDB (2015) Parnis et al. (2015)	Q Q	545 369
2-nitro-9H-fluorene $C_{13}H_9NO_2$ [607-57-8] XFOHWECQTFIEIX-UHFFFAOYSA-N	3.4×10^{1} 9.5×10^{1}		HSDB (2015) Parnis et al. (2015)	Q Q	545 369
5-*tert*-butyl-4,6-dinitro-1,2,3- trimethylbenzene $C_{13}H_{18}N_2O_4$ [145-39-1] MINYPECWDZURGR-UHFFFAOYSA-N	3.4×10^{1} 2.1 4.6×10^{-2} 1.1		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
penoxaline $C_{13}H_{19}N_3O_4$ (pendimethalin) [40487-42-1] CHIFOSRWCNZCFN-UHFFFAOYSA-N	1.2×10^{1} 2.7×10^{-1} 2.6×10^{-3} 4.8×10^{-3} 4.8 3.4×10^{1} 7.9×10^{-1}		Fendinger and Glotfelty (1990) Glotfelty et al. (1987) Barcelo and Hennion (1997) Goodarzi et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Maniere et al. (2011)	M V X Q Q Q ?	 567 568 67 165
2,6-dinitro-4-octylphenol $C_{14}H_{20}N_2O_5$ [4097-33-0] NYGISSDEOKKXOE-UHFFFAOYSA-N	1.6×10^{4}		HSDB (2015)	Q	99

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
musk ketone	3.0		Lee et al. (2012)	M	
$C_{14}H_{18}N_2O_5$	5.2×10^3		HSDB (2015)	Q	99
[81-14-1]	2.1×10^4		Zhang et al. (2010)	Q	287, 288
WXCMHFPAUCOJIG-UHFFFAOYSA-N	2.6×10^2		Zhang et al. (2010)	Q	287, 289
	8.4		Zhang et al. (2010)	Q	287, 290
	5.0×10^2		Zhang et al. (2010)	Q	287, 291
moskene	4.8×10^1		Zhang et al. (2010)	Q	287, 288
$C_{14}H_{18}N_2O_4$	1.4×10^1		Zhang et al. (2010)	Q	287, 289
[116-66-5]	7.5×10^{-1}		Zhang et al. (2010)	Q	287, 290
UHWURQRPEIFIAK-UHFFFAOYSA-N	2.5		Zhang et al. (2010)	Q	287, 291
nitrothal-isopropyl	5.7×10^2		Ebert et al. (2023)	?	316
$C_{14}H_{17}NO_6$					
[10552-74-6]					
VJAWBEFMCIINFU-UHFFFAOYSA-N					
9-ethyl-3-nitrocarbazole	3.3×10^2		Zhang et al. (2010)	Q	287, 288
$C_{14}H_{12}N_2O_2$	6.9×10^2		Zhang et al. (2010)	Q	287, 289
[86-20-4]	1.1×10^3		Zhang et al. (2010)	Q	287, 290
WONHLSYSHMRRGO-UHFFFAOYSA-N	2.5×10^2		Zhang et al. (2010)	Q	287, 291
2-nitroanthracene	1.0×10^2		Parnis et al. (2015)	Q	369
$C_{14}H_9NO_2$					
[3586-69-4]					
NZWGQBVOKHEKLD-UHFFFAOYSA-N					
9-nitroanthracene	1.6×10^1		Parnis et al. (2015)	Q	369
$C_{14}H_9NO_2$					
[602-60-8]					
LSIKFJXEYJIZNB-UHFFFAOYSA-N					
3-nitrophenanthrene	5.4×10^1		Parnis et al. (2015)	Q	369
$C_{14}H_9NO_2$					
[17024-19-0]					
CPRHWWUDRYJODK-UHFFFAOYSA-N					
9-nitrophenanthrene	3.2×10^1		Parnis et al. (2015)	Q	369
$C_{14}H_9NO_2$					
[954-46-1]					
QTTCNQHPKFAYEZ-UHFFFAOYSA-N					
binapacryl	2.2×10^2		Ebert et al. (2023)	?	316
$C_{15}H_{18}N_2O_6$					
[485-31-4]					
ZRDUSMYWDRPZRM-UHFFFAOYSA-N					
2-nitrofluoranthene	8.2×10^1		Parnis et al. (2015)	Q	369
$C_{16}H_9NO_2$					
[13177-29-2]					
VBCBFNMZBHKVQN-UHFFFAOYSA-N					

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-nitrofluoranthene $C_{16}H_9NO_2$ [892-21-7] PIHGQKMEAMSUNA-UHFFFAOYSA-N	1.1×10^{2}		Parnis et al. (2015)	Q	369
1-[(2,4-dinitrophenyl)azo]-2-naphthol $C_{16}H_{10}N_4O_5$ (C.I. pigment orange 5) [3468-63-1] HBHZKFOUIUMKHV-UHFFFAOYSA-N	1.1×10^{9}		HSDB (2015)	Q	99
3,7-dinitrofluoranthene $C_{16}H_8N_2O_4$ [105735-71-5] WAAHHGKGQYVTNS-UHFFFAOYSA-N	4.9×10^{4}		HSDB (2015)	Q	99
1,3-dinitropyrene $C_{16}H_8N_2O_4$ [75321-20-9] UJIPQBOHUQDIAA-UHFFFAOYSA-N	6.3×10^{3}		Parnis et al. (2015)	Q	369
1,6-dinitropyrene $C_{16}H_8N_2O_4$ [42397-64-8] GUXACCKTQWVTLG-UHFFFAOYSA-N	7.6×10^{4} 7.3×10^{3}		HSDB (2015) Parnis et al. (2015)	Q Q	99 369
1,8-dinitropyrene $C_{16}H_8N_2O_4$ [42397-65-9] BLYXNIHKOMELAP-UHFFFAOYSA-N	7.6×10^{4} 2.3×10^{4}		HSDB (2015) Parnis et al. (2015)	Q Q	99 369
1-nitropyrene $C_{16}H_9NO_2$ [5522-43-0] ALRLPDGCPYIVHP-UHFFFAOYSA-N	3.9×10^{2} 2.0×10^{2}		HSDB (2015) Parnis et al. (2015)	Q Q	99 369
2-nitropyrene $C_{16}H_9NO_2$ [789-07-1] MAZCGYFIOOIVHE-UHFFFAOYSA-N	9.0×10^{1}		Parnis et al. (2015)	Q	369
4-nitropyrene $C_{16}H_9NO_2$ [57835-92-4] UISKIUIWPSPSAV-UHFFFAOYSA-N	3.9×10^{2}		HSDB (2015)	Q	99

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{mol}{m^3\,Pa}\right]$	$\frac{d\ln H_s^{cp}}{d(1/T)}$ [K]	Reference	Type	Note
N,N-diethyl-4-[(4-nitrophenyl)azo]aniline	3.7		Duchowicz et al. (2020)	V	186
$C_{16}H_{18}N_4O_2$	1.5×10^3		Duchowicz et al. (2020)	Q	
[3025-52-3]					
LVQIWDUSUJTZJF-ISLYRVAYSA-N					
disperse red 1	1.2×10^8		Duchowicz et al. (2020)	V	186
$C_{16}H_{18}N_4O_3$	1.1×10^6		Duchowicz et al. (2020)	Q	
[2872-52-8]					
FOQABOMYTOFLPZ-ZCXUNETKSA-N					
1-[(4-methyl-2-nitrophenyl)azo]-2-naphthalenol	8.2×10^6		HSDB (2015)	Q	99
$C_{17}H_{13}N_3O_3$					
(C.I. Pigment Red 3)					
[2425-85-6]					
ZLFVRXUOSPRRKQ-UHFFFAOYSA-N					
phenyl 1-hydroxy-4-nitro-2-naphthoate	1.5×10^4		Zhang et al. (2010)	Q	287, 288
$C_{17}H_{11}NO_5$	6.7×10^5		Zhang et al. (2010)	Q	287, 289
[65208-34-6]	1.1×10^2		Zhang et al. (2010)	Q	287, 290
DMPUGHYNLCGVPX-UHFFFAOYSA-N	2.7×10^5		Zhang et al. (2010)	Q	287, 291
7-nitrobenz[a]anthracene	9.9×10^1		Parnis et al. (2015)	Q	369
$C_{18}H_{11}NO_2$					
[20268-51-3]					
KOPVBVBUIYTJBG-UHFFFAOYSA-N					
6-nitrochrysene	6.6×10^2		HSDB (2015)	Q	99
$C_{18}H_{11}NO_2$					
[7496-02-8]					
UAWLTQJFZUYROA-UHFFFAOYSA-N					
meptyldinocap	8.6×10^1		Maniere et al. (2011)	?	241, 165
$C_{18}H_{24}N_2O_6$					
[131-72-6]					
NIOPZPCMRQGZCE-WEVVVXLNSA-N					
1-nitrobenzo[a]pyrene	3.1×10^3		HSDB (2015)	Q	447
$C_{20}H_{11}NO_2$					
[70021-99-7]					
ICKISBPYFVBVQG-UHFFFAOYSA-N					
3-nitrobenzo[a]pyrene	3.1×10^3		HSDB (2015)	Q	447
$C_{20}H_{11}NO_2$					
[70021-98-6]					
CQIJHYPCKYZMIV-UHFFFAOYSA-N					

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
6-nitrobenzo[a]pyrene $C_{20}H_{11}NO_2$ [63041-90-7] NMMAFYSZGOFZCM-UHFFFAOYSA-N	3.1×10^{3} 3.3×10^{2}		HSDB (2015) Parnis et al. (2015)	Q Q	447 369
MCM:NPHEN1OOH $C_6H_5NO_4$ QKMAXSKQIHICGE-UHFFFAOYSA-N	2.8×10^{4} 3.0×10^{4} 3.3×10^{3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:NCATECHOL $C_6H_5NO_4$ XJNPNXSISMKQEX-UHFFFAOYSA-N	3.2×10^{7} 8.0×10^{7} 6.0×10^{6}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:NCRES1OOH $C_7H_7NO_4$ PUXUHFKGXFXGAC-UHFFFAOYSA-N	1.7×10^{4} 8.9×10^{3} 4.7		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:MNCATECH $C_7H_7NO_4$ DPKDSDOOIONLAG-UHFFFAOYSA-N	5.6×10^{3} 8.5×10^{5} 3.6		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:NEBNZ1OOH $C_8H_9NO_4$ WELXCAQABDDCET-UHFFFAOYSA-N	1.3×10^{4} 4.9×10^{3} 1.7		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:NMXYOL1OOH $C_8H_9NO_4$ WHVCHTZZXIECJY-UHFFFAOYSA-N	9.6×10^{3} 2.2×10^{4} 2.7		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:NOXYOL1OOH $C_8H_9NO_4$ WTJTXPQAQHBAPV-UHFFFAOYSA-N	9.6×10^{3} 1.2×10^{4} 8.9		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:NPXYOL1OOH $C_8H_9NO_4$ MKCNKDVBVLGUFV-UHFFFAOYSA-N	9.6×10^{3} 1.2×10^{4} 2.7		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:DM124OHNO2 $C_8H_9NO_3$ KGDIYDUZVHFMHQ-UHFFFAOYSA-N	2.3 2.4 5.6×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:DMPHOHNO2 $C_8H_9NO_3$ YXNYMZXPUWOUJT-UHFFFAOYSA-N	2.3 1.2×10^{1} 3.5×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:DNEBNZOL $C_8H_8N_2O_5$ SYWMIOFIFBKHTK-UHFFFAOYSA-N	1.2×10^{3} 9.6×10^{3} 2.1		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
MCM:DNMXYOL $C_8H_8N_2O_5$ MHXAYMPVZDCVJX-UHFFFAOYSA-N	1.1×10^{3} 2.1×10^{4} 1.9×10^{-1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:DNOXYOL	8.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_8N_2O_5$	1.6×10^{4}		Wang et al. (2017)	Q	80, 239
JCTQXQRGEDMCSI-UHFFFAOYSA-N	2.6		Wang et al. (2017)	Q	80, 240
MCM:DNPXYOL	8.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_8H_8N_2O_5$	6.5×10^{3}		Wang et al. (2017)	Q	80, 239
RROXWBBJMPCPHD-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	80, 240
MCM:EBNZOHNO2	3.5		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_3$	1.3×10^{1}		Wang et al. (2017)	Q	80, 239
RSETVJMGQZKFCF-UHFFFAOYSA-N	7.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:ENCATECH	4.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_4$	5.1×10^{5}		Wang et al. (2017)	Q	80, 239
CGDBCFCRALNPBR-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	80, 240
MCM:MXNCATECH	3.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_4$	4.1×10^{5}		Wang et al. (2017)	Q	80, 239
DNJZITGVNONOFW-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	80, 240
MCM:MXY1OHNO2	2.3		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_3$	1.7×10^{1}		Wang et al. (2017)	Q	80, 239
KJRCHILWKQLEBC-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:OXNCATECH	3.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_4$	8.0×10^{5}		Wang et al. (2017)	Q	80, 239
BBBHATWMUPCFKG-UHFFFAOYSA-N	3.1		Wang et al. (2017)	Q	80, 240
MCM:OXY1OHNO2	2.3		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_3$	2.6×10^{1}		Wang et al. (2017)	Q	80, 239
KXWOAPZXQJGYPU-UHFFFAOYSA-N	2.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:PXNCATECH	1.1×10^{7}		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_4$	2.5×10^{8}		Wang et al. (2017)	Q	80, 239
MAHUOFZDOBGDSU-UHFFFAOYSA-N	4.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:PXY1OHNO2	2.3		Wang et al. (2017)	Q	80, 238
$C_8H_9NO_3$	8.7		Wang et al. (2017)	Q	80, 239
VIQHHRZADKSPIM-UHFFFAOYSA-N	1.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:NIPBNZ1OOH	1.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_4$	3.6×10^{3}		Wang et al. (2017)	Q	80, 239
IXEXRYHUTBEDFT-UHFFFAOYSA-N	1.2		Wang et al. (2017)	Q	80, 240
MCM:NMETOL1OOH	8.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_4$	4.4×10^{3}		Wang et al. (2017)	Q	80, 239
OTBVEKBEKVMFBF-UHFFFAOYSA-N	2.1		Wang et al. (2017)	Q	80, 240
MCM:NOETOL1OOH	8.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_4$	6.5×10^{3}		Wang et al. (2017)	Q	80, 239
ZYYASKSQLLYACE-UHFFFAOYSA-N	3.2		Wang et al. (2017)	Q	80, 240

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:NPBNZ1OOH	1.2×10^{4}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_4$	3.6×10^{3}		Wang et al. (2017)	Q	80, 239
CVKCTJQZVRPANA-UHFFFAOYSA-N	1.5		Wang et al. (2017)	Q	80, 240
MCM:NPETOL1OOH	8.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_4$	3.2×10^{3}		Wang et al. (2017)	Q	80, 239
PGRGKKYGDUKVIK-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	80, 240
MCM:NT123L1OOH	5.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_4$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
QUQYRHULCDEZAA-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:NT124L1OOH	5.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_4$	4.6×10^{4}		Wang et al. (2017)	Q	80, 239
DLQITMPSPXAOFG-UHFFFAOYSA-N	2.9×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:DNIPBNZOL	1.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}N_2O_5$	3.6×10^{3}		Wang et al. (2017)	Q	80, 239
[29385-11-3]	1.4		Wang et al. (2017)	Q	80, 240
HBYHYLBZPLCIEE-UHFFFAOYSA-N	2.5×10^{1}		Raventos-Duran et al. (2010)	Q	271, 243
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	245
MCM:DNMETOL	8.7×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}N_2O_5$	2.4×10^{4}		Wang et al. (2017)	Q	80, 239
NLLBSWNZAUXBGJ-UHFFFAOYSA-N	1.3×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:DNOETOL	7.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}N_2O_5$	1.0×10^{4}		Wang et al. (2017)	Q	80, 239
AGMONASRVOHMRW-UHFFFAOYSA-N	1.9		Wang et al. (2017)	Q	80, 240
MCM:DNPBNZOL	1.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}N_2O_5$	5.8×10^{3}		Wang et al. (2017)	Q	80, 239
FCIYPWNHZQHVEQ-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	80, 240
MCM:DNPETOL	7.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}N_2O_5$	3.9×10^{3}		Wang et al. (2017)	Q	80, 239
DZWALJMRDDSGJQ-UHFFFAOYSA-N	8.9×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:DNT123BOL	6.2×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}N_2O_5$	1.7×10^{4}		Wang et al. (2017)	Q	80, 239
KTYJIHPJHVSEQH-UHFFFAOYSA-N	3.8		Wang et al. (2017)	Q	80, 240
MCM:DNT124BOL	4.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_9H_{10}N_2O_5$	1.4×10^{4}		Wang et al. (2017)	Q	80, 239
HCZZKJMHIZGVJN-UHFFFAOYSA-N	3.9×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:HOEMPHNO2	2.1		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_3$	1.0×10^{1}		Wang et al. (2017)	Q	80, 239
YSPMBFYZTNTHGD-UHFFFAOYSA-N	2.6×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A4.8: Nitro compounds (RNO_2) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:IPBNZOHNO2	3.2		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_3$	5.6		Wang et al. (2017)	Q	80, 239
RRFSVDKJKYCCEK-UHFFFAOYSA-N	6.5×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:IPNCATECH	4.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_4$	2.0×10^{5}		Wang et al. (2017)	Q	80, 239
MCPZUPZVJHDAPC-UHFFFAOYSA-N	1.6		Wang et al. (2017)	Q	80, 240
MCM:MET1OHNO2	2.1		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_3$	1.0×10^{1}		Wang et al. (2017)	Q	80, 239
QDGFKFKXXCXYOS-UHFFFAOYSA-N	8.7×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:MTNCATECH	2.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_4$	2.6×10^{5}		Wang et al. (2017)	Q	80, 239
CJFAOEWQLMJWBQ-UHFFFAOYSA-N	1.0		Wang et al. (2017)	Q	80, 240
MCM:OET1OHNO2	2.1		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_3$	1.5×10^{1}		Wang et al. (2017)	Q	80, 239
MEMHWZGPMLWUCR-UHFFFAOYSA-N	1.4×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:OTNCATECH	2.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_4$	4.6×10^{5}		Wang et al. (2017)	Q	80, 239
JWEUFFGZFSJOFB-UHFFFAOYSA-N	2.2		Wang et al. (2017)	Q	80, 240
MCM:PBNZOHNO2	2.8		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_3$	8.5		Wang et al. (2017)	Q	80, 239
SNIBPLNVBYUZKZ-UHFFFAOYSA-N	6.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:PET1OHNO2	2.1		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_3$	5.6		Wang et al. (2017)	Q	80, 239
DXOFURYTWRHSOS-UHFFFAOYSA-N	6.3×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:PNCATECH	3.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_4$	2.9×10^{5}		Wang et al. (2017)	Q	80, 239
UWDKGIAMIWLDOZ-UHFFFAOYSA-N	1.7		Wang et al. (2017)	Q	80, 240
MCM:PTNCATECH	8.9×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_4$	1.8×10^{8}		Wang et al. (2017)	Q	80, 239
POSTUROPYARVPT-UHFFFAOYSA-N	3.7×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:T123NCATEC	2.0×10^{3}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_4$	6.0×10^{5}		Wang et al. (2017)	Q	80, 239
NRIGBHNXEXAXSY-UHFFFAOYSA-N	2.0		Wang et al. (2017)	Q	80, 240
MCM:T124NCATEC	6.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_4$	4.8×10^{8}		Wang et al. (2017)	Q	80, 239
XNILZTOSMSXQOP-UHFFFAOYSA-N	8.7×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:TM123OHNO2	1.5		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_3$	3.3×10^{1}		Wang et al. (2017)	Q	80, 239
GRYTUHBAWMNFLK-UHFFFAOYSA-N	3.0×10^{-1}		Wang et al. (2017)	Q	80, 240

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Table A4.8: Nitro compounds (RNO_2) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
MCM:TM124OHNO2	9.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_9H_{11}NO_3$	2.4×10^{4}		Wang et al. (2017)	Q	80, 239
NKOCMNXLDSIDQC-UHFFFAOYSA-N	1.0×10^{3}		Wang et al. (2017)	Q	80, 240

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A5 Organic species with fluorine (F)

A5.1 Organic fluorine

Table A5.1: Organic fluorine

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
fluoromethane	6.1×10^{-4}	2100	Burkholder et al. (2019)	L	1
CH_3F	6.1×10^{-4}	2000	Burkholder et al. (2015)	L	
[593-53-3]	6.2×10^{-4}	2200	Brockbank (2013)	L	1, 596
NBVXSUQYWXRMNV-UHFFFAOYSA-N	6.1×10^{-4}	2000	Sander et al. (2011)	L	
	6.1×10^{-4}	2000	Sander et al. (2006)	L	
	5.8×10^{-4}	2200	Wilhelm et al. (1977)	L	
	5.8×10^{-4}	2100	Swain and Thornton (1962)	M	
	5.8×10^{-4}	2200	Glew and Moelwyn-Hughes (1953)	M	597
	5.8×10^{-4}		Duchowicz et al. (2020)	V	186
	5.1×10^{-4}		Mackay and Shiu (1981)	V	
	5.8×10^{-4}		Hine and Mookerjee (1975)	V	
	7.1×10^{-4}		Yaws (2003)	X	237, 80
	1.0×10^{-7}		Hayer et al. (2022)	Q	20
	2.6×10^{-3}		Duchowicz et al. (2020)	Q	
	8.7×10^{-5}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	6.7×10^{-4}		Gharagheizi et al. (2010)	Q	246
	9.2×10^{-5}		Hilal et al. (2008)	Q	
		2200	Kühne et al. (2005)	Q	
	5.1×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	7.7×10^{-4}		English and Carroll (2001)	Q	230, 231
	6.5×10^{-4}		Russell et al. (1992)	Q	279
	5.8×10^{-4}		Suzuki et al. (1992)	Q	232
	1.9×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	5.9×10^{-4}		Irmann (1965)	Q	
		2200	Kühne et al. (2005)	?	
	7.1×10^{-4}		Yaws (1999)	?	21, 80
	4.7×10^{-4}		Abraham and Weathersby (1994)	?	21
	7.0×10^{-4}		Yaws and Yang (1992)	?	21, 80
difluoromethane	6.4×10^{-4}	2100	Kutsuna (2017)	M	1
CH_2F_2	6.8×10^{-4}	2500	Anderson (2011)	M	
(R32)	3.0×10^{-4}	3500	Miguel et al. (2000)	M	
[75-10-5]	6.9×10^{-4}	2400	Maaßen (1995)	M	598
RWRIWBAIICGTTQ-UHFFFAOYSA-N	6.9×10^{-4}	2300	Reichl (1995)	M	599
	7.9×10^{-4}		Hayer et al. (2022)	Q	20
	1.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	8.4×10^{-4}		Hilal et al. (2008)	Q	
		2200	Kühne et al. (2005)	Q	
	3.1×10^{-2}		Yaffe et al. (2003)	Q	248, 249
		2400	Kühne et al. (2005)	?	

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.6×10^{-4}		Yaws (1999)	?	21
	8.6×10^{-4}		Yaws and Yang (1992)	?	21
trifluoromethane	1.3×10^{-4}	2500	Burkholder et al. (2019)	L	
CHF_3	1.2×10^{-4}	2200	Burkholder et al. (2019)	L	70
(R23)	1.3×10^{-4}	2500	Burkholder et al. (2015)	L	
[75-46-7]	1.2×10^{-4}	2200	Burkholder et al. (2015)	L	70
XPDWGBQVDMORPB-UHFFFAOYSA-N	1.3×10^{-4}	3300	Sander et al. (2011)	L	
	1.3×10^{-4}	3200	Wilhelm et al. (1977)	L	
	2.1×10^{-4}	2500	Miguel et al. (2000)	M	
	1.3×10^{-4}	2400	Zheng et al. (1997)	M	600
	1.2×10^{-4}	2400	Maaßen (1995)	M	601
	1.0×10^{-4}		Hine and Mookerjee (1975)	V	
	1.3×10^{-4}		Yaws (2003)	X	237
	1.0×10^{-4}		Irmann (1965)	C	
	1.3×10^{-4}		Hayer et al. (2022)	Q	20
	1.0×10^{-4}		Keshavarz et al. (2022)	Q	
	8.8×10^{-4}		Duchowicz et al. (2020)	Q	184
	1.3×10^{-4}	2700	Li et al. (2019)	Q	1
	4.0×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	1.3×10^{-4}		Gharagheizi et al. (2010)	Q	246
	2.0×10^{-4}		Hilal et al. (2008)	Q	
	4.0×10^{-5}		Modarresi et al. (2007)	Q	67
		2200	Kühne et al. (2005)	Q	
	1.2×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	1.1×10^{-4}		Irmann (1965)	Q	
	1.0×10^{-4}		Duchowicz et al. (2020)	?	185, 21
		3000	Kühne et al. (2005)	?	
	1.3×10^{-4}		Yaws (1999)	?	21
	1.3×10^{-4}		Yaws and Yang (1992)	?	21
tetrafluoromethane	2.1×10^{-6}	1800	Burkholder et al. (2019)	L	1
CF_4	1.7×10^{-6}	2300	Burkholder et al. (2019)	L	70
(carbontetrafluoride)	2.1×10^{-6}	1800	Burkholder et al. (2015)	L	1
[75-73-0]	1.7×10^{-6}	2300	Burkholder et al. (2015)	L	70
TXEYQDLBPFQVAA-UHFFFAOYSA-N	2.1×10^{-6}	2300	Warneck and Williams (2012)	L	
	2.1×10^{-6}	1800	Sander et al. (2011)	L	1
	2.1×10^{-6}	1800	Wilhelm et al. (1977)	L	
	2.0×10^{-6}	2000	Reichl (1995)	M	602
	2.1×10^{-6}	1800	Scharlin and Battino (1995)	M	603
	2.1×10^{-6}	1800	Scharlin and Battino (1994)	M	604
	2.1×10^{-6}		Park et al. (1982)	M	
	2.1×10^{-6}	1600	Cosgrove and Walkley (1981)	M	11
	2.0×10^{-6}	1900	Wen and Muccitelli (1979)	M	605
	2.1×10^{-6}	1800	Ashton et al. (1968)	M	606

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.0×10^{-6}	1500	Morrison and Johnstone (1954)	M	607
	1.9×10^{-6}		Hine and Mookerjee (1975)	V	
	3.3×10^{-6}		Pierotti (1965)	T	
	1.8×10^{-6}		Yaws (2003)	X	237
	1.9×10^{-6}		Irmann (1965)	C	
	2.8×10^{-6}		Hayer et al. (2022)	Q	20
	6.9×10^{-7}		Keshavarz et al. (2022)	Q	
	1.4×10^{-5}		Duchowicz et al. (2020)	Q	
	2.1×10^{-6}	1800	Li et al. (2019)	Q	1
	5.5×10^{-6}		Gharagheizi et al. (2012)	Q	
	2.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
	9.2×10^{-6}		Hilal et al. (2008)	Q	
	3.2×10^{-6}		Modarresi et al. (2007)	Q	67
		2200	Kühne et al. (2005)	Q	
	2.9×10^{-6}		Goss (2005)	Q	
	2.0×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	1.0×10^{-6}	-840	Bonifácio et al. (2001)	Q	
	1.2×10^{-8}		Katritzky et al. (1998)	Q	
	5.4×10^{-6}		Nirmalakhandan and Speece (1988)	Q	
	1.6×10^{-6}		Irmann (1965)	Q	
	1.9×10^{-6}		Duchowicz et al. (2020)	?	185, 21
		1900	Kühne et al. (2005)	?	
	1.9×10^{-6}		Yaws (1999)	?	21
	2.1×10^{-6}	1700	Yaws et al. (1999)	?	21
	1.8×10^{-6}		Yaws and Yang (1992)	?	21
fluoroethane C_2H_5F [353-36-6] UHCBBWUQDAVSMS-UHFFFAOYSA-N	4.6×10^{-4}		Yaws (2003)	X	237
	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
	4.8×10^{-4}		Hilal et al. (2008)	Q	
	3.2×10^{-4}		Modarresi et al. (2007)	Q	67
	4.6×10^{-4}		Yaws (1999)	?	21
	5.0×10^{-4}		Abraham and Weathersby (1994)	?	21
	4.4×10^{-4}		Yaws and Yang (1992)	?	21
1,1-difluoroethane $C_2H_4F_2$ (R152a) [75-37-6] NPNPZTNLOVBDOC-UHFFFAOYSA-N	4.9×10^{-4}	2600	Burkholder et al. (2019)	L	608, 70
	4.9×10^{-4}	2600	Burkholder et al. (2015)	L	609, 70
	4.9×10^{-4}	2800	Zheng et al. (1997)	M	610
	5.0×10^{-4}	2800	Maaßen (1995)	M	611
	4.9×10^{-4}	2700	Reichl (1995)	M	612
	4.2×10^{-4}	2300	McLinden (1989)	V	
	4.8×10^{-4}		Hine and Mookerjee (1975)	V	
	4.8×10^{-4}		Irmann (1965)	C	294
	5.7×10^{-4}		Hayer et al. (2022)	Q	20
	1.2×10^{-2}		Keshavarz et al. (2022)	Q	

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	2.9×10^{-4}		Hilal et al. (2008)	Q	
	1.4×10^{-4}		Modarresi et al. (2007)	Q	67
		2600	Kühne et al. (2005)	Q	
	9.0×10^{-4}		English and Carroll (2001)	Q	230, 231
	1.4×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	4.3×10^{-4}		Irmann (1965)	Q	
	4.9×10^{-4}		Duchowicz et al. (2020)	?	185, 21
		2800	Kühne et al. (2005)	?	
	3.9×10^{-4}		Yaws (1999)	?	21, 297
	3.7×10^{-4}		Yaws and Yang (1992)	?	21, 297
1,2-difluoroethane $C_2H_4F_2$ [624-72-6] AHFMSNDOYCFEPH-UHFFFAOYSA-N	2.5×10^{-5}		HSDB (2015)	Q	99
1,1,1,2-tetrafluoroethane	1.6×10^{-4}	2700	Burkholder et al. (2019)	L	70
$C_2H_2F_4$	1.6×10^{-4}	2700	Burkholder et al. (2015)	L	70
(R134a)	1.5×10^{-4}	3100	Ooki and Yokouchi (2011)	M	70
[811-97-2]	1.6×10^{-4}	2900	Zheng et al. (1997)	M	613
LVGUZGTVOIAKKC-UHFFFAOYSA-N	1.6×10^{-4}	3000	Maaßen (1995)	M	614
	1.6×10^{-4}	2900	Reichl (1995)	M	615
	1.9×10^{-4}	1400	Chang and Criddle (1995)	M	616
	1.4×10^{-4}	2600	McLinden (1989)	V	
	2.5×10^{-4}		Hayer et al. (2022)	Q	20
	1.5×10^{-4}	3100	Li et al. (2019)	Q	1
	6.5×10^{-6}		HSDB (2015)	Q	99
	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	1.2×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-6}		Raventos-Duran et al. (2010)	Q	245
	9.7×10^{-5}		Hilal et al. (2008)	Q	
	5.5×10^{-5}		Modarresi et al. (2007)	Q	67
1,1,2,2-tetrafluoroethane $C_2H_2F_4$ [359-35-3] WXGNWUVNYMJENI-UHFFFAOYSA-N	2.9×10^{-4}		Ebert et al. (2023)	?	318

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pentafluoroethane	3.1×10^{-4}	3300	Miguel et al. (2000)	M	
C_2HF_5	3.5×10^{-5}	3000	Reichl (1995)	M	617
(R125)	8.0×10^{-5}	4800	McLinden (1989)	V	
[354-33-6]	1.3×10^{-4}		Hayer et al. (2022)	Q	20
GTLACDSXYULKMZ-UHFFFAOYSA-N	3.5×10^{-5}	3000	Li et al. (2019)	Q	1
	2.0×10^{-4}		HSDB (2015)	Q	99
	3.2×10^{-6}		Zhang et al. (2010)	Q	287, 288
	2.0×10^{-5}		Zhang et al. (2010)	Q	287, 289
	5.7×10^{-5}		Zhang et al. (2010)	Q	287, 290
	2.1×10^{-5}		Zhang et al. (2010)	Q	287, 291
		2600	Kühne et al. (2005)	Q	
		2900	Kühne et al. (2005)	?	
hexafluoroethane	6.5×10^{-7}	2100	Bonifácio et al. (2001)	M	
C_2F_6	5.3×10^{-7}		Park et al. (1982)	M	
[76-16-4]	5.6×10^{-7}	2300	Wen and Muccitelli (1979)	M	618
WMIYKQLTONQJES-UHFFFAOYSA-N	5.8×10^{-7}		Yaws (2003)	X	237
	7.1×10^{-7}		Hayer et al. (2022)	Q	20
	9.3×10^{-7}		Keshavarz et al. (2022)	Q	
	2.2×10^{-5}		Duchowicz et al. (2020)	Q	
	5.8×10^{-7}	2600	Li et al. (2019)	Q	1
	1.5×10^{-5}		Gharagheizi et al. (2012)	Q	
	4.1×10^{-7}		Zhang et al. (2010)	Q	287, 288
	1.1×10^{-5}		Zhang et al. (2010)	Q	287, 289
	8.4×10^{-7}		Zhang et al. (2010)	Q	287, 290
	1.9×10^{-6}		Zhang et al. (2010)	Q	287, 291
	8.1×10^{-7}		Gharagheizi et al. (2010)	Q	246
	1.2×10^{-5}		Hilal et al. (2008)	Q	
	1.8×10^{-6}		Modarresi et al. (2007)	Q	67
		2600	Kühne et al. (2005)	Q	
	1.2×10^{-6}	1700	Bonifácio et al. (2001)	Q	
	4.9×10^{-7}		Duchowicz et al. (2020)	?	185, 21
		2900	Kühne et al. (2005)	?	
	5.8×10^{-7}		Yaws (1999)	?	21
	5.8×10^{-7}		Yaws and Yang (1992)	?	21
1-fluoropropane	6.3×10^{-4}		Yaws (2003)	X	237, 619
C_3H_7F	7.9×10^{-5}		Gharagheizi et al. (2012)	Q	
[460-13-9]	5.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
JRHNUZCXXOTJCA-UHFFFAOYSA-N	5.7×10^{-4}		Hilal et al. (2008)	Q	
	6.2×10^{-4}		Yaws (1999)	?	21, 619
	3.6×10^{-4}		Abraham and Weathersby (1994)	?	21
	6.1×10^{-4}		Yaws and Yang (1992)	?	21, 619

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Table A5.1: Organic fluorine (. . . continued)

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2-fluoropropane	6.0×10^{-4}		Yaws (2003)	X	237, 80
C_3H_7F	2.2×10^{-4}		Gharagheizi et al. (2012)	Q	
[420-26-8]	6.0×10^{-4}		Gharagheizi et al. (2010)	Q	246
PRNZBCYBKGCOFI-UHFFFAOYSA-N	2.5×10^{-4}		Hilal et al. (2008)	Q	
	5.9×10^{-4}		Yaws (1999)	?	21, 80
	3.8×10^{-4}		Abraham and Weathersby (1994)	?	21
	5.8×10^{-4}		Yaws and Yang (1992)	?	21, 80
1,1,1,2,2-pentafluoropropane	3.0×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
$C_3H_3F_5$					
[1814-88-6]					
FDOPVENYMZRARC-UHFFFAOYSA-N					
1,1,1,3,3,3-hexafluoropropane	1.2×10^{-6}		Zhang et al. (2010)	Q	287, 288
$C_3H_2F_6$	3.9×10^{-5}		Zhang et al. (2010)	Q	287, 289
[690-39-1]	1.8×10^{-4}		Zhang et al. (2010)	Q	287, 290
NSGXIBWMJZWTPY-UHFFFAOYSA-N	2.7×10^{-6}		Zhang et al. (2010)	Q	287, 291
1,1,1,2,3,3,3-heptafluoropropane	1.4×10^{-5}	3300	Reichl (1995)	M	620
C_3HF_7	2.2×10^{-4}		Hayer et al. (2022)	Q	20
(R227)	6.2×10^{-7}		HSDB (2015)	Q	99
[431-89-0]		2900	Kühne et al. (2005)	Q	
YFMFNYKEUDLDTL-UHFFFAOYSA-N		3300	Kühne et al. (2005)	?	
octafluoropropane	1.2×10^{-7}	6900	Wen and Muccitelli (1979)	M	
C_3F_8	3.0×10^{-7}		Duchowicz et al. (2020)	V	186
(R218)	3.0×10^{-7}		HSDB (2015)	V	
[76-19-7]	3.2×10^{-7}		Yaws (2003)	X	237, 80
QYSGYZVSCZSLHT-UHFFFAOYSA-N	1.1×10^{-3}		Hayer et al. (2022)	Q	20
	5.1×10^{-5}		Duchowicz et al. (2020)	Q	
	4.2×10^{-5}		Gharagheizi et al. (2012)	Q	
	7.7×10^{-8}		Zhang et al. (2010)	Q	287, 288
	1.0×10^{-5}		Zhang et al. (2010)	Q	287, 289
	3.8×10^{-7}		Zhang et al. (2010)	Q	287, 290
	4.5×10^{-7}		Zhang et al. (2010)	Q	287, 291
	3.0×10^{-7}		Gharagheizi et al. (2010)	Q	246
	1.1×10^{-5}		Hilal et al. (2008)	Q	
	3.1×10^{-7}		Yaws (1999)	?	21, 80
decafluorobutane	1.5×10^{-8}		HSDB (2015)	Q	99
C_4F_{10}					
[355-25-9]					
KAVGMUDTWQVPDF-UHFFFAOYSA-N					

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
octafluorocyclobutane	1.2×10^{-6}	3000	Clever et al. (2005)	L	621, 622
C_4F_8	1.3×10^{-6}	3300	Scharlin and Battino (1994)	M	623
[115-25-3]	1.2×10^{-6}		Park et al. (1982)	M	
BCCOBQSFUDVTJQ-UHFFFAOYSA-N	1.2×10^{-6}	3000	Wen and Muccitelli (1979)	M	624
	1.2×10^{-6}		Duchowicz et al. (2020)	V	186
	2.5×10^{-6}		Yaws (2003)	X	237, 372
	1.6×10^{-6}		Hayer et al. (2022)	Q	20
	3.9×10^{-3}		Duchowicz et al. (2020)	Q	
	1.0×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-7}		Zhang et al. (2010)	Q	287, 288
	1.6×10^{-6}		Zhang et al. (2010)	Q	287, 289
	2.2×10^{-6}		Zhang et al. (2010)	Q	287, 290
	1.0×10^{-6}		Zhang et al. (2010)	Q	287, 291
	2.6×10^{-6}		Gharagheizi et al. (2010)	Q	246
	9.2×10^{-6}		Hilal et al. (2008)	Q	
		4500	Kühne et al. (2005)	Q	
		3800	Kühne et al. (2005)	?	
	2.6×10^{-6}		Yaws (1999)	?	21, 372
	2.5×10^{-6}		Yaws and Yang (1992)	?	21, 372
1,1,1,2,2,3,4,5,5,5-decafluoropentane	4.4×10^{-8}		Zhang et al. (2010)	Q	287, 288
$C_5H_2F_{10}$	3.2×10^{-5}		Zhang et al. (2010)	Q	287, 289
[138495-42-8]	1.8×10^{-4}		Zhang et al. (2010)	Q	287, 290
RIQRGMUSBYGDBL-UHFFFAOYSA-N	9.0×10^{-7}		Zhang et al. (2010)	Q	287, 291
dodecafluoropentane	4.6×10^{-8}		Brockbank (2013)	L	
C_5F_{12}	6.1×10^{-6}		Hilal et al. (2008)	Q	
[678-26-2]					
NJCBUSHGCBERSK-UHFFFAOYSA-N					
tetradecafluorohexane	9.3×10^{-9}		Brockbank (2013)	L	
C_6F_{14}	5.4×10^{-10}		HSDB (2015)	Q	99
(perflexane)					
[355-42-0]					
ZJIJAJXFLBMLCK-UHFFFAOYSA-N					
fluorocyclohexane	1.3×10^{-3}		Hilal et al. (2008)	Q	
$C_6H_{11}F$					
[372-46-3]					
GOBGVVAHHOUMDK-UHFFFAOYSA-N					
1-fluoroheptane	2.7×10^{-4}		Hilal et al. (2008)	Q	
$C_7H_{15}F$					
[661-11-0]					
BITLXSQYFZTQGC-UHFFFAOYSA-N					

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexadecafluoroheptane C_7F_{16} [335-57-9] LGUZHRODIJCVOC-UHFFFAOYSA-N	3.0×10^{-9} 1.9×10^{-7}		Brockbank (2013) Hilal et al. (2008)	L Q	
1-fluorooctane $C_8H_{17}F$ [463-11-6] DHIVLKMGKIZOHF-UHFFFAOYSA-N	1.5×10^{-4}		Hilal et al. (2008)	Q	
perfluorooctane C_8F_{18} [307-34-6] YVBBRRALBYAZBM-UHFFFAOYSA-N	8.0×10^{-10}		Brockbank (2013)	L	
eicosafluorononane C_9F_{20} [375-96-2] UVWPNDVAQBNQBG-UHFFFAOYSA-N	4.5×10^{-9}		Hilal et al. (2008)	Q	
perfluoroundecane $C_{11}F_{24}$ [307-49-3] VCIVYCHKSHULON-UHFFFAOYSA-N	1.3×10^{-13} 1.2×10^{-11} 1.2×10^{-9} 6.0×10^{-12}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9, 10,10-henicosafluorododecane $C_{12}H_5F_{21}$ (perfluorodecyl ethane) [154478-87-2] HUPGRQWHZOWFPQ-UHFFFAOYSA-N	5.1×10^{-10}		Plassmann et al. (2010)	Q	
1,1,1,2,2,3,3,4,4,5,5,6,6- tridecafluorotetradecane $C_{14}H_{17}F_{13}$ [133331-77-8] WRYIIOKOQSICTB-UHFFFAOYSA-N	6.4×10^{-7}		Plassmann et al. (2010)	Q	
1,1,1,2,2,3,3,4,4,5,5,6,6- tridecafluoroicosane $C_{20}H_{29}F_{13}$ [154628-00-9] BREOHRVZEZMFOB-UHFFFAOYSA-N	2.5×10^{-7}		Plassmann et al. (2010)	Q	
1,1,1,2,2,3,3,4,4,5,5,6,6- tridecafluorodocosane $C_{22}H_{33}F_{13}$ [133310-71-1] ZKYMFADZZFTYJH-UHFFFAOYSA-N	2.0×10^{-7}		Plassmann et al. (2010)	Q	

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Table A5.1: Organic fluorine (. . . continued)

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1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluorotetracosane $C_{24}H_{33}F_{17}$ [117146-18-6] FTECWCULPOFDJS-UHFFFAOYSA-N	4.0×10^{-9}		Plassmann et al. (2010)	Q	
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10-henicosafluorohexacosane $C_{26}H_{33}F_{21}$ LZENXKBSJNMIKY-UHFFFAOYSA-N	3.2×10^{-11}		Plassmann et al. (2010)	Q	
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosafluorohexacosane $C_{26}H_{29}F_{25}$ [93454-73-0] OUASUHCMZXPMCH-UHFFFAOYSA-N	1.6×10^{-13}		Plassmann et al. (2010)	Q	
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosafluorooctacosane $C_{28}H_{33}F_{25}$ [93454-74-1] CZCMNCOQMXNFTL-UHFFFAOYSA-N	8.0×10^{-14}		Plassmann et al. (2010)	Q	
fluoroethene C_2H_3F (vinyl fluoride) [75-02-5] XUCNUKMRBVNAPB-UHFFFAOYSA-N	8.2×10^{-5}		HSDB (2015)	Q	99
1,1-difluoroethene $C_2H_2F_2$ [75-38-7] BQCIDUSAKPWEOX-UHFFFAOYSA-N	2.5×10^{-5} 2.6×10^{-5} 2.8×10^{-5} 2.8×10^{-5} 5.1×10^{-5} 2.9×10^{-5} 1.6×10^{-5} 2.6×10^{-5} 2.5×10^{-5}		HSDB (2015) Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Hilal et al. (2008) Yaffe et al. (2003) Katritzky et al. (1998) Yaws (1999) Yaws and Yang (1992)	V X Q Q Q Q Q ? ?	 237 246 248, 249 21 21
trifluoroethene C_2HF_3 [359-11-5] MIZLGWKEZAPEFJ-UHFFFAOYSA-N	2.3×10^{-5}		HSDB (2015)	Q	99

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Table A5.1: Organic fluorine (. . . continued)

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tetrafluoroethene	1.6×10^{-5}	2100	Wilhelm et al. (1977)	L	
C_2F_4	1.6×10^{-5}		HSDB (2015)	V	
[116-14-3]	1.6×10^{-5}		Yaws (2003)	X	237
BFKJFAAPBSQJPD-UHFFFAOYSA-N	9.8×10^{-6}		Irmann (1965)	C	38
	1.4×10^{-5}		Hayer et al. (2022)	Q	20
	2.8×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-5}		Gharagheizi et al. (2010)	Q	246
	1.9×10^{-5}		Hilal et al. (2008)	Q	
		2400	Kühne et al. (2005)	Q	
	2.8×10^{-5}		Yao et al. (2002)	Q	229
		2100	Kühne et al. (2005)	?	
	1.6×10^{-5}		Yaws (1999)	?	21
	1.6×10^{-5}		Yaws and Yang (1992)	?	21
3,3,3-trifluoropropene	1.3×10^{-5}		HSDB (2015)	Q	99
$C_3H_3F_3$					
[677-21-4]					
FDMFUZHCIRHGRG-UHFFFAOYSA-N					
hexafluoropropene	2.9×10^{-6}	2400	Wilhelm et al. (1977)	L	
C_3F_6	6.8×10^{-6}	2600	Maaßen (1995)	M	625
[116-15-4]	7.3×10^{-6}		Hayer et al. (2022)	Q	20
HCDGVLDPFQMKDK-UHFFFAOYSA-N	1.8×10^{-6}		HSDB (2015)	Q	99
	3.6×10^{-5}		Hilal et al. (2008)	Q	
		2800	Kühne et al. (2005)	Q	
		2400	Kühne et al. (2005)	?	
1,1,3,3,3-pentafluoro-2-(trifluoromethyl)-1-propene	2.9×10^{-7}		HSDB (2015)	Q	99
C_4F_8					
(perfluoroisobutylene)					
[382-21-8]					
DAFIBNSJXIGBQB-UHFFFAOYSA-N					
(perfluorobutyl)ethene	9.0×10^{-8}		HSDB (2015)	Q	99
$C_6H_3F_9$	8.8×10^{-8}		Zhang et al. (2010)	Q	287, 288
(4:2 FTO)	3.3×10^{-6}		Zhang et al. (2010)	Q	287, 289
[19430-93-4]	8.6×10^{-6}		Zhang et al. (2010)	Q	287, 290
GVEUEBXMTMZVSD-UHFFFAOYSA-N	3.6×10^{-7}		Zhang et al. (2010)	Q	287, 291
	2.5×10^{-6}	4100	Goss et al. (2006)	Q	
(*E*)-perfluoro(4-methyl-2-pentene)	6.4×10^{-8}		Ebert et al. (2023)	?	365
C_6F_{12}					
[3709-71-5]					
SAPOZTRFWJZUFT-OWOJBTEDSA-N					

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(perfluorohexyl)ethene $C_8H_3F_{13}$ (6:2 FTO) [25291-17-2] FYQFWFHDPNXORA-UHFFFAOYSA-N	1.1×10^{-4}	4900	Abusallout et al. (2022)	M	
	5.3×10^{-7}	4900	Goss et al. (2006)	Q	
(perfluorooctyl)ethene $C_{10}H_3F_{17}$ (8:2 FTO) [21652-58-4] NKAMGQZDVMQEJL-UHFFFAOYSA-N	1.4×10^{-7}	5700	Goss et al. (2006)	Q	
(perfluorodecyl)ethene $C_{12}H_3F_{21}$ (10:2 FTO) [30389-25-4] UCHSAVGOZUCXHC-UHFFFAOYSA-N	3.3×10^{-8}	6500	Goss et al. (2006)	Q	
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-pentacosafluorooctacos-13-ene $C_{28}H_{31}F_{25}$ LBVDHZOJOFOXJM-FOCLMDBBSA-N	8.0×10^{-11}		Plassmann et al. (2010)	Q	
fluorobenzene C_6H_5F [462-06-6] PYLWMHQQBFSUBP-UHFFFAOYSA-N	1.5×10^{-3}	4100	Brockbank (2013)	L	1
	1.6×10^{-3}		Mackay and Shiu (1981)	L	
	1.6×10^{-3}	3900	Hiatt (2013)	M	
	1.4×10^{-3}	4300	Dewulf et al. (1999)	M	
	1.1×10^{-3}		Li and Carr (1993)	M	
	1.5×10^{-3}	4400	Hartkopf and Karger (1973)	M	
	1.6×10^{-3}		Schüürmann (2000)	V	
	1.4×10^{-3}		Mackay et al. (1993)	V	
	1.6×10^{-3}		Yaws (2003)	X	237
	1.6×10^{-3}		Sieg et al. (2008)	C	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	8.6×10^{-3}		Duchowicz et al. (2020)	Q	299
	1.6×10^{-3}		Li et al. (2014)	Q	241
	2.2×10^{-3}		Li et al. (2014)	Q	241
	4.1×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.0×10^{-3}		Hilal et al. (2008)	Q	
	1.4×10^{-3}		Modarresi et al. (2007)	Q	67
		3700	Kühne et al. (2005)	Q	
	1.6×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	2.3×10^{-3}		Yao et al. (2002)	Q	229, 267
	1.3×10^{-3}		Katritzky et al. (1998)	Q	

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Table A5.1: Organic fluorine (. . . continued)

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	5.0×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	1.6×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		3800	Kühne et al. (2005)	?	
	1.6×10^{-3}		Yaws (1999)	?	21
	1.2×10^{-3}		Hoff et al. (1993)	?	21
	1.6×10^{-3}		Yaws and Yang (1992)	?	21
	1.5×10^{-3}		Abraham et al. (1990)	?	
1,2-difluorobenzene	1.3×10^{-3}	3700	Brockbank (2013)	L	1
$C_6H_4F_2$	1.2×10^{-3}	3500	Brockbank et al. (2013)	M	
(*o*-difluorobenzene)	1.4×10^{-3}		Yaws (2003)	X	237
[367-11-3]	3.6×10^{-3}		Gharagheizi et al. (2012)	Q	
GOYDNIKZWGIXJT-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.2×10^{-3}		Hilal et al. (2008)	Q	
	6.4×10^{-4}		Modarresi et al. (2007)	Q	67
	5.1×10^{-3}		Yao et al. (2002)	Q	229
	1.4×10^{-3}		Yaws (1999)	?	21
	1.4×10^{-3}		Yaws and Yang (1992)	?	21
1,3-difluorobenzene	3.6×10^{-3}		Gharagheizi et al. (2012)	Q	
$C_6H_4F_2$	1.3×10^{-3}		Hilal et al. (2008)	Q	
(*m*-difluorobenzene)	5.2×10^{-4}		Modarresi et al. (2007)	Q	67
[372-18-9]	1.3×10^{-4}		Yaws (1999)	?	21
UEMGWPRHOOEKTA-UHFFFAOYSA-N	1.3×10^{-4}		Yaws and Yang (1992)	?	21
1,4-difluorobenzene	1.6×10^{-3}	3900	Hiatt (2013)	M	
$C_6H_4F_2$	1.3×10^{-3}		Yaws (2003)	X	237
(*p*-difluorobenzene)	4.2×10^{-3}		Gharagheizi et al. (2012)	Q	
[540-36-3]	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
QUGUFLJIAFISSW-UHFFFAOYSA-N	1.8×10^{-3}		Hilal et al. (2008)	Q	
	3.5×10^{-4}		Modarresi et al. (2007)	Q	67
	9.5×10^{-4}		Yao et al. (2002)	Q	229
	1.3×10^{-3}		Yaws (1999)	?	21
	1.3×10^{-3}		Yaws and Yang (1992)	?	21
1,2,3,5-tetrafluorobenzene	5.1×10^{-4}		Duchowicz et al. (2020)	V	186
$C_6H_2F_4$	1.2×10^{-2}		Duchowicz et al. (2020)	Q	
[2367-82-0]	5.0×10^{-4}		Hilal et al. (2008)	Q	
UHHYOKRQTQBKSB-UHFFFAOYSA-N	9.4×10^{-5}		Modarresi et al. (2007)	Q	67
1,2,4,5-tetrafluorobenzene	5.6×10^{-4}		Duchowicz et al. (2020)	V	186
$C_6H_2F_4$	1.1×10^{-2}		Duchowicz et al. (2020)	Q	
[327-54-8]	7.0×10^{-4}		Hilal et al. (2008)	Q	
SDXUIOOHCIQXRP-UHFFFAOYSA-N	1.2×10^{-4}		Modarresi et al. (2007)	Q	67
pentafluorobenzene	7.5×10^{-4}	4800	Hiatt (2013)	M	
C_6HF_5					
[363-72-4]					
WACNXHCZHTVBJM-UHFFFAOYSA-N					

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hexafluorobenzene	3.0×10^{-4}	5100	Brockbank (2013)	L	1
C_6F_6	5.5×10^{-4}	5200	Hiatt (2013)	M	
[392-56-3]	2.9×10^{-4}		Schröder et al. (2011)	M	
ZQBFAOFFOQMSGJ-UHFFFAOYSA-N	1.1×10^{-4}		Schröder et al. (2011)	Q	626
(trifluoromethyl)-benzene	6.0×10^{-4}		Duchowicz et al. (2020)	V	186
$C_6H_5CF_3$	5.8×10^{-4}		HSDB (2015)	V	
(α,α,α-trifluorotoluene;	6.1×10^{-4}		Abraham et al. (1994a)	V	
benzotrifluoride)					
[98-08-8]	6.2×10^{-4}		Mackay and Shiu (1981)	V	
GETTZEONDQJALK-UHFFFAOYSA-N	5.9×10^{-4}		Yaws (2003)	X	237
	3.5×10^{-3}		Duchowicz et al. (2020)	Q	
	3.2×10^{-3}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	5.7×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.3×10^{-3}		Hilal et al. (2008)	Q	
	2.7×10^{-4}		Modarresi et al. (2007)	Q	67
	6.2×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	6.1×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	1.9×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	6.0×10^{-4}		Yaws (1999)	?	21
	6.0×10^{-4}		Yaws and Yang (1992)	?	21
decafluorobiphenyl	6.7×10^{-3}	3600	Hiatt (2013)	M	
$C_{10}F_{10}$					
[434-90-2]					
ONUFSRWQCKNVSL-UHFFFAOYSA-N					
carbonyl fluoride	3.5×10^{-1}		Mirabel et al. (1996)	M	
COF_2	9.9×10^{-3}		De Bruyn et al. (1995a)	M	449
[353-50-4]	2.0×10^{-1}		George et al. (1993)	X	627
IYRWEQXVUNLMAY-UHFFFAOYSA-N					
formyl fluoride	3.0×10^{-2}		Kanakidou et al. (1995)	E	
FCHO					
[1493-02-3]					
NHGVZTMBVDFPHJ-UHFFFAOYSA-N					
2-fluoroethanol	4.6×10^{-1}		Burkholder et al. (2019)	L	
C_2H_5FO	4.6×10^{-1}		Burkholder et al. (2015)	L	
[371-62-0]	4.6×10^{-1}		O'Farrell and Waghorne (2010)	M	
GGDYAKVUZMZKRV-UHFFFAOYSA-N	5.5		Duchowicz et al. (2020)	V	186
	1.9		Duchowicz et al. (2020)	Q	
	1.4		HSDB (2015)	Q	99
	2.5		Hilal et al. (2008)	Q	
	5.6		Modarresi et al. (2007)	Q	67

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2,2-difluoroethanol	9.3×10^{-1}		Burkholder et al. (2019)	L	
$C_2H_4F_2O$	9.3×10^{-1}		Burkholder et al. (2015)	L	
[359-13-7]	9.2×10^{-1}		O'Farrell and Waghorne (2010)	M	
VOGSDFLJZPNWHY-UHFFFAOYSA-N					
2,2,2-trifluoroethanol	4.7×10^{-1}	6200	Burkholder et al. (2019)	L	
CF_3CH_2OH	4.7×10^{-1}	6200	Burkholder et al. (2015)	L	
[75-89-8]	4.7×10^{-1}	6200	Sander et al. (2011)	L	
RHQDFWAXVIIEBN-UHFFFAOYSA-N	4.7×10^{-1}	6200	Chen et al. (2003)	M	
	4.3×10^{-1}		Eger et al. (1999)	M	14
	5.8×10^{-1}	5900	Rochester and Symonds (1973)	M	
	3.4×10^{-1}		Keshavarz et al. (2022)	Q	
	8.6×10^{-1}		Duchowicz et al. (2020)	Q	
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	3.5×10^{-1}		Zhang et al. (2010)	Q	287, 288
	2.4×10^{-1}		Zhang et al. (2010)	Q	287, 289
	3.8		Zhang et al. (2010)	Q	287, 290
	4.7×10^{-2}		Zhang et al. (2010)	Q	287, 291
	6.1×10^{-1}		Hilal et al. (2008)	Q	
	3.4		Modarresi et al. (2007)	Q	67
		6500	Kühne et al. (2005)	Q	
	7.7×10^{-1}		Goss (2005)	Q	628
	6.1×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	6.9×10^{-1}		English and Carroll (2001)	Q	230, 231
	1.6×10^{-2}		Katritzky et al. (1998)	Q	
	5.0×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	5.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		5600	Kühne et al. (2005)	?	
	5.7×10^{-1}		Abraham et al. (1990)	?	
1,1,1-trifluoro-2-propanol	1.3×10^{-1}		Eger et al. (1999)	M	14
$CF_3CHOHCH_3$	4.5×10^{-1}	6300	Rochester and Symonds (1973)	M	
[374-01-6]	4.6×10^{-1}		Keshavarz et al. (2022)	Q	
GILIYJDBJZWGBG-UHFFFAOYSA-N	1.1		Duchowicz et al. (2020)	Q	184
	3.1×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	4.9×10^{-1}		Modarresi et al. (2007)	Q	67
		6900	Kühne et al. (2005)	Q	
	5.2×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	4.5×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		6300	Kühne et al. (2005)	?	

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2,2,3,3-tetrafluoro-1-propanol	1.4	7000	Burkholder et al. (2019)	L	
$CHF_2CF_2CH_2OH$	1.4	7000	Burkholder et al. (2015)	L	
[76-37-9]	1.4	7000	Sander et al. (2011)	L	
NBUKAOOFKZFCGD-UHFFFAOYSA-N	1.4	7000	Chen et al. (2003)	M	
	7.5×10^{-1}		Eger et al. (1999)	M	14
	1.6	6700	Rochester and Symonds (1973)	M	
	4.6×10^{-1}		Keshavarz et al. (2022)	Q	
	8.3×10^{-1}		Duchowicz et al. (2020)	Q	
	1.2		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	6.0×10^{-1}		Hilal et al. (2008)	Q	
	1.0		Modarresi et al. (2007)	Q	67
		6900	Kühne et al. (2005)	Q	
	3.7×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	1.6		Duchowicz et al. (2020)	?	185, 21
		6600	Kühne et al. (2005)	?	
2,2,3,3,3-pentafluoro-1-propanol	1.4×10^{-1}	4300	Burkholder et al. (2019)	L	
$CF_3CF_2CH_2OH$	1.4×10^{-1}	4300	Burkholder et al. (2015)	L	
[422-05-9]	1.4×10^{-1}	4300	Sander et al. (2011)	L	
PSQZJKGXDGNDFP-UHFFFAOYSA-N	1.4×10^{-1}	4300	Chen et al. (2003)	M	
	6.9×10^{-2}		Eger et al. (1999)	M	14
	4.5×10^{-1}	6000	Rochester and Symonds (1973)	M	
	4.6×10^{-1}		Keshavarz et al. (2022)	Q	
	1.8×10^{-1}		Duchowicz et al. (2020)	Q	184
	2.0×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.3×10^{-1}		Hilal et al. (2008)	Q	
	4.8×10^{-1}		Modarresi et al. (2007)	Q	67
		6800	Kühne et al. (2005)	Q	
	4.4×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		6000	Kühne et al. (2005)	?	
1,1,1,3,3,3-hexafluoro-2-propanol	1.0×10^{-1}		Eger et al. (1999)	M	14
$CF_3CHOHCF_3$	2.4×10^{-1}	6700	Rochester and Symonds (1973)	M	
[920-66-1]	4.6×10^{-1}		Keshavarz et al. (2022)	Q	
BYEAHWXPCBROCE-UHFFFAOYSA-N	2.2		Duchowicz et al. (2020)	Q	
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	2.5×10^{-2}		Hilal et al. (2008)	Q	
	2.6×10^{-1}		Modarresi et al. (2007)	Q	67
		6800	Kühne et al. (2005)	Q	
	2.4×10^{-1}		Goss (2005)	Q	629
	2.3×10^{-1}		Nirmalakhandan and Speece (1988)	Q	
	2.3×10^{-1}		Duchowicz et al. (2020)	?	185, 21

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Table A5.1: Organic fluorine (. . . continued)

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		6700	Kühne et al. (2005)	?	
	2.3×10^{-1}		Abraham et al. (1990)	?	
trifluoroacetylfluoride	3.0×10^{-2}		Mirabel et al. (1996)	M	
CF_3COF	9.5×10^{-3}		De Bruyn et al. (1995a)	M	449
[354-34-7]	3.0×10^{-2}		George et al. (1994b)	M	630
DCEPGADSNJKOJK-UHFFFAOYSA-N	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	4.3×10^{-3}		Duchowicz et al. (2020)	Q	
	3.0×10^{-2}		Duchowicz et al. (2020)	?	185, 21
1-fluoro-2-propanone	4.6×10^{-1}		Burkholder et al. (2019)	L	
CH_2FCOCH_3	4.6×10^{-1}		Burkholder et al. (2015)	L	
(fluoroacetone)	4.6×10^{-1}		O'Farrell and Waghorne (2010)	M	
[430-51-3]					
MSWVMWGCNZQPIA-UHFFFAOYSA-N					
1,1,1-trifluoro-2-propanone	1.4	8900	Burkholder et al. (2019)	L	
CF_3COCH_3	1.4	8900	Burkholder et al. (2015)	L	
(1,1,1-trifluoroacetone)	1.4	8900	Sander et al. (2011)	L	
[421-50-1]	1.4	8900	Betterton (1991)	M	
FHUDAMLDXFJHJE-UHFFFAOYSA-N	1.4		Keshavarz et al. (2022)	Q	
	1.8×10^{-2}		Duchowicz et al. (2020)	Q	
	4.9		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	4.4×10^{-2}		Modarresi et al. (2007)	Q	67
	1.3		Duchowicz et al. (2020)	?	185, 21
1,1-difluoro-2-methoxyethane	1.3×10^{-2}		Duchowicz et al. (2020)	V	186
$C_3H_6F_2O$	2.2×10^{-2}		Duchowicz et al. (2020)	Q	
[461-57-4]					
CRGZRXUKXVTRNO-UHFFFAOYSA-N					
fluoroethanoic acid	8.0×10^{2}		Burkholder et al. (2019)	L	
CH_2FCOOH	8.0×10^{2}		Burkholder et al. (2015)	L	
(fluoroacetic acid)	8.0×10^{2}		Sander et al. (2011)	L	
[144-49-0]	8.0×10^{2}		Bowden et al. (1998a)	M	
QEWYKACRFQMRMB-UHFFFAOYSA-N	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	6.7×10^{1}		Duchowicz et al. (2020)	Q	184
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	271, 243
	9.9×10^{2}		Raventos-Duran et al. (2010)	Q	244
	9.9		Raventos-Duran et al. (2010)	Q	245
	5.4×10^{2}		Hilal et al. (2008)	Q	
	8.0×10^{2}		Duchowicz et al. (2020)	?	185, 21

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
difluoroethanoic acid	3.0×10^{2}	6900	Burkholder et al. (2019)	L	
CHF_2COOH	3.0×10^{2}	6900	Burkholder et al. (2015)	L	
(difluoroacetic acid)	3.0×10^{2}	6900	Sander et al. (2011)	L	
[381-73-7]	3.0×10^{2}	6900	Bowden et al. (1998a)	M	
PBWZKZYHONABLN-UHFFFAOYSA-N	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	8.5×10^{1}		Duchowicz et al. (2020)	Q	299
	4.9×10^{2}		Raventos-Duran et al. (2010)	Q	242, 243
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	244
	4.9		Raventos-Duran et al. (2010)	Q	245
	7.2×10^{1}		Hilal et al. (2008)	Q	
		7700	Kühne et al. (2005)	Q	
	3.0×10^{2}		Duchowicz et al. (2020)	?	185, 21
		6900	Kühne et al. (2005)	?	
trifluoroethanoic acid	5.7×10^{1}	4100	Burkholder et al. (2019)	L	
CF_3COOH	5.7×10^{1}	4100	Burkholder et al. (2015)	L	
(trifluoroacetic acid)	8.9×10^{1}	9300	Sander et al. (2011)	L	
[76-05-1]	5.7×10^{1}	4100	Kutsuna and Horia (2008)	M	
DTQVDTLACAAQTR-UHFFFAOYSA-N	8.3×10^{1}		Kwan (2001)	M	631
	8.8×10^{1}	9300	Bowden et al. (1996)	M	
	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	2.3		Abusallout et al. (2022)	Q	632
	1.9×10^{1}		Duchowicz et al. (2020)	Q	184
	6.2×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	2.5		Raventos-Duran et al. (2010)	Q	245
	2.3		Zhang et al. (2010)	Q	287, 288
	1.6×10^{-1}		Zhang et al. (2010)	Q	287, 289
	8.0		Zhang et al. (2010)	Q	287, 290
	3.9		Zhang et al. (2010)	Q	287, 291
	4.0×10^{-1}		Hilal et al. (2008)	Q	
	6.3×10^{1}		Modarresi et al. (2007)	Q	67
		7700	Kühne et al. (2005)	Q	
	8.9×10^{1}		Duchowicz et al. (2020)	?	185, 21
		9400	Kühne et al. (2005)	?	
perfluoropropanoic acid	8.8		Kwan (2001)	M	631
$C_3HF_5O_2$	4.3×10^{-1}		Abusallout et al. (2022)	Q	632
[422-64-0]					
LRMSQVBRUNSOJL-UHFFFAOYSA-N					
perfluorobutanoic acid	8.1×10^{-1}		Kwan (2001)	M	631
$C_4HF_7O_2$	8.2×10^{-2}		Abusallout et al. (2022)	Q	632
[375-22-4]	8.2×10^{-2}		Zhang et al. (2010)	Q	287, 288
YPJUNDFVDDCYIH-UHFFFAOYSA-N	7.2×10^{-1}		Zhang et al. (2010)	Q	287, 289
	2.5×10^{-1}		Zhang et al. (2010)	Q	287, 290
	6.4×10^{-1}		Zhang et al. (2010)	Q	287, 291

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
perfluoropentanoic acid $C_5HF_9O_2$ [2706-90-3] CXZGQIAOTKWCDB-UHFFFAOYSA-N	6.7×10^{-1} 1.6×10^{-2}		Kwan (2001) Abusallout et al. (2022)	M Q	631 632
perfluorohexanoic acid $C_6HF_{11}O_2$ [307-24-4] PXUULQAPEKKVAH-UHFFFAOYSA-N	1.1 3.0×10^{-3} 4.4×10^{-1} 1.2×10^{-1}		Kwan (2001) Abusallout et al. (2022) Arp et al. (2006) Arp et al. (2006)	M Q Q Q	631 632 633 634
perfluoroheptanoic acid $C_7HF_{13}O_2$ [375-85-9] ZWBAMYVPMDSJGQ-UHFFFAOYSA-N	1.7 5.8×10^{-4} 5.7×10^{-4} 5.0×10^{-2} 2.2×10^{-2} 5.6×10^{-3} 1.8×10^{-1} 5.7×10^{-2}		Kwan (2001) Abusallout et al. (2022) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Arp et al. (2006) Arp et al. (2006)	M Q Q Q Q Q Q Q	631 632 287, 288 287, 289 287, 290 287, 291 633 634
pentadecafluorooctanoic acid $C_8HF_{15}O_2$ (perfluorooctanoic acid; PFOA) [335-67-1] SNGREZUHAYWORS-UHFFFAOYSA-N	4.9×10^{-2} 4.0×10^{-1} 2.8 1.1×10^{-4} 1.1×10^{-4} 1.0×10^{-2} 1.2×10^{-2} 1.1×10^{-3} 1.1×10^{-4} 1.0×10^{-2} 2.1×10^{-2} 1.1×10^{-3} 9.5×10^{-2} 2.0×10^{-2}		Kutsuna and Hori (2008) Li et al. (2007) Kwan (2001) Abusallout et al. (2022) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Arp et al. (2006) Arp et al. (2006)	M M M Q Q Q Q Q Q Q Q Q Q Q	 631 632 287, 288 287, 289 287, 290 287, 291 287, 288 287, 289 287, 290 287, 291 633 634
perfluorononanoic acid $C_9HF_{17}O_2$ [375-95-1] UZUFPBIDKMEQEQ-UHFFFAOYSA-N	4.3×10^{-2} 5.3×10^{-3}		Arp et al. (2006) Arp et al. (2006)	Q Q	633 634
2H,2H-perfluorodecanoic acid $C_{10}H_3F_{17}O_2$ (8:2 FTCA) [27854-31-5] XTBXSCIWOVSSGB-UHFFFAOYSA-N	5.8×10^{-4}		Abusallout et al. (2022)	M	
perfluorodecanoic acid $C_{10}HF_{19}O_2$ [335-76-2] PCIUEQPBYFRTEM-UHFFFAOYSA-N	2.5×10^{-2} 1.1×10^{-3}		Arp et al. (2006) Arp et al. (2006)	Q Q	633 634

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Table A5.1: Organic fluorine (. . . continued)

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perfluoroundecanoic acid $C_{11}HF_{21}O_2$ [2058-94-8] SIDINRCMMRKXGQ-UHFFFAOYSA-N	1.3×10^{-2} 1.9×10^{-4}		Arp et al. (2006) Arp et al. (2006)	Q Q	633 634
perfluorododecanoic acid $C_{12}HF_{23}O_2$ [307-55-1] CXGONMQFMIYUJR-UHFFFAOYSA-N	6.4×10^{-3}		Plassmann et al. (2011)	E	
perfluorotetradecanoic acid $C_{14}HF_{27}O_2$ [376-06-7] RUDINRUXCKIXAJ-UHFFFAOYSA-N	1.6×10^{-3}		Plassmann et al. (2011)	E	
1,1,1,3,3,3-hexafluoro-2-propanone C_3F_6O [684-16-2] VBZWSGALLODQNC-UHFFFAOYSA-N	3.2×10^{-3}		HSDB (2015)	Q	99
desflurane $C_3H_2F_6O$ [57041-67-5] DPYMFVXJLLWWEU-UHFFFAOYSA-N	1.4×10^{-4} 9.0×10^{-5}		HSDB (2015) Abraham and Weathersby (1994)	Q ?	99 21
sevoflurane $C_4H_3F_7O$ [28523-86-6] DFEYYRMXOJXZRJ-UHFFFAOYSA-N	5.2×10^{-5} 1.5×10^{-4}		HSDB (2015) Abraham and Weathersby (1994)	Q ?	99 21
ethyl 2,2,2-trifluoroethyl ether $C_4H_7F_3O$ [461-24-5] ZKNHDJMXIUOHLX-UHFFFAOYSA-N	7.2×10^{-4}		Hilal et al. (2008)	Q	
iso-indoklon $C_4H_4F_6O$ (1,1,1,3,3,3-hexafluoro-2-methoxypropane) [13171-18-1] VNXYDFNVQBICRO-UHFFFAOYSA-N	5.6×10^{-5}		Abraham and Weathersby (1994)	?	21
di(2,2,2-trifluoroethyl) ether $C_4H_4F_6O$ (flurothyl) [333-36-8] KGPPDNUWZNWPSI-UHFFFAOYSA-N	9.2×10^{-3} 3.0×10^{-4}	-390	Fukuchi et al. (2002) Abraham and Weathersby (1994)	V ?	33 21

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(2,2,2-trifluoroethoxy)-ethene	5.4×10^{-4}	4000	Fogg and Sangster (2003)	L	
$CF_3CH_2OCHCH_2$	3.3×10^{-4}		Steward et al. (1973)	L	14
(fluoroxene; fluroxene)	5.5×10^{-4}	4000	Allott et al. (1973)	L	
[406-90-6]	5.5×10^{-4}	4300	Smith et al. (1981b)	M	
DLEGDLSLRSOURQ-UHFFFAOYSA-N	3.2×10^{-4}		Stoelting and Longshore (1972)	M	14
	3.3×10^{-4}		Munson et al. (1964)	M	14
	9.5×10^{-5}		Hilal et al. (2008)	Q	
	3.6×10^{-4}		Abraham and Weathersby (1994)	?	21
	5.1×10^{-4}		Abraham et al. (1990)	?	
2,2,2-trifluoroethyl methanoate	5.4×10^{-3}	4700	Burkholder et al. (2019)	L	
$HCOOCH_2CF_3$	5.4×10^{-3}	4700	Burkholder et al. (2015)	L	
[32042-38-9]	5.4×10^{-3}	4700	Sander et al. (2011)	L	
CAFROQYMUICGNO-UHFFFAOYSA-N	5.4×10^{-3}	4700	Kutsuna et al. (2005)	M	
2,2,2-trifluoroethyl ethanoate	5.5×10^{-3}	5200	Burkholder et al. (2019)	L	635
$CH_3COOCH_2CF_3$	5.5×10^{-3}	5200	Burkholder et al. (2015)	L	636
[406-95-1]	5.5×10^{-3}	5200	Sander et al. (2011)	L	
ZOWSJJBOQDKOHI-UHFFFAOYSA-N	5.7×10^{-3}	5300	Kutsuna et al. (2004)	M	
		6400	Kühne et al. (2005)	Q	
		5500	Kühne et al. (2005)	?	
trifluoroethanoic acid, methyl ester	1.1×10^{-3}	5300	Burkholder et al. (2019)	L	637, 638
CF_3COOCH_3	1.1×10^{-3}	5300	Burkholder et al. (2015)	L	639, 640
(methyl trifluoroacetate)	1.1×10^{-3}	5300	Sander et al. (2011)	L	641
[431-47-0]	1.2×10^{-3}	4900	Kutsuna et al. (2004)	M	
VMVNZNXAVJHNDJ-UHFFFAOYSA-N		6100	Kühne et al. (2005)	Q	
		5800	Kühne et al. (2005)	?	
trifluoroethanoic acid, ethyl ester	8.9×10^{-4}	4900	Burkholder et al. (2019)	L	
$CF_3COOC_2H_5$	8.9×10^{-4}	4900	Burkholder et al. (2015)	L	
(ethyl trifluoroacetate)	8.9×10^{-4}	4900	Sander et al. (2011)	L	
[383-63-1]	7.1×10^{-4}	4900	Kutsuna and Kaneyasu (2021)	M	
STSCVKRWJPWALQ-UHFFFAOYSA-N	8.9×10^{-4}	4900	Kutsuna et al. (2005)	M	
trifluoro(trifluoromethyl)-oxirane	9.3×10^{-6}	2400	Clever et al. (2005)	C	642, 643
C_3F_6O					
[428-59-1]					
PGFXOWRDDHCDTE-UHFFFAOYSA-N					
3,3,4,4,4-pentafluorobutan-1-ol	5.1×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_4H_5OF_5$	3.7×10^{-1}		Zhang et al. (2010)	Q	287, 289
[54949-74-5]	4.0×10^{-2}		Zhang et al. (2010)	Q	287, 290
JPMHUDBOKDBBLG-UHFFFAOYSA-N	1.5×10^{-3}		Zhang et al. (2010)	Q	287, 291
1,1,1,3,3,3-hexafluoro-2-methyl-2-propanol	1.8×10^{-2}		Eger et al. (1999)	M	14
$C_4H_4F_6O$					
[1515-14-6]					
FQDXJYBXPOMIBX-UHFFFAOYSA-N					

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Table A5.1: Organic fluorine (. . . continued)

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2,2,3,4,4,4-hexafluoro-1-butanol $C_4H_4F_6O$ [382-31-0] LVFXLZRISXUAIL-UHFFFAOYSA-N	3.2×10^{-1}		Eger et al. (1999)	M	14
2,2,3,3,4,4,4-heptafluoro-1-butanol $C_4H_3F_7O$ [375-01-9] WXJFKAZDSQLPBX-UHFFFAOYSA-N	2.1×10^{-2}		Eger et al. (1999)	M	14
3,3,4,4,5,5,5-heptafluoro-2-pentanol $C_5H_5F_7O$ [375-14-4] RBPHBIMHZSTIDT-UHFFFAOYSA-N	9.0×10^{-3}		Eger et al. (1999)	M	14
2,2,3,3,4,4,5,5-octafluoro-1-pentanol $C_5H_4F_8O$ [355-80-6] JUGSKHLZINSXPQ-UHFFFAOYSA-N	2.5×10^{-1}		Eger et al. (1999)	M	14
1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxybutane	9.9×10^{-6}		Zhang et al. (2010)	Q	287, 288
$C_5H_3F_9O$	1.3×10^{-5}		Zhang et al. (2010)	Q	287, 289
[163702-07-6]	8.4×10^{-6}		Zhang et al. (2010)	Q	287, 290
OKIYQFLILPKULA-UHFFFAOYSA-N	3.9×10^{-6}		Zhang et al. (2010)	Q	287, 291
1-ethoxy-1,1,2,3,3,3-hexafluoro-2-(trifluoromethyl)propane	7.5×10^{-6}		Zhang et al. (2010)	Q	287, 288
$C_6H_5F_9O$	4.7×10^{-5}		Zhang et al. (2010)	Q	287, 289
[163702-06-5]	8.0×10^{-6}		Zhang et al. (2010)	Q	287, 290
SQEGLLMNIBLLNQ-UHFFFAOYSA-N	3.3×10^{-6}		Zhang et al. (2010)	Q	287, 291
1H,1H,2H,2H-perfluorohexan-1-ol	1.3×10^{-3}		Abusallout et al. (2022)	M	
$C_6H_5F_9O$	6.6×10^{-3}	4500	Wu and Chang (2011)	M	11
(4:2 FTOH)	1.3×10^{-2}		Goss et al. (2006)	M	
[2043-47-2]	6.1×10^{-5}	5400	Lei et al. (2004)	M	327
JCMNMOBHVPONLD-UHFFFAOYSA-N	5.6×10^{-1}		Wu and Chang (2011)	V	
	1.8×10^{-3}		Abusallout et al. (2022)	Q	632
	1.8×10^{-3}		Zhang et al. (2010)	Q	287, 288
	1.3×10^{-1}		Zhang et al. (2010)	Q	287, 289
	8.2×10^{-3}		Zhang et al. (2010)	Q	287, 290
	2.4×10^{-4}		Zhang et al. (2010)	Q	287, 291
	4.3×10^{-4}		Arp et al. (2006)	Q	633
	3.1×10^{-5}		Arp et al. (2006)	Q	634
	7.2×10^{-3}	7200	Goss et al. (2006)	Q	

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2,3,3,4,4,5,5,6,6,6-undecafluoro-1-hexanol $C_6H_3F_{11}O$ [423-46-1] QZFZPVVDBGXQTB-UHFFFAOYSA-N	1.7×10^{-3}		Eger et al. (1999)	M	14
1-ethoxy-1,1,2,2,3,3,4,4,4-nonafluorobutane $C_6H_5F_9O$ [163702-05-4] DFUYAWQUODQGFF-UHFFFAOYSA-N	7.5×10^{-6} 1.2×10^{-5} 7.5×10^{-6} 3.0×10^{-6}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro-1-heptanol $C_7H_4F_{12}O$ [335-99-9] BYKNGMLDSIEFFG-UHFFFAOYSA-N	6.4×10^{-2}		Eger et al. (1999)	M	14
2,2,3,3,4,4,5,5,6,6,7,7,7-tridecafluoro-1-heptanol $C_7H_3F_{13}O$ [375-82-6] STLNAVFVCIRZLL-UHFFFAOYSA-N	6.0×10^{-4}		Eger et al. (1999)	M	14
1H,1H,2H,2H-perfluoro-1-octanol $C_8H_5F_{13}O$ (6:2 FTOH) [647-42-7] GRJRKPMIRMSBNK-UHFFFAOYSA-N	3.3×10^{-4} 1.7×10^{-4} 1.5×10^{-3} 8.5×10^{-5} 9.4×10^{-4} 3.9×10^{-1} 6.6×10^{-5} 6.5×10^{-5} 9.5×10^{-3} 3.4×10^{-3} 9.9×10^{-6} 2.8×10^{-4} 1.8×10^{-5} 1.8×10^{-3}	4700 2600 7000 8000	Abusallout et al. (2022) Wu and Chang (2011) Goss et al. (2006) Lei et al. (2004) Eger et al. (1999) Wu and Chang (2011) Abusallout et al. (2022) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Arp et al. (2006) Arp et al. (2006) Goss et al. (2006)	M M M M M V Q Q Q Q Q Q Q Q	 11 327 14 632 287, 288 287, 289 287, 290 287, 291 633 634
2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-1-octanol $C_8H_3F_{15}O$ [307-30-2] PJDOLCGOTSNFJM-UHFFFAOYSA-N	2.3×10^{-4}		Eger et al. (1999)	M	14
3-ethoxyperfluoro(2-methylhexane) $C_9H_5F_{15}O$ [297730-93-9] HHBBIOLEJRWIGU-UHFFFAOYSA-N	1.9×10^{-8}		Ebert et al. (2023)	?	365

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Table A5.1: Organic fluorine (. . . continued)

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methyl perfluoro(8-(fluoroformyl)-5-methyl-4,7-dioxanonanoate)	5.8×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{10}H_3F_{15}O_5$	5.1×10^{-4}		Zhang et al. (2010)	Q	287, 289
[69116-73-0]	2.6×10^{-4}		Zhang et al. (2010)	Q	287, 290
JOMJXRTUQWIHQD-UHFFFAOYSA-N	1.3×10^{-1}		Zhang et al. (2010)	Q	287, 291
3,3,4,4,5,5,6,6,6-nonafluorohexyl methacrylate	3.4×10^{-5}		Zhang et al. (2010)	Q	287, 288
$C_{10}H_9F_9O_2$	1.6×10^{-3}		Zhang et al. (2010)	Q	287, 289
[1799-84-4]	6.5×10^{-4}		Zhang et al. (2010)	Q	287, 290
TYNRPOFACABVSI-UHFFFAOYSA-N	3.4×10^{-5}		Zhang et al. (2010)	Q	287, 291
1H,1H,2H,2H-perfluorodecan-1-ol	2.0×10^{-4}		Abusallout et al. (2022)	M	
$C_{10}H_5F_{17}O$	2.0×10^{-4}	3100	Wu and Chang (2011)	M	11
(8:2 FTOH)	1.7×10^{-4}	8800	Lei et al. (2004)	M	327
[678-39-7]	2.4×10^{-1}		Wu and Chang (2011)	V	
JJUBFBTUBACDHW-UHFFFAOYSA-N	1.1×10^{-4}		Goss et al. (2006)	V	
	2.4×10^{-6}		Abusallout et al. (2022)	Q	632
	2.4×10^{-6}		Zhang et al. (2010)	Q	287, 288
	2.6×10^{-4}		Zhang et al. (2010)	Q	287, 289
	7.3×10^{-4}		Zhang et al. (2010)	Q	287, 290
	4.3×10^{-7}		Zhang et al. (2010)	Q	287, 291
	5.7×10^{-5}		Arp et al. (2006)	Q	633
	1.6×10^{-5}		Arp et al. (2006)	Q	634
	3.8×10^{-4}	8600	Goss et al. (2006)	Q	
2-methoxyperfluoro(2,5-di(propan-2-yl)oxolane) $C_{11}H_3F_{19}O_2$ [957209-18-6] YRGYOFYTTFLPQM-UHFFFAOYSA-N	1.0×10^{-8}		Ebert et al. (2023)	?	365
3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl acrylate	1.9×10^{-6}		Zhang et al. (2010)	Q	287, 288
$C_{11}H_7F_{13}O_2$	1.9×10^{-4}		Zhang et al. (2010)	Q	287, 289
[17527-29-6]	2.9×10^{-4}		Zhang et al. (2010)	Q	287, 290
VPKQPPJQTZJZDB-UHFFFAOYSA-N	2.4×10^{-6}		Zhang et al. (2010)	Q	287, 291
2-(perfluorohexyl)ethyl methacrylate	1.2×10^{-6}		Zhang et al. (2010)	Q	287, 288
$C_{12}H_9F_{13}O_2$	1.8×10^{-4}		Zhang et al. (2010)	Q	287, 289
[2144-53-8]	1.3×10^{-4}		Zhang et al. (2010)	Q	287, 290
CDXFIRXEAJABAZ-UHFFFAOYSA-N	1.5×10^{-6}		Zhang et al. (2010)	Q	287, 291

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Table A5.1: Organic fluorine (. . . continued)

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1,1,2,2-tetrahydroperfluoro dodecanol	1.4×10^{-4}		Abusallout et al. (2022)	M	
$C_{12}H_5F_{21}O$	1.3×10^{-4}	2700	Wu and Chang (2011)	M	11
(10:2 FTOH)	2.5×10^{-1}		Wu and Chang (2011)	V	
[865-86-1]	9.0×10^{-8}		Abusallout et al. (2022)	Q	632
FLXYIZWPNQYPIT-UHFFFAOYSA-N	8.6×10^{-8}		Zhang et al. (2010)	Q	287, 288
	2.7×10^{-6}		Zhang et al. (2010)	Q	287, 289
	1.5×10^{-4}		Zhang et al. (2010)	Q	287, 290
	1.6×10^{-8}		Zhang et al. (2010)	Q	287, 291
	4.6×10^{-5}		Arp et al. (2006)	Q	633
	5.2×10^{-5}		Arp et al. (2006)	Q	634
	1.0×10^{-4}	9600	Goss et al. (2006)	Q	
	1.0×10^{-5}		Arp et al. (2006)	E	644
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl acrylate	1.3×10^{-3}		Abusallout et al. (2022)	M	
$C_{13}H_7F_{17}O_2$	7.0×10^{-8}		Zhang et al. (2010)	Q	287, 288
[27905-45-9]	1.1×10^{-5}		Zhang et al. (2010)	Q	287, 289
QUKRIOLKOHUUBM-UHFFFAOYSA-N	1.1×10^{-4}		Zhang et al. (2010)	Q	287, 290
	9.9×10^{-8}		Zhang et al. (2010)	Q	287, 291
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl methacrylate	4.4×10^{-8}		Zhang et al. (2010)	Q	287, 288
$C_{14}H_9F_{17}O_2$	1.0×10^{-5}		Zhang et al. (2010)	Q	287, 289
[1996-88-9]	5.4×10^{-5}		Zhang et al. (2010)	Q	287, 290
HBZFBSFGXQBQTB-UHFFFAOYSA-N	6.4×10^{-8}		Zhang et al. (2010)	Q	287, 291
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecan-1-ol	3.1×10^{-9}		Zhang et al. (2010)	Q	287, 288
$C_{14}H_5F_{25}O$	1.1×10^{-8}		Zhang et al. (2010)	Q	287, 289
[39239-77-5]	3.1×10^{-5}		Zhang et al. (2010)	Q	287, 290
QBBJBWKVSJWYQK-UHFFFAOYSA-N	6.9×10^{-10}		Zhang et al. (2010)	Q	287, 291
2-(perfluorodecyl)ethyl acrylate	2.5×10^{-9}		Zhang et al. (2010)	Q	287, 288
$C_{15}H_7F_{21}O_2$	3.1×10^{-7}		Zhang et al. (2010)	Q	287, 289
[17741-60-5]	2.4×10^{-5}		Zhang et al. (2010)	Q	287, 290
FIAHOPQKBBASOY-UHFFFAOYSA-N	3.7×10^{-9}		Zhang et al. (2010)	Q	287, 291
1,1,2,2-tetrahydroperfluoro-1-hexadecanol	1.1×10^{-10}		Zhang et al. (2010)	Q	287, 288
$C_{16}H_5OF_{29}$	1.4×10^{-11}		Zhang et al. (2010)	Q	287, 289
[60699-51-6]	6.1×10^{-6}		Zhang et al. (2010)	Q	287, 290
ZDUOTHMDVYXZBS-UHFFFAOYSA-N	2.9×10^{-11}		Zhang et al. (2010)	Q	287, 291

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Table A5.1: Organic fluorine (. . . continued)

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2-(perfluorodecyl)ethyl methacrylate	1.6×10^{-9}		Zhang et al. (2010)	Q	287, 288
$C_{16}H_9F_{21}O_2$	3.1×10^{-7}		Zhang et al. (2010)	Q	287, 289
[2144-54-9]	1.1×10^{-5}		Zhang et al. (2010)	Q	287, 290
FQHLOOOXLDQLPF-UHFFFAOYSA-N	2.4×10^{-9}		Zhang et al. (2010)	Q	287, 291
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-pentacosafluorotetradecyl prop-2-enoate	9.0×10^{-11}		Zhang et al. (2010)	Q	287, 288
$C_{17}H_7F_{25}O_2$	5.0×10^{-9}		Zhang et al. (2010)	Q	287, 289
[34395-24-9]	2.7×10^{-3}		Zhang et al. (2010)	Q	287, 290
SWTZSHBOMGAQKX-UHFFFAOYSA-N	1.6×10^{-10}		Zhang et al. (2010)	Q	287, 291
profluthrin $C_{17}H_{18}F_4O_2$ [223419-20-3] AGMMRUPNXPWLGF-AATRIKPKSA-N	2.5×10^{-2}		Ebert et al. (2023)	?	318
2-perfluorododecylethyl methacrylate	5.8×10^{-11}		Zhang et al. (2010)	Q	287, 288
$C_{18}H_9F_{25}O_2$	5.0×10^{-9}		Zhang et al. (2010)	Q	287, 289
[6014-75-1]	2.3×10^{-6}		Zhang et al. (2010)	Q	287, 290
LFEGLDRNIDJMKB-UHFFFAOYSA-N	9.9×10^{-11}		Zhang et al. (2010)	Q	287, 291
1,1,2,2-tetrahydroperfluoro-1-octadecanol	4.1×10^{-12}		Zhang et al. (2010)	Q	287, 288
$C_{18}H_5OF_{33}$	6.7×10^{-15}		Zhang et al. (2010)	Q	287, 289
[65104-67-8]	1.2×10^{-6}		Zhang et al. (2010)	Q	287, 290
UYSGWTCETIRUHO-UHFFFAOYSA-N	1.1×10^{-12}		Zhang et al. (2010)	Q	287, 291
metofluthrin $C_{18}H_{20}F_4O_3$ [240494-70-6] KVIZNNVXXNFLMU-AATRIKPKSA-N	1.0		HSDB (2015)	V	
1,1,2,2-tetrahydroperfluorohexadecyl acrylate	3.3×10^{-12}		Zhang et al. (2010)	Q	287, 288
$C_{19}H_7F29O_2$	4.1×10^{-11}		Zhang et al. (2010)	Q	287, 289
[34362-49-7]	6.5×10^{-4}		Zhang et al. (2010)	Q	287, 290
KLOHTAIHCCMZIL-UHFFFAOYSA-N	6.9×10^{-12}		Zhang et al. (2010)	Q	287, 291
fluoxymesterone $C_{20}H_{29}FO_3$ [76-43-7] YLRFCQOZQXIBAB-YXVJBPKESA-N	1.6×10^{4}		HSDB (2015)	Q	99

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Table A5.1: Organic fluorine (. . . continued)

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dexamethasone $C_{22}H_{29}FO_5$ [50-02-2] UREBDLICKHMUKA-GCMAGEFQSA-N	1.4×10^{2}		HSDB (2015)	Q	99
1,1,2,2-tetrahydroperfluoroeicosyl alcohol	1.5×10^{-13}		Zhang et al. (2010)	Q	287, 288
$C_{20}H_5OF_{37}$	2.2×10^{-18}		Zhang et al. (2010)	Q	287, 289
[65104-65-6]	2.4×10^{-7}		Zhang et al. (2010)	Q	287, 290
FDCQNVKWWMNRQN-UHFFFAOYSA-N	4.6×10^{-14}		Zhang et al. (2010)	Q	287, 291
2-hydroxyfluorobenzene	3.1		Abraham et al. (1994a)	R	
C_6H_5FO	4.3		Keshavarz et al. (2022)	Q	
(*o*-fluorophenol)	5.1×10^{1}		Duchowicz et al. (2020)	Q	299
[367-12-4]	2.3		Hilal et al. (2008)	Q	
HFHFGHLXUCOHLN-UHFFFAOYSA-N	2.9		Modarresi et al. (2007)	Q	67
	3.1		Yaffe et al. (2003)	Q	248, 249
	2.1×10^{2}		Nirmalakhandan et al. (1997)	Q	
	3.1		Duchowicz et al. (2020)	?	185, 21
4-hydroxyfluorobenzene	1.4×10^{1}		Abraham et al. (1994a)	R	
C_6H_5FO	4.3		Keshavarz et al. (2022)	Q	
(*p*-fluorophenol)	1.3×10^{2}		Duchowicz et al. (2020)	Q	
[371-41-5]	7.9		Hilal et al. (2008)	Q	
RHMPLDJJXGPMEX-UHFFFAOYSA-N	3.3		Modarresi et al. (2007)	Q	67
	1.4×10^{1}		Yaffe et al. (2003)	Q	248, 249
	2.1×10^{1}		English and Carroll (2001)	Q	230, 231
	2.1×10^{2}		Nirmalakhandan et al. (1997)	Q	
	1.4×10^{1}		Duchowicz et al. (2020)	?	185, 21
3-fluorophenol C_6H_5FO [372-20-3] SJTBRFHBXDZMPS-UHFFFAOYSA-N	9.0		Hilal et al. (2008)	Q	
2,6-difluorophenol $C_6H_4F_2O$ [28177-48-2] CKKOVFGIBXCEIJ-UHFFFAOYSA-N	7.0×10^{-1}		Hilal et al. (2008)	Q	
4,4'-(hexafluoroisopropylidene)diphenol	1.7×10^{4}		HSDB (2015)	Q	447
$C_{15}H_{10}F_6O_2$	1.7×10^{4}		Zhang et al. (2010)	Q	287, 288
[1478-61-1]	1.4×10^{6}		Zhang et al. (2010)	Q	287, 289
ZFVMWEVVKGLCIJ-UHFFFAOYSA-N	2.1×10^{5}		Zhang et al. (2010)	Q	287, 290
	5.3×10^{3}		Zhang et al. (2010)	Q	287, 291

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
flocoumafen $C_{33}H_{25}F_3O_4$ [90035-08-8] KKBGNYHHEIAGOH-UHFFFAOYSA-N	1.4×10^{7}		HSDB (2015)	Q	99
2,3,3,3-tetrafluoro-2-(trifluoromethyl)propanenitrile C_4F_7N [42532-60-5] AASDJASZOZGYMM-UHFFFAOYSA-N	1.6×10^{-8}		Ebert et al. (2023)	?	365
2-fluoroaniline C_6H_6FN [348-54-9] FTZQXOJYPFINKJ-UHFFFAOYSA-N	1.4		Ebert et al. (2023)	?	318
4-fluoroaniline C_6H_6FN [371-40-4] KRZCOLNOCZKSDF-UHFFFAOYSA-N	1.6		HSDB (2015)	Q	447
3-(trifluoromethyl)aniline $C_7H_6F_3N$ [98-16-8] VIUDTWATMPPKEL-UHFFFAOYSA-N	3.9×10^{-1}		Ebert et al. (2023)	?	316
perfluorotributylamine $C_{12}F_{27}N$ [311-89-7] RVZRBWKZFJCCIB-UHFFFAOYSA-N	1.8×10^{-10} 1.8×10^{-10} 3.4×10^{-10} 1.8×10^{-9} 2.7×10^{-10}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	99 287, 288 287, 289 287, 290 287, 291
N-ethyl-1-[3-(trifluoromethyl)phenyl]-2-propanamine $C_{12}H_{16}F_3N$ (fenfluramine) [458-24-2] DBGIVFWFUFKIQN-UHFFFAOYSA-N	3.7×10^{-1}		HSDB (2015)	Q	99
tris(undecafluoropentyl)amine $C_{15}F_{33}N$ [338-84-1] AQZYBQIAUSKCCS-UHFFFAOYSA-N	1.2×10^{-12} 1.0×10^{-12} 3.4×10^{-10} 2.1×10^{-12}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
indaziflam A $C_{16}H_{20}FN_5$ [730979-19-8] YFONKFDEZLYQDH-OPQQBVKSSA-N	1.8×10^{5}		Ebert et al. (2023)	?	318

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Table A5.1: Organic fluorine (. . . continued)

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indaziflam B $C_{16}H_{20}FN_5$ [730979-32-5] YFONKFDEZLYQDH-OUJBWJOFSA-N	5.3×10^{5}		Ebert et al. (2023)	?	318
cinacalcet $C_{22}H_{22}F_3N$ [226256-56-0] VDHAWDNDOKGFTD-MRXNPFEDSA-N	4.5×10^{1}		HSDB (2015)	Q	99
hydramethylnon $C_{25}H_{24}F_6N_4$ [67485-29-4] IQVNEKKDSLOHHK-FNCQTZNRSA-N	4.5 4.5 2.7×10^{6}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
2-fluoroacetamide C_2H_4FNO [640-19-7] FVTWJXMFYOXOKK-UHFFFAOYSA-N	4.4×10^{2}		HSDB (2015)	Q	99
5-fluorouracil $C_4H_3FN_2O_2$ [51-21-8] GHASVSINZRGABV-UHFFFAOYSA-N	5.8×10^{4}		HSDB (2015)	Q	99
perfluoro-N-methylmorpholine $C_5F_{11}NO$ [382-28-5] PQMAKJUXOOVROI-UHFFFAOYSA-N	6.4×10^{-8}		Ebert et al. (2023)	?	365
1-fluoro-2,4-dinitrobenzene $C_6H_3FN_2O_4$ [70-34-8] LOTKRQAVGJMPNV-UHFFFAOYSA-N	1.0×10^{2}		HSDB (2015)	Q	447
5-fluoro-2-nitrophenol $C_6H_4FNO_3$ [446-36-6] QQURWFRNETXFTN-UHFFFAOYSA-N	5.0×10^{-1} 5.8	 4100 6200	Tremp et al. (1993) Schwarzenbach et al. (1988) Kühne et al. (2005) Kühne et al. (2005)	M V Q ?	12 12
4-nitro-3-(trifluoromethyl)phenol $C_7H_4F_3NO_3$ [88-30-2] ZEFMBAFMCSYJOO-UHFFFAOYSA-N	5.2×10^{2} 5.2×10^{2} 6.7×10^{3} 3.9×10^{4} 1.2×10^{3}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	99 287, 288 287, 289 287, 290 287, 291
1-nitro-3-(trifluoromethyl)benzene $C_7H_4F_3NO_2$ [98-46-4] WHNAMGUAXHGCHH-UHFFFAOYSA-N	5.3×10^{-2} 2.0×10^{-1} 5.7×10^{-2} 8.2×10^{-3}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291

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Table A5.1: Organic fluorine (. . . continued)

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1-isocyanato-3-(trifluoromethyl)-benzene	4.8×10^{-3}		Zhang et al. (2010)	Q	287, 288
$C_8H_4F_3NO$	2.5		Zhang et al. (2010)	Q	287, 289
[329-01-1]	1.3×10^{-3}		Zhang et al. (2010)	Q	287, 290
SXJYSIBLFGQAND-UHFFFAOYSA-N	6.4×10^{-2}		Zhang et al. (2010)	Q	287, 291
flonicamid	2.4×10^{7}		HSDB (2015)	V	
$C_9H_6F_3N_3O$	2.4×10^{7}		Maniere et al. (2011)	?	241, 165
[158062-67-0]					
RLQJEEJISHYWON-UHFFFAOYSA-N					
trifluridine	1.0×10^{11}		HSDB (2015)	Q	99
$C_{10}H_{11}F_3N_2O_5$					
[70-00-8]					
VSQQQLOSPVPRAZ-RRKCRQDMSA-N					
N-(4-amino-2-hydroxyphenyl)-2,2,3,3,4,4,4-heptafluorobutanamide	2.0×10^{8}		Zhang et al. (2010)	Q	287, 288
$C_{10}H_7F_7N_2O_2$	2.3×10^{7}		Zhang et al. (2010)	Q	287, 289
[847-51-8]	1.5×10^{5}		Zhang et al. (2010)	Q	287, 290
STPOJASQXPXVMS-UHFFFAOYSA-N	5.7×10^{6}		Zhang et al. (2010)	Q	287, 291
fluometuron	5.8×10^{3}		Mackay et al. (2006d)	V	
$C_{10}H_{11}F_3N_2O$	3.8×10^{3}		HSDB (2015)	C	
[2164-17-2]					
RZILCCPWPBTYDO-UHFFFAOYSA-N					
dinitramine	7.1		HSDB (2015)	V	
$C_{11}H_{13}F_3N_4O_4$	6.5		Mackay et al. (2006d)	V	
[29091-05-2]	6.2		Suntio et al. (1988)	V	12
OFDYMSKSGFSLLM-UHFFFAOYSA-N					
5-methyl-N-[4-(trifluoromethyl)phenyl]-4-isoxazolecarboxamide $C_{12}H_9F_3N_2O_2$ (leflunomide) [75706-12-6]	8.0×10^{4}		HSDB (2015)	Q	99
VHOGYURTWQBHIL-UHFFFAOYSA-N					
fludioxonil	1.9×10^{4}		Duchowicz et al. (2020)	V	186
$C_{12}H_6F_2N_2O_2$	1.6×10^{4}		Duchowicz et al. (2020)	Q	
[131341-86-1]	1.9×10^{4}		Maniere et al. (2011)	?	241, 165
MUJOIMFVNIBMKC-UHFFFAOYSA-N					
fluconazole	9.9×10^{7}		HSDB (2015)	Q	99
$C_{13}H_{12}F_2N_6O$					
[86386-73-4]					
RFHAOTPXVQNOHP-UHFFFAOYSA-N					

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ethalfluralin $C_{13}H_{14}F_3N_3O_4$ [55283-68-6] PTFJIKYUEPWBMS-UHFFFAOYSA-N	7.6×10^{-2}		HSDB (2015)	V	
benfluralin $C_{13}H_{16}F_3N_3O_4$ (benefin) [1861-40-1] SMDHCQAYESWHAE-UHFFFAOYSA-N	3.4×10^{-2}		HSDB (2015)	V	
			Mackay et al. (2006d)	V	558
	7.5×10^{-1}		Suntio et al. (1988)	V	12
	1.1×10^{-1}		Maniere et al. (2011)	?	12, 165
trifluralin $C_{13}H_{16}F_3N_3O_4$ [1582-09-8] ZSDSQXJSNMTJDA-UHFFFAOYSA-N	9.5×10^{-2}		Rice et al. (1997b)	M	12
	9.1×10^{-1}		Watanabe (1993)	M	
	1.9×10^{-1}		Fendinger et al. (1989)	M	72
	1.7×10^{-1}		Fendinger et al. (1989)	M	645
			Mackay et al. (2006d)	V	558
	2.5×10^{-1}		Suntio et al. (1988)	V	12
	3.8		Sanders and Seiber (1983)	V	87
	2.5×10^{-3}		Barcelo and Hennion (1997)	X	567
	9.6×10^{-2}		HSDB (2015)	C	
	8.3×10^{-4}		Goodarzi et al. (2010)	Q	568
	1.7		Hilal et al. (2008)	Q	
	2.6×10^{-1}		Modarresi et al. (2007)	Q	67
		5000	Kühne et al. (2005)	Q	
		2100	Kühne et al. (2005)	?	
prodiamine $C_{13}H_{17}F_3N_4O_4$ [29091-21-2] RSVPPPHXAASNOL-UHFFFAOYSA-N	1.3		Ebert et al. (2023)	?	316
fluorodifen $C_{13}H_7F_3N_2O_5$ [15457-05-3] HHMCAJWVGYGUEF-UHFFFAOYSA-N			Mackay et al. (2006d)	V	558
	6.5×10^{2}		MacBean (2012a)	?	
profluralin $C_{14}H_{16}F_3N_3O_4$ [26399-36-0] ITVQAKZNYJEWKS-UHFFFAOYSA-N	3.4×10^{-2}		HSDB (2015)	V	
	3.2×10^{-2}		Mackay et al. (2006d)	V	
	2.6×10^{-2}		Suntio et al. (1988)	V	12
	3.4×10^{-2}		MacBean (2012a)	?	
flumequine $C_{14}H_{12}FNO_3$ [42835-25-6] DPSPPJIUMHPXMA-UHFFFAOYSA-N	3.7×10^{7}		HSDB (2015)	Q	99
fluazifop $C_{15}H_{12}F_3NO_4$ [69335-91-7] YUVKUEAFAVKILW-UHFFFAOYSA-N	3.4×10^{7}		Ebert et al. (2023)	?	316

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
fluazifop-p $C_{15}H_{12}F_3NO_4$ [83066-88-0] YUVKUEAFAVKILW-SECBINFHSA-N	1.0×10^6		Ebert et al. (2023)	?	316
prosulfuron $C_{15}H_{16}F_3N_5O_4S$ [94125-34-5] LTUNNEGNEKBSEH-UHFFFAOYSA-N	$>3.3\times10^3$		Maniere et al. (2011)	?	165
flurprimidol $C_{15}H_{15}N_2O_2F_3$ [56425-91-3] VEVZCONIUDBCDC-UHFFFAOYSA-N	7.5×10^3 2.5×10^4		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
flutriafol $C_{16}H_{13}F_2N_3O$ [76674-21-0] JWUCHKBSVLQQCO-UHFFFAOYSA-N	6.1×10^7 7.6×10^4 7.9×10^5		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	186 12, 165
flunitrazepam $C_{16}H_{12}FN_3O_3$ [1622-62-4] PPTYJKAXVCCBDU-UHFFFAOYSA-N	4.3×10^5		HSDB (2015)	Q	99
cyhalofop $C_{16}H_{12}FNO_4$ [122008-78-0] ROBSGBGTWRRYSK-SNVBAGLBSA-N	1.7×10^5		Ebert et al. (2023)	?	318
benzpyrimoxan $C_{16}H_{15}F_3N_2O_3$ [1449021-97-9] ZYXYTGQFPZEUFX-UHFFFAOYSA-N	1.1×10^3		Ebert et al. (2023)	?	318
tolprocarb $C_{16}H_{21}F_3N_2O_3$ [911499-62-2] RSOBJVBYZCMJOS-CYBMUJFWSA-N	6.5×10^4		Ebert et al. (2023)	?	318
flutolanil $C_{17}H_{16}F_3NO_2$ [66332-96-5] PTCGDEVVHUXTMP-UHFFFAOYSA-N	3.1×10^3 2.5 6.1×10^4		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	186 241, 165
beflubutamid $C_{18}H_{17}F_4NO_2$ [113614-08-7] FFQPZWRNXKPNPX-UHFFFAOYSA-N	9.1×10^3		Maniere et al. (2011)	?	241, 165

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
fluxapyroxad $C_{18}H_{12}F_5N_3O$ [907204-31-3] SXSGXWCSHSVPGB-UHFFFAOYSA-N	3.3×10^{6}		Maniere et al. (2011)	?	12, 165
flurtamone $C_{18}H_{14}F_3NO_2$ [96525-23-4] NYRMIJKDBAQCHC-UHFFFAOYSA-N	1.6×10^{8}		Ebert et al. (2023)	?	318
picoxystrobin $C_{18}H_{16}F_3NO_4$ [117428-22-5] IBSNKSODLGJUMQ-SDNWHVSQSA-N	1.4×10^{3}		Ebert et al. (2023)	?	316
sedaxane $C_{18}H_{19}F_2N_3O$ [874967-67-6] XQJQCBDIXRIYRP-UHFFFAOYSA-N	2.5×10^{5}		Maniere et al. (2011)	?	165
penflufen $C_{18}H_{24}FN_3O$ [494793-67-8] GOFJDXZZHFNFLV-UHFFFAOYSA-N	3.2×10^{4}		Ebert et al. (2023)	?	318
fluazifop-p-butyl $C_{19}H_{20}F_3NO_4$ [79241-46-6] VAIZTNZGPYBOGF-CYBMUJFWSA-N	2.0×10^{1}		Maniere et al. (2011)	?	12, 165
picolinafen $C_{19}H_{12}F_4N_2O_2$ [137641-05-5] CWKFPEBMTGKLKX-UHFFFAOYSA-N	6.2×10^{2}		Maniere et al. (2011)	?	12, 165
diflufenican $C_{19}H_{11}F_5N_2O_2$ [83164-33-4] WYEHFWKAOXOVJD-UHFFFAOYSA-N	6.4×10^{1} 1.1×10^{3} 3.0×10^{1} $<8.5\times10^{1}$		Keshavarz et al. (2022) Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	Q Q ? ?	 185, 21 241, 165
fluazifop-butyl $C_{19}H_{20}F_3NO_4$ [69806-50-4] VAIZTNZGPYBOGF-UHFFFAOYSA-N	4.7×10^{1}		HSDB (2015)	V	
flumioxazin $C_{19}H_{15}FN_2O_4$ [103361-09-7] FOUWCSDKDDHKQP-UHFFFAOYSA-N	1.6×10^{1} 1.6×10^{1}		HSDB (2015) Maniere et al. (2011)	V ?	 12, 165

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
fluridone $C_{19}H_{14}F_3NO$ [59756-60-4] YWBVHLJPRPCRSD-UHFFFAOYSA-N	1.2×10^3 2.8×10^3 1.9×10^2		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Duchowicz et al. (2020)	V V V Q	186 558
cyhalofop-butyl $C_{20}H_{20}FNO_4$ [122008-85-9] TYIYMOAHACZAMQ-CQSZACIVSA-N	1.0×10^3 1.1×10^3		MacBean (2012b) Maniere et al. (2011)	X ?	350 241, 165
raltegravir $C_{20}H_{21}FN_6O_5$ [518048-05-0] CZFFBEXEKNGXKS-UHFFFAOYSA-N	1.1×10^{17}		HSDB (2015)	Q	99
fluacrypyrim $C_{20}H_{21}N_2O_5F_3$ [229977-93-9] MXWAGQASUDSFBG-RVDMUPIBSA-N	3.0×10^2		MacBean (2012a)	?	12
trifloxystrobin $C_{20}H_{19}F_3N_2O_4$ [141517-21-7] ONCZDRURRATYFI-UHFFFAOYSA-N	4.3×10^2 4.3×10^2		MacBean (2012b) Maniere et al. (2011)	X ?	350 165
isopyrazam $C_{20}H_{23}F_2N_3O$ [881685-58-1] XTDZGXBTXBEZDN-UHFFFAOYSA-N	5.3×10^3 2.7×10^4		Maniere et al. (2011) Maniere et al. (2011)	? ?	241, 165 241, 165
syn-isopyrazam $C_{20}H_{23}F_2N_3O$ [683777-13-1] XTDZGXBTXBEZDN-HEHGZKQESA-N	5.2×10^6		Ebert et al. (2023)	?	318
anti-isopyrazam $C_{20}H_{23}F_2N_3O$ [683777-14-2] XTDZGXBTXBEZDN-XEZPLFJOSA-N	2.6×10^6		Ebert et al. (2023)	?	318
etoxazole $C_{21}H_{23}F_2NO_2$ [153233-91-1] IXSZQYVWNJNRAL-UHFFFAOYSA-N	9.6×10^1 9.9×10^1 1.7×10^2 2.8×10^1		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Maniere et al. (2011)	V V Q ?	186 165
droperidol $C_{22}H_{22}FN_3O_2$ [548-73-2] RMEDXOLNCUSCGS-UHFFFAOYSA-N	3.7×10^{11}		HSDB (2015)	Q	99

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
paliperidone $C_{23}H_{27}FN_4O_3$ [144598-75-4] PMXMIIMHBWHSKN-UHFFFAOYSA-N	1.2×10^{15}		HSDB (2015)	Q	99
risperidone $C_{23}H_{27}FN_4O_2$ [106266-06-2] RAPZEAPATHNIPO-UHFFFAOYSA-N	4.5×10^{10}		HSDB (2015)	Q	99
ezetimibe $C_{24}H_{21}F_2NO_3$ [163222-33-1] OLNTVTPDXPETLC-XPWALMASSA-N	2.2×10^{12}		HSDB (2015)	Q	99
cyflumetofen $C_{24}H_{24}F_3NO_4$ [400882-07-7] AWSZRJQNBMEZOI-UHFFFAOYSA-N	$>1.1\times10^{1}$		Maniere et al. (2011)	?	241, 165
acrinathrin $C_{26}H_{21}F_6NO_5$ [101007-06-1] YLFSVIMMRPNPFK-WEQBUNFVSA-N	9.3×10^{1}		Maniere et al. (2011)	?	12, 165
cerivastatin $C_{26}H_{34}FNO_5$ [145599-86-6] SEERZIQQUAZTOL-ANMDKAQQSA-N	1.7×10^{13}		HSDB (2015)	Q	99
flucythrinate, isomer 1 $C_{26}H_{23}F_2NO_4$ [70124-77-5] GBIHOLCMZGAKNG-UHFFFAOYSA-N	1.1×10^{2} 9.3×10^{2}		HSDB (2015) Mackay et al. (2006d)	V V	
PFBHA-methanal $H_2C{=}NOCH_2C_6F_5$ [86356-73-2] SRTQFRQWTUMMTC-UHFFFAOYSA-N	1.6×10^{-2}	7200	Destaillats and Charles (2002)	M	
PFBHA-ethanal $CH_3CH{=}NOCH_2C_6F_5$ [114611-59-5] AKDRYEADQPNLOH-UHFFFAOYSA-N	1.9×10^{-2}	5400	Destaillats and Charles (2002)	M	
PFBHA-propanone $(CH_3)_2C{=}NOCH_2C_6F_5$ [899828-53-6] DLIFNTQMBOCKTL-UHFFFAOYSA-N	1.1×10^{-2}	3800	Destaillats and Charles (2002)	M	

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
PFBHA-butanone $(C_2H_5)(CH_3)C{=}NOCH_2C_6F_5$ LNDQFOSWZJYEIC-UHFFFAOYSA-N	$4.7{\times}10^{-3}$	6000	Destaillats and Charles (2002)	M	
PFBHA-2-pentanone $(C_3H_7)(CH_3)C{=}NOCH_2C_6F_5$ YKQOTQPNOJSJFA-UHFFFAOYSA-N	$3.7{\times}10^{-3}$	2200	Destaillats and Charles (2002)	M	
PFBHA-hexanal $C_5H_{11}CH{=}NOCH_2C_6F_5$ GPAVMFOMYSGJDM-UHFFFAOYSA-N	$5.8{\times}10^{-3}$		Destaillats and Charles (2002)	M	
PFBHA-octanal $C_7H_{15}CH{=}NOCH_2C_6F_5$ RLSQIXNUITTXKZ-UHFFFAOYSA-N	$7.9{\times}10^{-3}$		Destaillats and Charles (2002)	M	
PFBHA-decanal $C_9H_{19}CH{=}NOCH_2C_6F_5$ NUGDFCWVLOJWOP-UHFFFAOYSA-N	$2.4{\times}10^{-2}$		Destaillats and Charles (2002)	M	
PFBHA-propenal $CH_2CHCH{=}NOCH_2C_6F_5$ ICDUEGOPUWNJNF-UHFFFAOYSA-N	$9.5{\times}10^{-3}$	5400	Destaillats and Charles (2002)	M	
(E)-PFBHA-propenal $C_{10}H_6F_5NO$ [932710-55-9] ICDUEGOPUWNJNF-HQYXKAPLSA-N	$9.5{\times}10^{-3}$		Ebert et al. (2023)	?	579
PFBHA-crotonaldehyde $CH_3CHCHCH{=}NOCH_2C_6F_5$ [932710-52-6] QNPFFCQTVXPCLD-UHFFFAOYSA-N	$6.8{\times}10^{-3}$	3400	Destaillats and Charles (2002)	M	
PFBHA-benzaldehyde $C_6H_5CH{=}NOCH_2C_6F_5$ UKSAZCDAGVHMRF-UHFFFAOYSA-N	$5.0{\times}10^{-3}$	2000	Destaillats and Charles (2002)	M	
PFBHA-4-methyl-benzaldehyde $C_8H_8{=}NOCH_2C_6F_5$ UCASBURGYXMQLW-UHFFFAOYSA-N	$6.6{\times}10^{-3}$		Destaillats and Charles (2002)	M	
PFBHA-9-fluorenone $C_{13}H_8{=}NOCH_2C_6F_5$ UABDVZDYKDIZFO-UHFFFAOYSA-N	$1.1{\times}10^{-2}$		Destaillats and Charles (2002)	M	
PFBHA-ethanedial $(HC{=}NOCH_2C_6F_5)_2$ [618858-54-1] VNVBOBJSRGZDCW-UHFFFAOYSA-N	$1.6{\times}10^{-2}$		Destaillats and Charles (2002)	M	

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Table A5.1: Organic fluorine (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
PFBHA-1-hydroxypropanone $(CH_2OH)(CH_3)C{=}NOCH_2C_6F_5$ BCTASVPUYLXFBW-UHFFFAOYSA-N	$2.7{\times}10^{-2}$		Destaillats and Charles (2002)	M	
PFBHA-3-hydroxy-3-methyl-2-butanone $(HOC_3H_6)(CH_3)C{=}NOCH_2C_6F_5$ VNWPJWLGZUDTBZ-UHFFFAOYSA-N	$1.2{\times}10^{-2}$		Destaillats and Charles (2002)	M	

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A6 Organic species with chlorine (Cl)

A6.1 Chlorocarbons (C, H, Cl)

Table A6.1: Chlorocarbons (C, H, Cl)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chloromethane	1.0×10^{-3}	2900	Schwardt et al. (2021)	L	1
CH_3Cl	1.0×10^{-3}	2900	Burkholder et al. (2019)	L	1
(methyl chloride)	8.7×10^{-4}	3400	Burkholder et al. (2019)	L	70
[74-87-3]	1.1×10^{-3}	3300	Burkholder et al. (2015)	L	
NEHMKBQYUWJMIP-UHFFFAOYSA-N	8.7×10^{-4}	3400	Burkholder et al. (2015)	L	70
	1.0×10^{-3}	2800	Brockbank (2013)	L	1
	1.3×10^{-3}	3300	Sander et al. (2011)	L	646
	1.1×10^{-3}	3300	Warneck (2007)	L	
	1.3×10^{-3}	3300	Sander et al. (2006)	L	647
	1.1×10^{-3}	3300	Staudinger and Roberts (2001)	L	
	1.1×10^{-3}		Mackay and Shiu (1981)	L	
	1.0×10^{-3}	2800	Wilhelm et al. (1977)	L	
	7.9×10^{-4}	2400	Hiatt (2013)	M	
	9.1×10^{-4}	2000	Chen et al. (2012)	M	
	8.8×10^{-4}	3200	Moore (2000)	M	70
	9.3×10^{-4}	3300	Moore et al. (1995)	M	70
	8.5×10^{-4}	2800	Reichl (1995)	M	648
	1.1×10^{-3}	3000	Elliott and Rowland (1993)	M	
	1.2×10^{-3}	4200	Gossett (1987)	M	
	1.4×10^{-3}		Pearson and McConnell (1975)	M	649, 12
	1.1×10^{-3}	2600	Swain and Thornton (1962)	M	
	9.9×10^{-4}	2500	Boggs and Buck (1958)	M	
	1.0×10^{-3}	2900	Glew and Moelwyn-Hughes (1953)	M	650
	1.0×10^{-3}		Mackay et al. (2006b)	V	
	4.2×10^{-4}		Lide and Frederikse (1995)	V	
	1.0×10^{-3}		Mackay et al. (1993)	V	
	1.1×10^{-3}		Dilling (1977)	V	651
	1.2×10^{-3}		Dilling (1977)	V	12
	9.9×10^{-4}		Hine and Mookerjee (1975)	V	
	1.2×10^{-3}		Yaws (2003)	X	237
	2.9×10^{-4}	-630	Goldstein (1982)	X	298
	2.5×10^{-5}		Ryan et al. (1988)	C	
	1.1×10^{-3}		Hayer et al. (2022)	Q	20
	2.7×10^{-4}		Wang et al. (2017)	Q	80, 238
	1.4×10^{-3}		Wang et al. (2017)	Q	80, 239
	1.8×10^{-3}		Wang et al. (2017)	Q	80, 240
	9.9×10^{-4}		Li et al. (2014)	Q	241
	6.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.0×10^{-3}		Hilal et al. (2008)	Q	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.9×10^{-3}		Modarresi et al. (2007)	Q	67
		2600	Kühne et al. (2005)	Q	
	1.1×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	8.6×10^{-4}		Yao et al. (2002)	Q	229
	1.0×10^{-3}		English and Carroll (2001)	Q	230, 231
	3.7×10^{-4}		Katritzky et al. (1998)	Q	
	8.6×10^{-4}		Suzuki et al. (1992)	Q	232
	3.9×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	8.6×10^{-4}		Irmann (1965)	Q	
	1.1×10^{-3}		Mackay et al. (2006b)	?	
		2700	Kühne et al. (2005)	?	
	1.2×10^{-3}		Yaws (1999)	?	21
	6.9×10^{-4}		Abraham and Weathersby (1994)	?	21
	1.2×10^{-3}		Yaws and Yang (1992)	?	21
	1.0×10^{-3}		Abraham et al. (1990)	?	
dichloromethane	3.9×10^{-3}	3500	Schwardt et al. (2021)	L	1
CH_2Cl_2	3.9×10^{-3}	3700	Burkholder et al. (2019)	L	
(methylene chloride)	3.5×10^{-3}	3900	Burkholder et al. (2019)	L	70
[75-09-2]	3.9×10^{-3}	3700	Burkholder et al. (2015)	L	
YMWUJEATGCHHMB-UHFFFAOYSA-N	3.5×10^{-3}	3900	Burkholder et al. (2015)	L	70
	3.7×10^{-3}	3300	Brockbank (2013)	L	1
	3.6×10^{-3}	4100	Sander et al. (2011)	L	
	3.9×10^{-3}	3700	Warneck (2007)	L	
	3.6×10^{-3}	4100	Sander et al. (2006)	L	
	3.6×10^{-3}	4100	Staudinger and Roberts (2001)	L	
	3.6×10^{-3}	4100	Staudinger and Roberts (1996)	L	
	3.8×10^{-3}		Mackay and Shiu (1981)	L	
	4.0×10^{-3}	3900	Hiatt (2013)	M	
	3.5×10^{-3}	2300	Chen et al. (2012)	M	
	3.6×10^{-3}	3700	Ooki and Yokouchi (2011)	M	70
	3.2×10^{-3}		Helburn et al. (2008)	M	
	4.3×10^{-3}	3500	Lutsyk et al. (2005)	M	
	3.3×10^{-3}	4200	Moore (2000)	M	70
	3.9×10^{-3}		David et al. (2000)	M	72
	3.4×10^{-3}		McIntosh and Heffron (2000)	M	14
	4.1×10^{-3}		Ryu and Park (1999)	M	
	3.4×10^{-3}		Chiang et al. (1998)	M	652, 12
	3.7		Welke et al. (1998)	M	
	5.1×10^{-3}		Hovorka and Dohnal (1997)	M	12
	3.7×10^{-3}	3200	Kondoh and Nakajima (1997)	M	
	4.3×10^{-3}	3500	Park et al. (1997)	M	
	4.1×10^{-3}		Hoff et al. (1993)	M	
	3.8×10^{-3}		Li et al. (1993)	M	
	3.9×10^{-3}	3400	Wright et al. (1992)	M	653
	3.9×10^{-3}	3500	Tse et al. (1992)	M	
	4.4×10^{-3}		Yu (1992)	M	12
	3.4×10^{-3}		Guitart et al. (1989)	M	14

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.4×10^{-3}	4200	Ashworth et al. (1988)	M	278
	4.6×10^{-3}	3800	Gossett (1987)	M	
	5.7×10^{-3}		Hellmann (1987)	M	87
	5.2×10^{-3}		Yurteri et al. (1987)	M	12
	3.8×10^{-3}	4500	Gossett et al. (1985)	M	
	3.4×10^{-3}	4200	Lincoff and Gossett (1984)	M	
	3.0×10^{-3}	3600	Leighton and Calo (1981)	M	
	3.1×10^{-3}		Warner et al. (1980)	M	
	2.8×10^{-3}		Sato and Nakajima (1979b)	M	14
	3.3×10^{-3}		Pearson and McConnell (1975)	M	649, 12
	4.2×10^{-3}	4400	Hartkopf and Karger (1973)	M	
	4.1×10^{-3}	4000	Rex (1906)	M	
	2.7×10^{-3}		Mackay et al. (2006b)	V	
	3.5×10^{-3}	4100	Fogg and Sangster (2003)	V	
	4.0×10^{-3}		Park et al. (1997)	V	
	5.9×10^{-3}		Mackay et al. (1993)	V	
	2.9×10^{-3}		Hwang et al. (1992)	V	
	3.2×10^{-3}		Warner et al. (1980)	V	
	4.0×10^{-3}		Dilling (1977)	V	651
	1.2×10^{-2}		Dilling (1977)	V	153
	4.3×10^{-3}		Hine and Mookerjee (1975)	V	
	4.0×10^{-3}		Dilling et al. (1975)	V	
	4.0×10^{-3}		Yaws (2003)	X	237
	3.1×10^{-3}	3600	Goldstein (1982)	X	298
	4.2×10^{-3}		Harrison et al. (1993)	C	
	3.4×10^{-3}		Harrison et al. (1993)	C	
	4.7×10^{-3}		Ryan et al. (1988)	C	
	3.1×10^{-3}		Shen (1982)	C	
	3.7×10^{-3}		Dilling (1977)	C	
	3.7×10^{-3}		Dilling et al. (1975)	C	
	5.6×10^{-3}		Hayer et al. (2022)	Q	20
	8.8×10^{-3}		Keshavarz et al. (2022)	Q	
	2.6×10^{-3}		Duchowicz et al. (2020)	Q	
	6.2×10^{-4}		Wang et al. (2017)	Q	80, 238
	1.4×10^{-2}		Wang et al. (2017)	Q	80, 239
	9.3×10^{-3}		Wang et al. (2017)	Q	80, 240
	2.9×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	4.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
	9.0×10^{-3}		Hilal et al. (2008)	Q	
	1.8×10^{-3}		Modarresi et al. (2007)	Q	67
		3000	Kühne et al. (2005)	Q	
	3.8×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	3.0×10^{-3}		Yao et al. (2002)	Q	229
	1.8×10^{-3}		English and Carroll (2001)	Q	230, 260

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.4×10^{-4}		Katritzky et al. (1998)	Q	
	2.2×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	3.0×10^{-3}		Duchowicz et al. (2020)	?	185, 21
	3.3×10^{-3}		Mackay et al. (2006b)	?	
		3900	Kühne et al. (2005)	?	
	4.0×10^{-3}		Yaws (1999)	?	21
	2.9×10^{-3}		Abraham and Weathersby (1994)	?	21
	3.3×10^{-3}		Mackay et al. (1993)	?	
	4.0×10^{-3}		Yaws and Yang (1992)	?	21
	3.7×10^{-3}		Abraham et al. (1990)	?	
dichloromethane-d2 CD_2Cl_2 (methylene chloride-d2) [1665-00-5] YMWUJEATGCHHMB-DICFDUPASA-N	3.8×10^{-3}	4600	Hiatt (2013)	M	
trichloromethane $CHCl_3$ (chloroform) [67-66-3] HEDRZPFGACZZDS-UHFFFAOYSA-N	2.7×10^{-3}	4200	Schwardt et al. (2021)	L	1
	2.6×10^{-3}	4300	Burkholder et al. (2019)	L	
	2.0×10^{-3}	4400	Burkholder et al. (2019)	L	70
	2.6×10^{-3}	4300	Burkholder et al. (2015)	L	
	2.0×10^{-3}	4400	Burkholder et al. (2015)	L	70
	2.3×10^{-3}	4200	Brockbank (2013)	L	1, 654
	2.5×10^{-3}	4500	Sander et al. (2011)	L	
	2.6×10^{-3}	4300	Warneck (2007)	L	
	2.5×10^{-3}	4500	Sander et al. (2006)	L	
	2.5×10^{-3}	4500	Staudinger and Roberts (2001)	L	
	2.5×10^{-3}	4500	Staudinger and Roberts (1996)	L	
	2.6×10^{-3}		Mackay and Shiu (1981)	L	
	1.6×10^{-3}		Steward et al. (1973)	L	14
	2.6×10^{-3}	3900	Allott et al. (1973)	L	
	2.8×10^{-3}	4500	Hiatt (2013)	M	
	2.5×10^{-3}	3900	Chen et al. (2012)	M	
	3.1×10^{-3}		Ruiz-Bevia and Fernandez-Torres (2010)	M	
	2.7×10^{-3}	4500	Lutsyk et al. (2005)	M	
	1.4×10^{-3}		Zhang et al. (2002)	M	14
	2.3×10^{-3}	4200	Görgényi et al. (2002)	M	655
	2.0×10^{-3}	4600	Moore (2000)	M	70
	2.4×10^{-3}		David et al. (2000)	M	72
	2.7×10^{-3}		Ryu and Park (1999)	M	
	3.0×10^{-3}		Dohnal and Hovorka (1999)	M	12
	3.0×10^{-3}		Chiang et al. (1998)	M	12
	3.4×10^{-3}		Welke et al. (1998)	M	
	3.2×10^{-3}		Hovorka and Dohnal (1997)	M	12
	2.7×10^{-3}	3400	Kondoh and Nakajima (1997)	M	
	2.6×10^{-3}	3400	Park et al. (1997)	M	
	2.2×10^{-3}	4700	Turner et al. (1996)	M	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{-3}	4200	Moore et al. (1995)	M	656, 70
	2.6×10^{-3}	4400	Dewulf et al. (1995)	M	
	2.5×10^{-3}		Hoff et al. (1993)	M	
	2.4×10^{-3}		Li et al. (1993)	M	
	2.6×10^{-3}	4000	Wright et al. (1992)	M	657
	4.8×10^{-3}	7300	Tancrède and Yanagisawa (1990)	M	
	2.4×10^{-3}	2000	Lamarche and Droste (1989)	M	345
	2.1×10^{-3}		Guitart et al. (1989)	M	14
	2.3×10^{-3}	5000	Ashworth et al. (1988)	M	278
	2.7×10^{-3}	4600	Gossett (1987)	M	
	2.6×10^{-3}	4300	Munz and Roberts (1987)	M	
	2.9×10^{-3}		Hellmann (1987)	M	87
	3.3×10^{-3}		Munz and Roberts (1986)	M	
	2.5×10^{-3}	4300	Gossett et al. (1985)	M	
	2.5×10^{-3}	5200	Nicholson et al. (1984)	M	
	2.3×10^{-3}	4200	Lincoff and Gossett (1984)	M	
	2.0×10^{-3}	3900	Hunter-Smith et al. (1983)	M	70, 658
	2.5×10^{-3}	4000	Leighton and Calo (1981)	M	
	1.5×10^{-3}	5600	Ervin et al. (1980)	M	
	2.9×10^{-3}		Warner et al. (1980)	M	
	2.4×10^{-3}	7200	Balls (1980)	M	
	1.4×10^{-3}		Sato and Nakajima (1979b)	M	14
	3.5×10^{-3}		Pearson and McConnell (1975)	M	649, 12
	2.8×10^{-3}	5100	Hartkopf and Karger (1973)	M	
	1.6×10^{-3}		Bachofen and Farhi (1971)	M	14
	2.6×10^{-3}	4600	Rex (1906)	M	
	2.6×10^{-3}		Mackay et al. (2006b)	V	
	2.6×10^{-3}	4400	Fogg and Sangster (2003)	V	
	2.5×10^{-3}		Park et al. (1997)	V	
	2.6×10^{-3}		Mackay et al. (1993)	V	
	2.6×10^{-3}		Hwang et al. (1992)	V	
	5.5×10^{-3}		McLachlan et al. (1990)	V	373
	3.1×10^{-3}		Warner et al. (1980)	V	
	2.8×10^{-3}		Smith and Bomberger (1980)	V	24
	2.5×10^{-3}		Dilling (1977)	V	651
	9.0×10^{-3}		Dilling (1977)	V	153
	2.3×10^{-3}		Hine and Mookerjee (1975)	V	
	2.5×10^{-3}		Dilling et al. (1975)	V	
	2.2×10^{-3}	4700	Winkler (1906)	V	
	2.5×10^{-3}	4100	Barr and Newsham (1987)	X	298
	3.0×10^{-3}	4400	Goldstein (1982)	X	298
	2.4×10^{-3}		Harrison et al. (1993)	C	
	3.4×10^{-3}		Harrison et al. (1993)	C	
	3.4×10^{-3}		Ryan et al. (1988)	C	
	2.7×10^{-3}		Nicholson et al. (1984)	C	
	2.1×10^{-3}		Nicholson et al. (1984)	C	12
	2.9×10^{-3}		Shen (1982)	C	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.1×10^{-3}		Dilling (1977)	C	
	3.1×10^{-3}		Dilling et al. (1975)	C	
	2.6×10^{-3}		Hayer et al. (2022)	Q	20
	1.1×10^{-3}		Wang et al. (2017)	Q	80, 238
	4.3×10^{-3}		Wang et al. (2017)	Q	80, 239
	4.5×10^{-3}		Wang et al. (2017)	Q	80, 240
	3.7×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.2×10^{-3}		Hilal et al. (2008)	Q	
	1.3×10^{-3}		Modarresi et al. (2007)	Q	67
		3300	Kühne et al. (2005)	Q	
	4.1×10^{-3}		Yao et al. (2002)	Q	229
	1.0×10^{-3}		English and Carroll (2001)	Q	230, 274
	2.6×10^{-4}		Katritzky et al. (1998)	Q	
	3.9×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	2.3×10^{-3}		Arbuckle (1983)	Q	
	2.3×10^{-3}		Mackay et al. (2006b)	?	
		4300	Kühne et al. (2005)	?	
	2.4×10^{-3}		Yaws (1999)	?	21
	1.6×10^{-3}		Abraham and Weathersby (1994)	?	21
	2.3×10^{-3}		Mackay et al. (1993)	?	
	2.4×10^{-3}		Yaws and Yang (1992)	?	21
	2.5×10^{-3}		Abraham et al. (1990)	?	
tetrachloromethane	3.4×10^{-4}	4200	Schwardt et al. (2021)	L	1
CCl_4	3.6×10^{-4}	4300	Burkholder et al. (2019)	L	
(carbontetrachloride)	2.6×10^{-4}	4200	Burkholder et al. (2019)	L	70
[56-23-5]	3.6×10^{-4}	4300	Burkholder et al. (2015)	L	
VZGDMQKNWNREIO-UHFFFAOYSA-N	2.6×10^{-4}	4200	Burkholder et al. (2015)	L	70
	3.5×10^{-4}	4200	Brockbank (2013)	L	1, 659
	3.4×10^{-4}	4200	Sander et al. (2011)	L	
	3.6×10^{-4}	4300	Warneck (2007)	L	
	3.4×10^{-4}	4200	Sander et al. (2006)	L	
	3.4×10^{-4}	4200	Staudinger and Roberts (2001)	L	
	3.4×10^{-4}	4200	Staudinger and Roberts (1996)	L	
	5.0×10^{-4}		Mackay and Shiu (1981)	L	
	5.0×10^{-4}	4500	Hiatt (2013)	M	
	3.0×10^{-4}	4400	Chen et al. (2012)	M	
	3.4×10^{-4}	3800	Lutsyk et al. (2005)	M	
	3.8×10^{-4}		Ryu and Park (1999)	M	
	4.0×10^{-4}		Chiang et al. (1998)	M	12
	2.9×10^{-4}	3700	Bullister and Wisegarver (1998)	M	660
	4.4×10^{-4}	1900	Kondoh and Nakajima (1997)	M	
	3.9×10^{-4}	2600	Park et al. (1997)	M	
	3.8×10^{-4}	4400	Dewulf et al. (1995)	M	
	3.6×10^{-4}		Hoff et al. (1993)	M	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

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	3.3×10^{-4}	3600	Hansen et al. (1993)	M	281
	2.3×10^{-4}		Li and Carr (1993)	M	
	2.9×10^{-4}	4500	Wright et al. (1992)	M	661
	3.8×10^{-4}	3600	Tse et al. (1992)	M	
	3.4×10^{-4}	4100	Tancrède and Yanagisawa (1990)	M	
	2.8×10^{-4}	5600	Bissonette et al. (1990)	M	
	3.3×10^{-4}	4000	Ashworth et al. (1988)	M	278
	3.3×10^{-4}	4400	Gossett (1987)	M	
	3.3×10^{-4}	4300	Munz and Roberts (1987)	M	
	3.3×10^{-4}		Hellmann (1987)	M	87
	4.3×10^{-4}		Yurteri et al. (1987)	M	12
	4.2×10^{-4}		Munz and Roberts (1986)	M	
	4.1×10^{-4}	3200	Hunter-Smith et al. (1983)	M	658
	3.6×10^{-4}	4400	Leighton and Calo (1981)	M	
	3.3×10^{-4}		Warner et al. (1980)	M	
	3.2×10^{-4}	3300	Balls (1980)	M	
	9.7×10^{-5}		Sato and Nakajima (1979b)	M	14
	4.5×10^{-4}		Pearson and McConnell (1975)	M	649, 12
	3.7×10^{-4}	5200	Hartkopf and Karger (1973)	M	
	3.5×10^{-4}	4400	Rex (1906)	M	
	3.4×10^{-4}		Mackay et al. (2006b)	V	
	3.6×10^{-4}	4200	Fogg and Sangster (2003)	V	
	4.3×10^{-4}		Park et al. (1997)	V	
	3.4×10^{-4}		Mackay et al. (1993)	V	
	3.4×10^{-4}		Hwang et al. (1992)	V	
	6.7×10^{-5}		Ballschmiter and Wittlinger (1991)	V	
	3.5×10^{-4}		Warner et al. (1980)	V	
	4.6×10^{-4}		Smith and Bomberger (1980)	V	24
	3.4×10^{-4}		Dilling (1977)	V	
	3.4×10^{-4}		Hine and Mookerjee (1975)	V	
	2.0×10^{-4}		Pierotti (1965)	T	
	3.4×10^{-4}		Yaws (2003)	X	237
	3.3×10^{-4}	1100	Goldstein (1982)	X	298
	3.8×10^{-4}		Harrison et al. (1993)	C	
	2.1×10^{-4}		Harrison et al. (1993)	C	
	4.5×10^{-4}		Ryan et al. (1988)	C	
	3.3×10^{-4}		Shen (1982)	C	
	4.6×10^{-4}		Dilling (1977)	C	
	3.7×10^{-4}		Liss and Slater (1974)	C	
	4.9×10^{-4}		Hayer et al. (2022)	Q	20
	5.4×10^{-4}		Keshavarz et al. (2022)	Q	
	6.3×10^{-4}		Duchowicz et al. (2020)	Q	
	3.4×10^{-4}		Li et al. (2014)	Q	241
	3.2×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
	5.4×10^{-4}		Hilal et al. (2008)	Q	
	2.3×10^{-4}		Modarresi et al. (2007)	Q	67

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		3700	Kühne et al. (2005)	Q	
	3.5×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	2.1×10^{-4}		English and Carroll (2001)	Q	230, 231
	3.4×10^{-5}		Katritzky et al. (1998)	Q	
	3.5×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	4.1×10^{-4}		Arbuckle (1983)	Q	
	3.6×10^{-4}		Duchowicz et al. (2020)	?	185, 21
	1.2×10^{-4}		MacBean (2012a)	?	
	3.3×10^{-4}		Mackay et al. (2006b)	?	
		4300	Kühne et al. (2005)	?	
	3.4×10^{-4}		Yaws (1999)	?	21
	1.0×10^{-4}		Abraham and Weathersby (1994)	?	21
	3.3×10^{-4}		Mackay et al. (1993)	?	
	3.3×10^{-4}		Yaws and Yang (1992)	?	21
	3.5×10^{-4}		Abraham et al. (1990)	?	
	4.3×10^{-4}		Mackay and Yeun (1983)	?	
	1.1×10^{-3}		Chiou et al. (1980)	?	79
chloroethane	8.1×10^{-4}	3000	Schwardt et al. (2021)	L	1
C_2H_5Cl	8.1×10^{-4}	2900	Burkholder et al. (2019)	L	1
[75-00-3]	8.3×10^{-4}	2800	Burkholder et al. (2015)	L	
HRYZWHHZPQKTII-UHFFFAOYSA-N	8.1×10^{-4}	2900	Brockbank (2013)	L	1
	8.3×10^{-4}	2800	Warneck (2007)	L	
	8.4×10^{-4}	2900	Staudinger and Roberts (2001)	L	
	8.3×10^{-4}	2900	Staudinger and Roberts (1996)	L	
	5.0×10^{-3}		Mackay and Shiu (1981)	L	
	4.7×10^{-4}		Steward et al. (1973)	L	14
	7.3×10^{-4}	3500	Allott et al. (1973)	L	
	8.5×10^{-4}	3200	Hiatt (2013)	M	
	7.6×10^{-4}	3100	Chen et al. (2012)	M	
	8.9×10^{-4}	3200	Maaßen (1995)	M	662
	9.3×10^{-4}	3300	Reichl (1995)	M	663
	7.9×10^{-4}	2600	Ashworth et al. (1988)	M	278
	8.8×10^{-4}	3100	Gossett (1987)	M	
	5.5×10^{-3}		Mackay et al. (2006b)	V	
	5.5×10^{-3}		Mackay et al. (1993)	V	
	5.6×10^{-4}		Hwang et al. (1992)	V	
	8.8×10^{-4}		Dilling (1977)	V	
	1.2×10^{-3}		Hine and Mookerjee (1975)	V	
	1.4×10^{-3}		Yaws (2003)	X	237, 12
	6.8×10^{-4}	750	Goldstein (1982)	X	298
	6.6×10^{-4}		Ryan et al. (1988)	C	
	6.3×10^{-4}		Irmann (1965)	C	
	8.0×10^{-4}		Hayer et al. (2022)	Q	20
	2.2×10^{-4}		Wang et al. (2017)	Q	80, 238
	1.4×10^{-3}		Wang et al. (2017)	Q	80, 239
	1.7×10^{-3}		Wang et al. (2017)	Q	80, 240
	7.9×10^{-4}		Gharagheizi et al. (2012)	Q	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	9.3×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.2×10^{-3}		Hilal et al. (2008)	Q	
	1.0×10^{-3}		Modarresi et al. (2007)	Q	67
		3000	Kühne et al. (2005)	Q	
	1.1×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	4.8×10^{-4}		Yao et al. (2002)	Q	229
	9.7×10^{-4}		English and Carroll (2001)	Q	230, 231
	9.0×10^{-4}		Katritzky et al. (1998)	Q	
	6.1×10^{-4}		Suzuki et al. (1992)	Q	232
	7.9×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	7.6×10^{-4}		Irmann (1965)	Q	
	9.8×10^{-4}		Mackay et al. (2006b)	?	
		2900	Kühne et al. (2005)	?	
	1.4×10^{-3}		Yaws (1999)	?	21, 12
	4.8×10^{-4}		Abraham and Weathersby (1994)	?	21
	9.8×10^{-4}		Mackay et al. (1993)	?	
	1.4×10^{-3}		Yaws and Yang (1992)	?	21, 12
	1.2×10^{-3}		Abraham et al. (1990)	?	
1,1-dichloroethane $CHCl_2CH_3$ [75-34-3] SCYULBFZEHDVBN-UHFFFAOYSA-N	1.7×10^{-3}	3900	Schwardt et al. (2021)	L	1
	1.7×10^{-3}	4000	Burkholder et al. (2019)	L	1
	1.5×10^{-3}	3900	Burkholder et al. (2019)	L	70
	1.7×10^{-3}	4100	Burkholder et al. (2015)	L	
	1.5×10^{-3}	3900	Burkholder et al. (2015)	L	70
	1.7×10^{-3}	4000	Brockbank (2013)	L	1
	1.7×10^{-3}	4100	Warneck (2007)	L	
	1.8×10^{-3}	4100	Fogg and Sangster (2003)	L	
	1.6×10^{-3}	3700	Staudinger and Roberts (2001)	L	
	1.5×10^{-3}	3600	Staudinger and Roberts (1996)	L	
	1.7×10^{-3}		Mackay and Shiu (1981)	L	
	2.0×10^{-3}	3900	Hiatt (2013)	M	
	1.9×10^{-3}	3300	Chen et al. (2012)	M	
	2.0×10^{-3}		Bobadilla et al. (2003)	M	
	1.6×10^{-3}	3900	Görgényi et al. (2002)	M	664
	2.2×10^{-3}		Hovorka and Dohnal (1997)	M	12
	1.8×10^{-3}	2600	Kondoh and Nakajima (1997)	M	
	2.0×10^{-3}	4300	Dewulf et al. (1995)	M	
	1.5×10^{-3}	4900	Wright et al. (1992)	M	665
	1.7×10^{-3}	3700	Tse et al. (1992)	M	
	1.7×10^{-3}	2100	Lamarche and Droste (1989)	M	345
	1.5×10^{-3}	3100	Ashworth et al. (1988)	M	278
	1.8×10^{-3}	4100	Gossett (1987)	M	
	1.3×10^{-3}	4900	Ervin et al. (1980)	M	
	1.8×10^{-3}		Warner et al. (1980)	M	
	1.0×10^{-3}		Sato and Nakajima (1979b)	M	14

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.8×10^{-3}	4400	Rex (1906)	M	
	1.7×10^{-3}		Mackay et al. (2006b)	V	
	1.6×10^{-3}		Mackay et al. (1993)	V	
	1.8×10^{-3}		Warner et al. (1980)	V	
	1.7×10^{-3}		Smith and Bomberger (1980)	V	24
	1.7×10^{-3}		Dilling (1977)	V	
	1.7×10^{-3}		Hine and Mookerjee (1975)	V	
	1.7×10^{-3}		Yaws (2003)	X	237
	1.7×10^{-3}	3800	Barr and Newsham (1987)	X	298
	1.8×10^{-3}	1700	Goldstein (1982)	X	298
	2.4×10^{-3}		Ryan et al. (1988)	C	
	1.8×10^{-3}		Shen (1982)	C	
	5.1×10^{-4}		Wang et al. (2017)	Q	80, 238
	4.2×10^{-3}		Wang et al. (2017)	Q	80, 239
	6.5×10^{-3}		Wang et al. (2017)	Q	80, 240
	2.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-3}		Gharagheizi et al. (2010)	Q	246
	3.2×10^{-3}		Hilal et al. (2008)	Q	
	1.4×10^{-3}		Modarresi et al. (2007)	Q	67
		3300	Kühne et al. (2005)	Q	
	1.8×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	5.0×10^{-4}		English and Carroll (2001)	Q	230, 274
	1.1×10^{-3}		Katritzky et al. (1998)	Q	
	1.4×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.8×10^{-3}		Mackay et al. (2006b)	?	
		3900	Kühne et al. (2005)	?	
	1.7×10^{-3}		Yaws (1999)	?	21
	1.1×10^{-3}		Abraham and Weathersby (1994)	?	21
	1.6×10^{-3}		Mackay et al. (1993)	?	
	1.7×10^{-3}		Yaws and Yang (1992)	?	21
	1.7×10^{-3}		Abraham et al. (1990)	?	
1,2-dichloroethane CH_2ClCH_2Cl [107-06-2] WSLDOOZREJYCGB-UHFFFAOYSA-N	7.5×10^{-3}	4400	Schwardt et al. (2021)	L	1
	8.9×10^{-3}	4300	Burkholder et al. (2019)	L	
	7.6×10^{-3}	3700	Burkholder et al. (2019)	L	70
	8.9×10^{-3}	4300	Burkholder et al. (2015)	L	
	7.6×10^{-3}	3700	Burkholder et al. (2015)	L	70
	8.4×10^{-3}	4200	Brockbank (2013)	L	1
	8.9×10^{-3}	4300	Warneck (2007)	L	
	9.1×10^{-3}	4300	Fogg and Sangster (2003)	L	
	7.8×10^{-3}	4200	Staudinger and Roberts (2001)	L	
	7.1×10^{-3}	4200	Staudinger and Roberts (1996)	L	
	9.1×10^{-3}		Mackay and Shiu (1981)	L	
	8.2×10^{-3}	4400	Hiatt (2013)	M	
	9.1×10^{-3}	6100	Chen et al. (2012)	M	

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Table A6.1: Chlorocarbons (C, H, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.4×10^{-3}		Ayuttaya et al. (2001)	M	340
	5.7×10^{-4}		Ayuttaya et al. (2001)	M	341
	4.2×10^{-3}		Ayuttaya et al. (2001)	M	342
	8.1×10^{-3}		Ayuttaya et al. (2001)	M	343
	7.5×10^{-3}		Welke et al. (1998)	M	
	1.1×10^{-2}		Hovorka and Dohnal (1997)	M	12
	6.2×10^{-3}	3700	Kondoh and Nakajima (1997)	M	
	9.3×10^{-3}	4600	Dewulf et al. (1995)	M	
	8.3×10^{-3}		Hoff et al. (1993)	M	
	8.2×10^{-3}		Li et al. (1993)	M	
	8.4×10^{-3}	4300	Wright et al. (1992)	M	666
	8.0×10^{-3}	3600	Tse et al. (1992)	M	
	6.4×10^{-3}	4500	Bissonette et al. (1990)	M	
	5.8×10^{-3}	3000	Lamarche and Droste (1989)	M	345
	7.6×10^{-3}		Guitart et al. (1989)	M	14
	6.4×10^{-3}	1500	Ashworth et al. (1988)	M	33, 278
	8.4×10^{-3}	3500	Leighton and Calo (1981)	M	
	9.0×10^{-3}		Warner et al. (1980)	M	
	4.4×10^{-3}		Sato and Nakajima (1979b)	M	14
	1.1×10^{-2}		Pearson and McConnell (1975)	M	649, 12
	7.9×10^{-3}	4400	Hartkopf and Karger (1973)	M	
	7.2×10^{-3}		Saylor et al. (1938)	M	38
	8.6×10^{-3}	4400	Rex (1906)	M	
	8.2×10^{-3}		Mackay et al. (2006b)	V	
	8.3×10^{-3}		Mackay et al. (1993)	V	
	7.3×10^{-3}		Warner et al. (1980)	V	
	8.1×10^{-3}		Dilling (1977)	V	
	7.5×10^{-3}		Hine and Mookerjee (1975)	V	
	8.3×10^{-3}		Yaws (2003)	X	237
	8.5×10^{-3}	3700	Barr and Newsham (1987)	X	298
	9.0×10^{-3}	2400	Goldstein (1982)	X	298
	8.6×10^{-3}		Harrison et al. (1993)	C	
	9.0×10^{-3}		Harrison et al. (1993)	C	
	1.1×10^{-2}		Ryan et al. (1988)	C	
	9.0×10^{-3}		Shen (1982)	C	
	1.0×10^{-2}		Dilling (1977)	C	
	1.1×10^{-2}		Hayer et al. (2022)	Q	20
	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	3.8×10^{-3}		Duchowicz et al. (2020)	Q	184
	1.5×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.2×10^{-2}		Wang et al. (2017)	Q	80, 239
	2.0×10^{-2}		Wang et al. (2017)	Q	80, 240
	7.5×10^{-3}		Li et al. (2014)	Q	241
	6.6×10^{-3}		Ghargheizi et al. (2012)	Q	
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^{-2}		Gharagheizi et al. (2010)	Q	246
	1.0×10^{-2}		Hilal et al. (2008)	Q	
	5.1×10^{-3}		Modarresi et al. (2007)	Q	67
		3300	Kühne et al. (2005)	Q	
	8.2×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	3.4×10^{-3}		English and Carroll (2001)	Q	230, 231
	2.2×10^{-3}		Katritzky et al. (1998)	Q	
	7.7×10^{-3}		Russell et al. (1992)	Q	279
	1.8×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	8.4×10^{-3}		Duchowicz et al. (2020)	?	185, 21
	4.2×10^{-3}		MacBean (2012a)	?	
	7.0×10^{-3}		Mackay et al. (2006b)	?	
		3600	Kühne et al. (2005)	?	
	8.4×10^{-3}		Yaws (1999)	?	21
	4.5×10^{-3}		Abraham and Weathersby (1994)	?	21
	7.0×10^{-3}		Mackay et al. (1993)	?	
	8.3×10^{-3}		Yaws and Yang (1992)	?	21
	8.2×10^{-3}		Abraham et al. (1990)	?	
	1.2×10^{-2}		Chiou et al. (1980)	?	79
1,2-dichloroethane-d4 CD_2ClCD_2Cl [17060-07-0] WSLDOOZREJYCGB-LNLMKGTHSA-N	8.7×10^{-3}	4300	Hiatt (2013)	M	
1,1,1-trichloroethane	6.0×10^{-4}	3800	Schwardt et al. (2021)	L	1
CH_3CCl_3	6.0×10^{-4}	3700	Burkholder et al. (2019)	L	
(methylchloroform; MCF)	4.2×10^{-4}	4200	Burkholder et al. (2019)	L	70
[71-55-6]	6.0×10^{-4}	3700	Burkholder et al. (2015)	L	
UOCLXMDMGBRAIB-UHFFFAOYSA-N	4.2×10^{-4}	4200	Burkholder et al. (2015)	L	70
	5.8×10^{-4}	4100	Brockbank (2013)	L	1
	6.0×10^{-4}	3700	Warneck (2007)	L	
	6.2×10^{-4}	3900	Fogg and Sangster (2003)	L	
	5.9×10^{-4}	4000	Staudinger and Roberts (2001)	L	
	5.8×10^{-4}	3900	Staudinger and Roberts (1996)	L	
	3.6×10^{-4}		Mackay and Shiu (1981)	L	
	6.9×10^{-4}	4000	Hiatt (2013)	M	
	5.4×10^{-4}	4100	Chen et al. (2012)	M	
	6.2×10^{-4}	3500	Vane and Giroux (2000)	M	
	7.1×10^{-4}		Chiang et al. (1998)	M	12
	7.9×10^{-4}		Hovorka and Dohnal (1997)	M	12
	6.7×10^{-4}	1900	Kondoh and Nakajima (1997)	M	
	4.8×10^{-4}		Turner et al. (1996)	M	
	6.7×10^{-4}	4100	Dewulf et al. (1995)	M	
	5.5×10^{-4}	2500	Robbins et al. (1993)	M	667
	5.3×10^{-4}		Hoff et al. (1993)	M	
	5.9×10^{-4}	3100	Hansen et al. (1993)	M	281
	5.7×10^{-4}		Li et al. (1993)	M	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	6.0×10^{-4}	3300	Wright et al. (1992)	M	668
	6.3×10^{-4}	3700	Tse et al. (1992)	M	
	7.9×10^{-4}	1300	Kolb et al. (1992)	M	277
	5.1×10^{-4}	5200	Bissonette et al. (1990)	M	
	3.2×10^{-4}		Guitart et al. (1989)	M	14
	5.7×10^{-4}	3400	Ashworth et al. (1988)	M	278
	5.9×10^{-4}	4100	Gossett (1987)	M	
	5.8×10^{-4}	4100	Munz and Roberts (1987)	M	
	6.3×10^{-4}		Yurteri et al. (1987)	M	12
	5.7×10^{-4}	4200	Gossett et al. (1985)	M	
	5.9×10^{-4}	4300	Lincoff and Gossett (1984)	M	
	7.6×10^{-4}	3200	Hunter-Smith et al. (1983)	M	658
	4.9×10^{-4}	4400	Leighton and Calo (1981)	M	
	2.7×10^{-4}	7000	Ervin et al. (1980)	M	
	2.0×10^{-3}		Warner et al. (1980)	M	
	3.6×10^{-4}		Sato and Nakajima (1979b)	M	14
	2.9×10^{-4}		Pearson and McConnell (1975)	M	649, 12
	5.9×10^{-4}		Mackay et al. (2006b)	V	
	6.8×10^{-4}		Mackay et al. (1993)	V	
	7.0×10^{-4}	4700	McLinden (1989)	V	
	2.4×10^{-3}		Warner et al. (1980)	V	
	3.4×10^{-4}		Dilling (1977)	V	651
	4.0×10^{-4}		Dilling (1977)	V	12
	1.1×10^{-3}		Dilling (1977)	V	153
	6.1×10^{-4}		Hine and Mookerjee (1975)	V	
	5.9×10^{-4}		Dilling et al. (1975)	V	
	4.5×10^{-4}		Yaws (2003)	X	237
	5.8×10^{-4}	4000	Barr and Newsham (1987)	X	298
	2.2×10^{-3}	1700	Goldstein (1982)	X	298
	3.1×10^{-4}		Ryan et al. (1988)	C	
	2.0×10^{-3}		Shen (1982)	C	
	2.3×10^{-4}		Wang et al. (2017)	Q	80, 238
	7.6×10^{-4}		Wang et al. (2017)	Q	80, 239
	2.0×10^{-3}		Wang et al. (2017)	Q	80, 240
	2.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	4.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
	9.0×10^{-4}		Hilal et al. (2008)	Q	
	1.3×10^{-3}		Modarresi et al. (2007)	Q	67
		3700	Kühne et al. (2005)	Q	
	6.1×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	7.9×10^{-4}		English and Carroll (2001)	Q	230, 260
	5.4×10^{-4}		Katritzky et al. (1998)	Q	
	2.3×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.6×10^{-3}		Arbuckle (1983)	Q	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.7×10^{-4}		Mackay et al. (2006b)	?	
		3700	Kühne et al. (2005)	?	
	4.6×10^{-4}		Yaws (1999)	?	21
	3.8×10^{-4}		Abraham and Weathersby (1994)	?	21
	5.7×10^{-4}		Mackay et al. (1993)	?	
	5.6×10^{-4}		Abraham et al. (1990)	?	
	1.6×10^{-3}		Chiou et al. (1980)	?	79
1,1,2-trichloroethane	1.1×10^{-2}	4400	Schwardt et al. (2021)	L	1
$CHCl_2CH_2Cl$	1.1×10^{-2}	4100	Burkholder et al. (2019)	L	
[79-00-5]	1.1×10^{-2}	4100	Burkholder et al. (2015)	L	
UBOXGVDOUJQMTN-UHFFFAOYSA-N	1.1×10^{-2}	4400	Brockbank (2013)	L	1, 669
	1.1×10^{-2}	4100	Warneck (2007)	L	
	1.2×10^{-2}	4200	Fogg and Sangster (2003)	L	
	1.1×10^{-2}	4900	Staudinger and Roberts (2001)	L	
	1.1×10^{-2}	4900	Staudinger and Roberts (1996)	L	
	8.3×10^{-3}		Mackay and Shiu (1981)	L	
	7.3×10^{-3}	2400	Schwardt et al. (2021)	M	670, 11
	1.4×10^{-2}	5400	Hiatt (2013)	M	
	1.2×10^{-2}		Bobadilla et al. (2003)	M	
	1.1×10^{-2}	4700	Dewulf et al. (1999)	M	
	1.5×10^{-2}		Dohnal and Hovorka (1999)	M	12
	1.5×10^{-2}		Hovorka and Dohnal (1997)	M	12
	1.1×10^{-2}	5100	Kondoh and Nakajima (1997)	M	
	1.2×10^{-2}	5900	Hansen et al. (1993)	M	281
	1.1×10^{-2}	4300	Wright et al. (1992)	M	671
	1.1×10^{-2}	4100	Tse et al. (1992)	M	
	1.0×10^{-2}	4800	Ashworth et al. (1988)	M	278
	1.2×10^{-2}	3700	Leighton and Calo (1981)	M	
	6.6×10^{-3}		Sato and Nakajima (1979b)	M	14
	1.1×10^{-2}		Mackay et al. (2006b)	V	
	1.0×10^{-2}		Mackay et al. (1993)	V	
	1.1×10^{-2}		Dilling (1977)	V	
	1.1×10^{-2}		Hine and Mookerjee (1975)	V	
	1.1×10^{-2}		Yaws (2003)	X	237
	1.1×10^{-2}	4300	Barr and Newsham (1987)	X	298
	1.2×10^{-2}	2700	Goldstein (1982)	X	298
	1.3×10^{-3}		Ryan et al. (1988)	C	
	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	7.7×10^{-3}		Duchowicz et al. (2020)	Q	
	4.9×10^{-3}		Wang et al. (2017)	Q	80, 238
	2.1×10^{-2}		Wang et al. (2017)	Q	80, 239
	4.1×10^{-2}		Wang et al. (2017)	Q	80, 240
	1.1×10^{-2}		Li et al. (2014)	Q	241
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	1.6×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.0×10^{-2}		Gharagheizi et al. (2010)	Q	246

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.5×10^{-2}		Hilal et al. (2008)	Q	
	6.7×10^{-3}		Modarresi et al. (2007)	Q	67
		3700	Kühne et al. (2005)	Q	
	8.6×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.9×10^{-3}		Katritzky et al. (1998)	Q	
	3.3×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	7.6×10^{-3}		Arbuckle (1983)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	1.1×10^{-2}		Mackay et al. (2006b)	?	
		4200	Kühne et al. (2005)	?	
	1.1×10^{-2}		Yaws (1999)	?	21
	6.9×10^{-3}		Abraham and Weathersby (1994)	?	21
	1.1×10^{-2}		Mackay et al. (1993)	?	
	1.0×10^{-2}		Yaws and Yang (1992)	?	21
	1.2×10^{-2}		Abraham et al. (1990)	?	
1,1,2-trichloroethane-d3 $CDCl_2CD_2Cl$ [171086-93-4] UBOXGVDOUJQMTN-FUDHJZNOSA-N	1.3×10^{-2}	5100	Hiatt (2013)	M	
1,1,1,2-tetrachloroethane CCl_3CH_2Cl [630-20-6] QVLAWKAXOMEXPM-UHFFFAOYSA-N	5.0×10^{-3}	6700	Schwardt et al. (2021)	L	1
	4.2×10^{-3}	4600	Burkholder et al. (2019)	L	
	4.2×10^{-3}	4600	Burkholder et al. (2015)	L	
	4.2×10^{-3}	4900	Brockbank (2013)	L	1
	4.2×10^{-3}	4600	Warneck (2007)	L	
	2.4×10^{-2}	3200	Staudinger and Roberts (2001)	L	
	3.6×10^{-3}		Mackay and Shiu (1981)	L	
	4.5×10^{-3}	11000	Schwardt et al. (2021)	M	672
	4.8×10^{-3}	4800	Hiatt (2013)	M	
	4.3×10^{-3}	4100	Kondoh and Nakajima (1997)	M	
	4.0×10^{-3}	4400	Wright et al. (1992)	M	673
	4.5×10^{-3}	4600	Tse et al. (1992)	M	
	2.1×10^{-3}		Sato and Nakajima (1979b)	M	14
	4.0×10^{-3}		Mackay et al. (2006b)	V	
	4.2×10^{-3}	5000	Fogg and Sangster (2003)	V	
	4.1×10^{-3}		Mackay et al. (1993)	V	
	3.7×10^{-3}		Dilling (1977)	V	
	4.1×10^{-3}		Yaws (2003)	X	237
	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	184
	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
	3.9×10^{-3}		Hilal et al. (2008)	Q	
	6.0×10^{-3}		Modarresi et al. (2007)	Q	67

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		4100	Kühne et al. (2005)	Q	
	3.8×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	4.5×10^{-3}		English and Carroll (2001)	Q	230, 231
	1.2×10^{-3}		Katritzky et al. (1998)	Q	
	5.4×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	3.9×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4600	Kühne et al. (2005)	?	
	4.1×10^{-3}		Yaws (1999)	?	21
	2.2×10^{-3}		Abraham and Weathersby (1994)	?	21
	3.5×10^{-3}		Abraham et al. (1990)	?	
1,1,2,2-tetrachloroethane $CHCl_2CHCl_2$ [79-34-5] QPFMBZIOSGYJDE-UHFFFAOYSA-N	2.3×10^{-2}	3700	Schwardt et al. (2021)	L	1
	2.3×10^{-2}	4800	Burkholder et al. (2019)	L	
	2.3×10^{-2}	4800	Burkholder et al. (2015)	L	
	2.4×10^{-2}	5000	Brockbank (2013)	L	1
	2.4×10^{-2}	4800	Warneck (2007)	L	
	2.4×10^{-2}	3200	Staudinger and Roberts (1996)	L	
	2.1×10^{-2}		Mackay and Shiu (1981)	L	
	3.3×10^{-2}	7200	Hiatt (2013)	M	
	3.0×10^{-2}		Hovorka and Dohnal (1997)	M	12
	2.3×10^{-2}	6800	Kondoh and Nakajima (1997)	M	674
	2.9×10^{-2}		Li and Carr (1993)	M	
	2.2×10^{-2}	3100	Wright et al. (1992)	M	675
	2.6×10^{-2}	4800	Tse et al. (1992)	M	
	2.2×10^{-2}	2900	Ashworth et al. (1988)	M	42, 278
	2.7×10^{-2}	3500	Leighton and Calo (1981)	M	
	1.4×10^{-2}		Sato and Nakajima (1979b)	M	14
	2.1×10^{-2}		Mackay et al. (2006b)	V	
	2.2×10^{-2}		Mackay et al. (1993)	V	
	2.1×10^{-2}		Dilling (1977)	V	
	2.2×10^{-2}		Hine and Mookerjee (1975)	V	
	2.8×10^{-2}		Yaws (2003)	X	237
	1.8×10^{-2}	4200	Barr and Newsham (1987)	X	298
	2.3×10^{-2}	3000	Goldstein (1982)	X	298
	2.5×10^{-2}		Ryan et al. (1988)	C	
	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	1.5×10^{-2}		Duchowicz et al. (2020)	Q	299
	1.6×10^{-2}		Wang et al. (2017)	Q	80, 238
	2.7×10^{-2}		Wang et al. (2017)	Q	80, 239
	9.3×10^{-2}		Wang et al. (2017)	Q	80, 240
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	2.8×10^{-2}		Gharagheizi et al. (2010)	Q	246
	1.9×10^{-2}		Hilal et al. (2008)	Q	
	5.5×10^{-3}		Modarresi et al. (2007)	Q	67
		4100	Kühne et al. (2005)	Q	
	2.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^{-3}		Katritzky et al. (1998)	Q	
	6.1×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	2.7×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	3.9×10^{-2}		Mackay et al. (2006b)	?	
		4500	Kühne et al. (2005)	?	
	2.8×10^{-2}		Yaws (1999)	?	21
	1.4×10^{-2}		Abraham and Weathersby (1994)	?	21
	3.9×10^{-2}		Mackay et al. (1993)	?	
	3.0×10^{-2}		Yaws and Yang (1992)	?	21
	2.6×10^{-2}		Abraham et al. (1990)	?	
	3.0×10^{-2}		Chiou et al. (1980)	?	79
pentachloroethane	4.1×10^{-3}	7700	Burkholder et al. (2019)	L	676
$CHCl_2CCl_3$	4.2×10^{-3}	7700	Brockbank (2013)	L	1
[76-01-7]	4.5×10^{-3}		Mackay and Shiu (1981)	L	
BNIXVQGCZULYKV-UHFFFAOYSA-N	5.9×10^{-3}	5400	Hiatt (2013)	M	
	5.1×10^{-3}		Duchowicz et al. (2020)	V	186
	5.2×10^{-3}		HSDB (2015)	V	
	4.1×10^{-3}		Mackay et al. (2006b)	V	
	4.0×10^{-3}		Mackay et al. (1993)	V	
	5.3×10^{-3}		Meylan and Howard (1991)	V	
	4.0×10^{-3}		Dilling (1977)	V	
	4.0×10^{-3}		Hine and Mookerjee (1975)	V	
	6.2×10^{-3}		Duchowicz et al. (2020)	Q	
	4.0×10^{-3}		Li et al. (2014)	Q	241
	2.0×10^{-2}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	6.1×10^{-3}		Hilal et al. (2008)	Q	
	3.6×10^{-3}		Modarresi et al. (2007)	Q	67
	4.0×10^{-4}		Katritzky et al. (1998)	Q	
	1.9×10^{-2}		Meylan and Howard (1991)	Q	
	1.0×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	5.1×10^{-3}		Yaws (1999)	?	21
	5.4×10^{-3}		Yaws and Yang (1992)	?	21
	4.2×10^{-3}		Abraham et al. (1990)	?	
hexachloroethane	2.7×10^{-3}	5700	Burkholder et al. (2019)	L	
C_2Cl_6	2.6×10^{-3}	5600	Burkholder et al. (2015)	L	
[67-72-1]	2.8×10^{-3}	6100	Brockbank (2013)	L	1
VHHHONWQHHHLTI-UHFFFAOYSA-N	2.5×10^{-3}	5600	Staudinger and Roberts (1996)	L	
	1.2×10^{-3}	2600	Ashworth et al. (1988)	M	33, 278
	2.5×10^{-3}	5600	Munz and Roberts (1987)	M	
	3.4×10^{-3}		Munz and Roberts (1986)	M	
	1.0×10^{-3}		Warner et al. (1980)	M	
	4.2×10^{-3}		Mackay et al. (2006b)	V	
	3.6×10^{-3}		Lide and Frederikse (1995)	V	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.5×10^{-2}		Hwang et al. (1992)	V	
	2.2×10^{-4}		Ballschmiter and Wittlinger (1991)	V	
	7.7×10^{-4}		Mackay and Shiu (1981)	V	
	8.1×10^{-3}		Dilling (1977)	V	
	4.3×10^{-3}		Hine and Mookerjee (1975)	V	
	3.9×10^{-4}		Yaws (2003)	X	237
	1.0×10^{-3}	2100	Goldstein (1982)	X	298
	9.8×10^{-4}		Ryan et al. (1988)	C	
	1.0×10^{-3}		Shen (1982)	C	
	7.3×10^{-4}		Keshavarz et al. (2022)	Q	
	2.5×10^{-3}		Duchowicz et al. (2020)	Q	
	2.4×10^{-3}		Zhang et al. (2010)	Q	287, 288
	1.8×10^{-3}		Zhang et al. (2010)	Q	287, 289
	1.9×10^{-3}		Zhang et al. (2010)	Q	287, 290
	3.9×10^{-3}		Zhang et al. (2010)	Q	287, 291
	3.7×10^{-4}		Gharagheizi et al. (2010)	Q	246
	3.9×10^{-3}		Hilal et al. (2008)	Q	
	9.3×10^{-4}		Modarresi et al. (2007)	Q	67
	8.0×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	2.4×10^{-4}		Yao et al. (2002)	Q	229
	1.0×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	2.5×10^{-3}		Duchowicz et al. (2020)	?	185, 21
	1.2×10^{-3}		Mackay et al. (2006b)	?	
	3.9×10^{-4}		Yaws (1999)	?	21
	1.2×10^{-3}		Mackay et al. (1993)	?	
	4.4×10^{-4}		Yaws and Yang (1992)	?	21
1-chloropropane	7.6×10^{-4}	4500	Brockbank (2013)	L	1
C_3H_7Cl	6.9×10^{-4}		Li et al. (1993)	M	
[540-54-5]	4.3×10^{-4}		Sato and Nakajima (1979b)	M	14
SNMVRZFUUCLYTO-UHFFFAOYSA-N	7.7×10^{-4}	4400	Rex (1906)	M	
	7.5×10^{-4}		Duchowicz et al. (2020)	V	186
	7.6×10^{-4}		HSDB (2015)	V	
	6.9×10^{-4}		Mackay et al. (2006b)	V	
	7.1×10^{-4}		Mackay et al. (1993)	V	
	7.1×10^{-4}		Abraham (1984)	V	
	7.3×10^{-4}		Hine and Mookerjee (1975)	V	
	9.2×10^{-4}		Yaws (2003)	X	237, 12
	1.3×10^{-3}		Duchowicz et al. (2020)	Q	
	7.3×10^{-4}		Li et al. (2014)	Q	241
	4.3×10^{-4}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	6.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.1×10^{-3}		Hilal et al. (2008)	Q	
	1.0×10^{-3}		Modarresi et al. (2007)	Q	67
		3300	Kühne et al. (2005)	Q	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

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			Yaffe et al. (2003)	Q	356
	2.8×10^{-4}		Yao et al. (2002)	Q	229
	7.3×10^{-4}		English and Carroll (2001)	Q	230, 231
	1.2×10^{-3}		Katritzky et al. (1998)	Q	
	4.7×10^{-4}		Suzuki et al. (1992)	Q	232
	6.2×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
		3500	Kühne et al. (2005)	?	
	7.5×10^{-4}		Yaws (1999)	?	21, 12
	4.4×10^{-4}		Abraham and Weathersby (1994)	?	21
	9.1×10^{-4}		Yaws and Yang (1992)	?	21, 12
	7.0×10^{-4}		Abraham et al. (1990)	?	
2-chloropropane	5.7×10^{-4}	4400	Brockbank (2013)	L	1
C_3H_7Cl	5.4×10^{-4}		Li et al. (1993)	M	
[75-29-6]	5.6×10^{-4}	4300	Rex (1906)	M	
ULYZAYCEDJDHCC-UHFFFAOYSA-N	5.6×10^{-4}		Duchowicz et al. (2020)	V	186
	5.5×10^{-4}		HSDB (2015)	V	
	5.6×10^{-4}		Mackay et al. (2006b)	V	
	5.5×10^{-4}		Mackay et al. (1993)	V	
	6.1×10^{-4}		Hine and Mookerjee (1975)	V	
	6.8×10^{-4}		Yaws (2003)	X	237, 12
	5.9×10^{-4}		Duchowicz et al. (2020)	Q	
	9.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	4.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
	6.0×10^{-4}		Hilal et al. (2008)	Q	
	8.1×10^{-4}		Modarresi et al. (2007)	Q	67
	6.1×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	6.2×10^{-4}		English and Carroll (2001)	Q	230, 260
	1.5×10^{-3}		Katritzky et al. (1998)	Q	
	9.5×10^{-4}		Russell et al. (1992)	Q	279
	4.1×10^{-4}		Suzuki et al. (1992)	Q	232
	5.1×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	5.6×10^{-4}		Yaws (1999)	?	21, 12
	6.8×10^{-4}		Yaws and Yang (1992)	?	21, 12
	6.1×10^{-4}		Abraham et al. (1990)	?	
1,1-dichloropropane	2.6×10^{-3}		Duchowicz et al. (2020)	V	186
$C_3H_6Cl_2$	3.3×10^{-3}		Duchowicz et al. (2020)	V	186
[78-99-9]	2.6×10^{-3}		HSDB (2015)	V	
WIHMGGWNMISDNJ-UHFFFAOYSA-N	2.7×10^{-3}		Duchowicz et al. (2020)	Q	
	2.7×10^{-3}		Duchowicz et al. (2020)	Q	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-dichloropropane	3.7×10^{-3}	4100	Schwardt et al. (2021)	L	1
$C_3H_6Cl_2$	3.4×10^{-3}	4300	Burkholder et al. (2019)	L	
[78-87-5]	3.4×10^{-3}	4300	Burkholder et al. (2015)	L	
KNKRKFALVUDBJE-UHFFFAOYSA-N	3.4×10^{-3}	4000	Brockbank (2013)	L	1
	3.4×10^{-3}	4300	Staudinger and Roberts (2001)	L	
	3.4×10^{-3}	4300	Staudinger and Roberts (1996)	L	
	4.3×10^{-3}	4400	Hiatt (2013)	M	
	4.2×10^{-3}		Bobadilla et al. (2003)	M	
	3.5×10^{-3}	4300	Dewulf et al. (1999)	M	
	4.4×10^{-3}		Dohnal and Hovorka (1999)	M	12
	5.5×10^{-3}		Welke et al. (1998)	M	
	4.6×10^{-3}		Hovorka and Dohnal (1997)	M	12
	4.3×10^{-3}	3700	Kondoh and Nakajima (1997)	M	
	3.6×10^{-3}	4200	Wright et al. (1992)	M	677
	3.8×10^{-3}	3800	Tse et al. (1992)	M	
	3.0×10^{-3}	3800	Bissonette et al. (1990)	M	
	3.8×10^{-3}	4700	Ashworth et al. (1988)	M	33, 278
	4.9×10^{-3}		Albanese et al. (1987)	M	
	3.4×10^{-3}	4300	Leighton and Calo (1981)	M	
	3.5×10^{-3}		Warner et al. (1980)	M	
	2.1×10^{-3}		Sato and Nakajima (1979b)	M	14
	3.7×10^{-3}		Mackay et al. (2006b)	V	
	3.7×10^{-3}		Mackay et al. (1993)	V	
	3.6×10^{-3}		Warner et al. (1980)	V	
	3.4×10^{-3}		Hine and Mookerjee (1975)	V	
	3.5×10^{-3}		Yaws (2003)	X	237
	3.4×10^{-3}	2100	Goldstein (1982)	X	298
	3.5×10^{-3}		Horvath and Getzen (1999)	C	
	3.4×10^{-3}		Ryan et al. (1988)	C	
	3.5×10^{-3}		Shen (1982)	C	
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	1.8×10^{-3}		Duchowicz et al. (2020)	Q	184
	1.4×10^{-3}		Wang et al. (2017)	Q	80, 238
	6.2×10^{-3}		Wang et al. (2017)	Q	80, 239
	8.9×10^{-3}		Wang et al. (2017)	Q	80, 240
	4.7×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	4.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
	5.4×10^{-3}		Hilal et al. (2008)	Q	
	3.6×10^{-3}		Modarresi et al. (2007)	Q	67
		3700	Kühne et al. (2005)	Q	
	3.8×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	2.1×10^{-3}		English and Carroll (2001)	Q	230, 231
	2.8×10^{-3}		Katritzky et al. (1998)	Q	
	1.2×10^{-3}		Nirmalakhandan and Speece (1988)	Q	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.5×10^{-3}		Duchowicz et al. (2020)	?	185, 21
	8.5×10^{-4}		MacBean (2012a)	?	
	3.5×10^{-3}		Mackay et al. (2006b)	?	
		4000	Kühne et al. (2005)	?	
	3.5×10^{-3}		Yaws (1999)	?	21
	2.2×10^{-3}		Abraham and Weathersby (1994)	?	21
	3.5×10^{-3}		Mackay et al. (1993)	?	
	3.7×10^{-3}		Yaws and Yang (1992)	?	21
	3.4×10^{-3}		Abraham et al. (1990)	?	
	4.8×10^{-3}		Mackay and Yeun (1983)	?	
	5.9×10^{-3}		Chiou et al. (1980)	?	79
1,2-dichloropropane-d6 $C_3D_6Cl_2$ [93952-08-0] KNKRKFALVUDBJE-LIDOUZCJSA-N	3.6×10^{-3}	4600	Hiatt (2013)	M	
1,3-dichloropropane $C_3H_6Cl_2$ [142-28-9] YHRUOJUYPBUZOS-UHFFFAOYSA-N	1.0×10^{-2}	3900	Burkholder et al. (2019)	L	
	1.0×10^{-2}	3900	Burkholder et al. (2015)	L	
	1.2×10^{-2}	3100	Brockbank (2013)	L	1
	1.3×10^{-2}	5300	Hiatt (2013)	M	
	1.1×10^{-2}	5000	Kondoh and Nakajima (1997)	M	
	8.5×10^{-3}		Albanese et al. (1987)	M	
	1.0×10^{-2}	3900	Leighton and Calo (1981)	M	
	9.9×10^{-3}		Hine and Mookerjee (1975)	V	
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	3.6×10^{-3}		Duchowicz et al. (2020)	Q	299
	1.8×10^{-2}		Hilal et al. (2008)	Q	
	5.8×10^{-3}		Modarresi et al. (2007)	Q	67
		3700	Kühne et al. (2005)	Q	
	5.6×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	3.0×10^{-3}		Katritzky et al. (1998)	Q	
	1.4×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.0×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		3900	Kühne et al. (2005)	?	
	1.0×10^{-2}		Yaws (1999)	?	21
	9.9×10^{-3}		Yaws and Yang (1992)	?	21
	9.9×10^{-3}		Abraham et al. (1990)	?	
2,2-dichloropropane $C_3H_6Cl_2$ [594-20-7] ZEOVXNVKXIPWMS-UHFFFAOYSA-N	4.4×10^{-4}	7400	Hiatt (2013)	M	
	8.1×10^{-4}	3900	Bakierowska and Trzeszczyński (2003)	M	
	7.1×10^{-4}	630	Kondoh and Nakajima (1997)	M	
		3700	Kühne et al. (2005)	Q	
		3900	Kühne et al. (2005)	?	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1,1-trichloropropane	3.1×10^{-3}		Duchowicz et al. (2020)	V	186
$C_3H_5Cl_3$	3.8×10^{-3}		Yaws et al. (2005)	X	446
[7789-89-1]	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
AVGQTJUPLKNPQP-UHFFFAOYSA-N	1.1×10^{-3}		Hilal et al. (2008)	Q	
	3.1×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	6.5×10^{-4}		Katritzky et al. (1998)	Q	
1,1,2-trichloropropane	3.1×10^{-2}		Duchowicz et al. (2020)	V	186
$C_3H_5Cl_3$	1.4×10^{-2}		Yaws et al. (2005)	X	446
[598-77-6]	4.0×10^{-3}		Duchowicz et al. (2020)	Q	
GRSQYISVQKPZCW-UHFFFAOYSA-N	7.9×10^{-3}		Hilal et al. (2008)	Q	
	3.1×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.4×10^{-3}		Katritzky et al. (1998)	Q	
1,2,3-trichloropropane	3.6×10^{-2}	3700	Burkholder et al. (2019)	L	
$C_3H_5Cl_3$	3.6×10^{-2}	3700	Burkholder et al. (2015)	L	
[96-18-4]	3.3×10^{-2}	1900	Brockbank (2013)	L	1
CFXQEHVMCRXUSD-UHFFFAOYSA-N	3.6×10^{-2}	3700	Staudinger and Roberts (2001)	L	
	3.4×10^{-2}	3700	Staudinger and Roberts (1996)	L	
	4.2×10^{-2}	7200	Hiatt (2013)	M	
	2.8×10^{-2}	5300	Kondoh and Nakajima (1997)	M	
	4.4×10^{-2}	4000	Tancrède and Yanagisawa (1990)	M	
	3.3×10^{-2}		Albanese et al. (1987)	M	
	2.9×10^{-2}	3500	Leighton and Calo (1981)	M	
	2.6×10^{-2}		Mackay et al. (2006b)	V	
	2.6×10^{-2}		Mackay et al. (1993)	V	
	3.1×10^{-2}		Dilling (1977)	V	
	2.6×10^{-2}		Yaws (2003)	X	237
	2.2×10^{-2}		Yaws et al. (2005)	X	446
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	5.3×10^{-3}		Duchowicz et al. (2020)	Q	
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	2.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	1.4×10^{-2}		Modarresi et al. (2007)	Q	67
		4000	Kühne et al. (2005)	Q	
	2.9×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	3.9×10^{-3}		Katritzky et al. (1998)	Q	
	2.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		4100	Kühne et al. (2005)	?	
	2.6×10^{-2}		Yaws (1999)	?	21
	2.9×10^{-2}		Yaws and Yang (1992)	?	21

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1,2,2,3-pentachloropropane	1.4×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_3H_3Cl_5$	7.3×10^{-2}		Zhang et al. (2010)	Q	287, 289
[16714-68-4]	6.2×10^{-1}		Zhang et al. (2010)	Q	287, 290
IYFMQUDCYNWFTL-UHFFFAOYSA-N	8.6×10^{-3}		Zhang et al. (2010)	Q	287, 291
1-chloro-2-methylpropane	8.3×10^{-3}		Mackay and Shiu (1981)	L	
C_4H_9Cl	5.0×10^{-4}		Duchowicz et al. (2020)	V	186
[513-36-0]	5.0×10^{-4}		Duchowicz et al. (2020)	Q	
QTBFPMKWQKYFLR-UHFFFAOYSA-N	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	7.3×10^{-4}		Hilal et al. (2008)	Q	
	8.5×10^{-4}		Modarresi et al. (2007)	Q	67
	8.6×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	6.3×10^{-4}		Yaws and Yang (1992)	?	21, 12
2-chloro-2-methylpropane	1.6×10^{-4}	5600	Clarke et al. (1962)	M	
C_4H_9Cl	7.7×10^{-4}		Duchowicz et al. (2020)	V	186
(*tert*-butyl chloride)	1.2×10^{-3}		Yaws (2003)	X	237, 80
[507-20-0]	2.2×10^{-4}		Duchowicz et al. (2020)	Q	
NBRKLOOSMBRFMH-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.2×10^{-4}		Hilal et al. (2008)	Q	
	6.5×10^{-4}		Modarresi et al. (2007)	Q	67
	6.9×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	3.1×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	7.7×10^{-4}		Yaws (1999)	?	21, 80
	6.4×10^{-5}		Abraham et al. (1990)	?	
1-chlorobutane	5.6×10^{-4}	4500	Brockbank (2013)	L	1
C_4H_9Cl	6.7×10^{-4}		Dohnal and Hovorka (1999)	M	12
(butyl chloride)	5.3×10^{-4}		Li et al. (1993)	M	
[109-69-3]	5.9×10^{-4}	3500	Leighton and Calo (1981)	M	
VFWCMGCRMGJXDK-UHFFFAOYSA-N	3.3×10^{-4}		Sato and Nakajima (1979b)	M	14
	4.8×10^{-4}		Mackay et al. (2006b)	V	
	4.8×10^{-4}		Mackay et al. (1993)	V	
	5.3×10^{-4}		Abraham (1984)	V	
	5.1×10^{-4}		Hine and Mookerjee (1975)	V	
	5.9×10^{-4}		Yaws (2003)	X	237
	4.4×10^{-4}		Keshavarz et al. (2022)	Q	
	1.3×10^{-3}		Duchowicz et al. (2020)	Q	
	3.1×10^{-4}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	4.5×10^{-4}		Gharagheizi et al. (2010)	Q	246

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

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	9.0×10^{-4}		Hilal et al. (2008)	Q	
	8.7×10^{-4}		Modarresi et al. (2007)	Q	67
		3700	Kühne et al. (2005)	Q	
	6.1×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	1.9×10^{-4}		Yao et al. (2002)	Q	229
	5.4×10^{-4}		English and Carroll (2001)	Q	230, 231
	1.4×10^{-3}		Katritzky et al. (1998)	Q	
	1.3×10^{-3}		Russell et al. (1992)	Q	279
	3.6×10^{-4}		Suzuki et al. (1992)	Q	232
	5.0×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	5.9×10^{-4}		Duchowicz et al. (2020)	?	185, 21
	6.5×10^{-4}		Mackay et al. (2006b)	?	
		3700	Kühne et al. (2005)	?	
	5.9×10^{-4}		Yaws (1999)	?	21
	3.4×10^{-4}		Abraham and Weathersby (1994)	?	21
	6.5×10^{-4}		Mackay et al. (1993)	?	
	5.6×10^{-4}		Hoff et al. (1993)	?	21
	5.8×10^{-4}		Yaws and Yang (1992)	?	21
	5.3×10^{-4}		Abraham et al. (1990)	?	
2-chlorobutane	4.1×10^{-4}	4500	Brockbank (2013)	L	1
C_4H_9Cl	4.1×10^{-4}	4500	Leighton and Calo (1981)	M	
(*sec*-butyl chloride)	5.3×10^{-4}		Mackay et al. (2006b)	V	
[78-86-4]	5.3×10^{-4}		Mackay et al. (1993)	V	
BSPCSKHALVHRSR-UHFFFAOYSA-N	5.1×10^{-4}		Yaws (2003)	X	237
	4.4×10^{-4}		Keshavarz et al. (2022)	Q	
	5.9×10^{-4}		Duchowicz et al. (2020)	Q	299
	5.3×10^{-4}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	3.7×10^{-4}		Gharagheizi et al. (2010)	Q	246
	6.2×10^{-4}		Hilal et al. (2008)	Q	
	8.2×10^{-4}		Modarresi et al. (2007)	Q	67
		3700	Kühne et al. (2005)	Q	
	4.2×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	1.3×10^{-4}		Yao et al. (2002)	Q	229
	4.7×10^{-4}		English and Carroll (2001)	Q	230, 274
	1.9×10^{-3}		Katritzky et al. (1998)	Q	
	4.2×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	4.1×10^{-4}		Duchowicz et al. (2020)	?	185, 21
	4.4×10^{-4}		Mackay et al. (2006b)	?	
		4500	Kühne et al. (2005)	?	
	5.2×10^{-4}		Yaws (1999)	?	21
	4.4×10^{-4}		Mackay et al. (1993)	?	
	5.3×10^{-4}		Yaws and Yang (1992)	?	21
	4.0×10^{-4}		Abraham et al. (1990)	?	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

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1,1-dichlorobutane	1.3×10^{-3}		Duchowicz et al. (2020)	V	186
$C_4H_8Cl_2$	1.3×10^{-3}		Hine and Mookerjee (1975)	V	
[541-33-3]	2.7×10^{-3}		Duchowicz et al. (2020)	Q	
SEQRDAAUNCRFIT-UHFFFAOYSA-N	2.5×10^{-3}		Hilal et al. (2008)	Q	
	9.2×10^{-4}		Modarresi et al. (2007)	Q	67
	1.4×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.6×10^{-3}		English and Carroll (2001)	Q	230, 260
	1.3×10^{-3}		Katritzky et al. (1998)	Q	
	9.2×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
1,4-dichlorobutane	2.0×10^{-2}	3600	Brockbank (2013)	L	1
$C_4H_8Cl_2$	1.2×10^{-2}		Albanese et al. (1987)	M	
[110-56-5]	2.0×10^{-2}	3100	Leighton and Calo (1981)	M	
KJDRSWPQXHESDQ-UHFFFAOYSA-N	2.2×10^{-2}		Keshavarz et al. (2022)	Q	
	3.6×10^{-3}		Duchowicz et al. (2020)	Q	299
	2.6×10^{-2}		Hilal et al. (2008)	Q	
	4.5×10^{-3}		Modarresi et al. (2007)	Q	67
		4000	Kühne et al. (2005)	Q	
	2.0×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.9×10^{-3}		English and Carroll (2001)	Q	230, 231
	3.9×10^{-3}		Katritzky et al. (1998)	Q	
	1.1×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	2.0×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		3700	Kühne et al. (2005)	?	
	2.0×10^{-2}		Abraham et al. (1990)	?	
2,3-dichlorobutane	1.4×10^{-3}		Duchowicz et al. (2020)	V	186
$C_4H_8Cl_2$	2.5×10^{-3}		Yaws et al. (2005)	X	446
[7581-97-7]	8.4×10^{-4}		Duchowicz et al. (2020)	Q	
RMISVOPUIFJTEO-UHFFFAOYSA-N	2.8×10^{-3}		Hilal et al. (2008)	Q	
	2.5×10^{-3}		Modarresi et al. (2007)	Q	67
	1.4×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	3.1×10^{-3}		Katritzky et al. (1998)	Q	
1-chloropentane	4.1×10^{-4}	4000	Brockbank (2013)	L	1
$C_5H_{11}Cl$	4.2×10^{-4}		Li et al. (1993)	M	
[543-59-9]	4.1×10^{-4}	4700	Leighton and Calo (1981)	M	
SQCZQTSHSZLZIQ-UHFFFAOYSA-N	2.7×10^{-4}		Sato and Nakajima (1979b)	M	14
	4.5×10^{-4}		Mackay et al. (2006b)	V	
	4.5×10^{-4}		Mackay et al. (1993)	V	
	4.5×10^{-4}		Abraham (1984)	V	
	4.3×10^{-4}		Amoore and Buttery (1978)	V	
	4.5×10^{-4}		Hine and Mookerjee (1975)	V	
	1.9×10^{-4}		Yaws (2003)	X	237
	5.9×10^{-4}		Keshavarz et al. (2022)	Q	
	1.3×10^{-3}		Duchowicz et al. (2020)	Q	299
	2.5×10^{-4}		Gharagheizi et al. (2012)	Q	
	2.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
	7.3×10^{-4}		Hilal et al. (2008)	Q	

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	7.1×10^{-4}		Modarresi et al. (2007)	Q	67
		4000	Kühne et al. (2005)	Q	
	4.2×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	4.1×10^{-4}		English and Carroll (2001)	Q	230, 231
	1.6×10^{-3}		Katritzky et al. (1998)	Q	
	2.8×10^{-4}		Suzuki et al. (1992)	Q	232
	3.9×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	4.1×10^{-4}		Duchowicz et al. (2020)	?	185, 21
	4.2×10^{-4}		Mackay et al. (2006b)	?	
		4400	Kühne et al. (2005)	?	
	1.9×10^{-4}		Yaws (1999)	?	21
	2.8×10^{-4}		Abraham and Weathersby (1994)	?	21
	4.2×10^{-4}		Mackay et al. (1993)	?	
	2.0×10^{-4}		Yaws and Yang (1992)	?	21
	4.5×10^{-4}		Abraham et al. (1990)	?	
2-chloropentane $C_5H_{11}Cl$ [625-29-6] NFRKUDYZEVQXTE-UHFFFAOYSA-N	6.7×10^{-4}		Duchowicz et al. (2020)	V	186
	3.6×10^{-4}		Hine and Mookerjee (1975)	V	
	5.8×10^{-4}		Duchowicz et al. (2020)	Q	
	4.8×10^{-4}		Hilal et al. (2008)	Q	
	6.0×10^{-4}		Modarresi et al. (2007)	Q	67
	6.7×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	3.6×10^{-4}		English and Carroll (2001)	Q	230, 274
	2.2×10^{-3}		Katritzky et al. (1998)	Q	
	2.5×10^{-4}		Suzuki et al. (1992)	Q	232
	3.3×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	3.6×10^{-4}		Abraham et al. (1990)	?	
3-chloropentane $C_5H_{11}Cl$ [616-20-6] CXQSCYIVCSCSES-UHFFFAOYSA-N	3.8×10^{-4}		Duchowicz et al. (2020)	V	186
	3.8×10^{-4}		Meylan and Howard (1991)	V	
	3.8×10^{-4}		Hine and Mookerjee (1975)	V	
	5.8×10^{-4}		Duchowicz et al. (2020)	Q	
	4.7×10^{-4}		Hilal et al. (2008)	Q	
	5.9×10^{-4}		Modarresi et al. (2007)	Q	67
	4.5×10^{-4}		English and Carroll (2001)	Q	230, 260
	2.5×10^{-4}		Suzuki et al. (1992)	Q	232
	3.9×10^{-4}		Meylan and Howard (1991)	Q	
	3.4×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	3.8×10^{-4}		Abraham et al. (1990)	?	
1,2-dichloropentane $C_5H_{10}Cl_2$ [1674-33-5] PPLBPDUKNRCHGG-UHFFFAOYSA-N	4.8×10^{-3}		Yaws et al. (2005)	X	446
	3.1×10^{-3}		Hilal et al. (2008)	Q	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,5-dichloropentane	1.0×10^{-2}	4000	Brockbank (2013)	L	1
$C_5H_{10}Cl_2$	1.8×10^{-2}	1600	Leighton and Calo (1981)	M	
[628-76-2]	2.9×10^{-2}		Keshavarz et al. (2022)	Q	
LBKDGROORAKTLC-UHFFFAOYSA-N	3.6×10^{-3}		Duchowicz et al. (2020)	Q	184
	2.0×10^{-2}		Hilal et al. (2008)	Q	
	3.8×10^{-3}		Modarresi et al. (2007)	Q	67
		4400	Kühne et al. (2005)	Q	
	1.8×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	4.2×10^{-3}		Katritzky et al. (1998)	Q	
	1.8×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		4100	Kühne et al. (2005)	?	
2,3-dichloropentane	2.9×10^{-3}		Yaws et al. (2005)	X	446
$C_5H_{10}Cl_2$	2.8×10^{-3}		Hilal et al. (2008)	Q	
[600-11-3]					
HVFJQRZGBBKTPL-UHFFFAOYSA-N					
2-chloro-2-methylbutane	3.1×10^{-3}		Yaws (1999)	?	21
$C_5H_{11}Cl$	3.0×10^{-3}		Yaws and Yang (1992)	?	21
[594-36-5]					
CRNIHJHMEQZAAS-UHFFFAOYSA-N					
1-chlorohexane	3.1×10^{-4}		Li et al. (1993)	M	
$C_6H_{13}Cl$	4.1×10^{-4}	4500	Leighton and Calo (1981)	M	
[544-10-5]	8.0×10^{-4}		Keshavarz et al. (2022)	Q	
MLRVZFYXUZQSRU-UHFFFAOYSA-N	1.3×10^{-3}		Duchowicz et al. (2020)	Q	299
	6.1×10^{-4}		Hilal et al. (2008)	Q	
	6.1×10^{-4}		Modarresi et al. (2007)	Q	67
		4300	Kühne et al. (2005)	Q	
	3.5×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	3.1×10^{-4}		English and Carroll (2001)	Q	230, 231
	1.7×10^{-3}		Katritzky et al. (1998)	Q	
	3.1×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	4.1×10^{-4}		Duchowicz et al. (2020)	?	185, 21
		4400	Kühne et al. (2005)	?	
	4.0×10^{-4}		Abraham et al. (1990)	?	
2-chlorohexane	5.0×10^{-4}		Yaws et al. (2005)	X	446
$C_6H_{13}Cl$	4.2×10^{-4}		Hilal et al. (2008)	Q	
[638-28-8]					
GLCIPJOIEVLTPR-UHFFFAOYSA-N					
3-chlorohexane	5.0×10^{-4}		Yaws et al. (2005)	X	446
$C_6H_{13}Cl$	5.0×10^{-4}		Hilal et al. (2008)	Q	
[2346-81-8]					
BXSMMAVTEURRGG-UHFFFAOYSA-N					

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloroheptane	2.5×10^{-4}		Abraham (1984)	V	
$C_7H_{15}Cl$	5.1×10^{-4}		Hilal et al. (2008)	Q	
[629-06-1]	5.1×10^{-4}		Modarresi et al. (2007)	Q	67
DZMDPHNGKBEVRE-UHFFFAOYSA-N	2.3×10^{-4}		English and Carroll (2001)	Q	230, 231
	2.4×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	2.5×10^{-4}		Abraham et al. (1990)	?	
2-chloroheptane	3.9×10^{-4}		Yaws et al. (2005)	X	446
$C_7H_{15}Cl$	3.4×10^{-4}		Hilal et al. (2008)	Q	
[1001-89-4]					
PTSLUOSUHFGQHV-UHFFFAOYSA-N					
3-chloroheptane	3.6×10^{-4}		Yaws et al. (2005)	X	446
$C_7H_{15}Cl$	3.4×10^{-4}		Hilal et al. (2008)	Q	
[999-52-0]					
DMKNOEJJJSHSML-UHFFFAOYSA-N					
4-chloroheptane	3.6×10^{-4}		Yaws et al. (2005)	X	446
$C_7H_{15}Cl$	3.5×10^{-4}		Hilal et al. (2008)	Q	
[998-95-8]					
MGSGWAXIEMEWCQ-UHFFFAOYSA-N					
1-chlorooctane	2.6×10^{-4}		Duchowicz et al. (2020)	V	186
$C_8H_{17}Cl$	1.9×10^{-4}	6100	Sarraute et al. (2004)	V	
[111-85-3]	2.6×10^{-4}		Yaws et al. (2005)	X	446
CNDHHGUSRIZDSL-UHFFFAOYSA-N	1.3×10^{-3}		Duchowicz et al. (2020)	Q	
	1.6×10^{-4}		HSDB (2015)	Q	99
	4.2×10^{-4}		Hilal et al. (2008)	Q	
	2.6×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	1.8×10^{-3}		Katritzky et al. (1998)	Q	
2-chlorooctane	2.7×10^{-4}		Yaws et al. (2005)	X	446
$C_8H_{17}Cl$	3.1×10^{-4}		Hilal et al. (2008)	Q	
[628-61-5]					
HKDCIIMOALDWHF-UHFFFAOYSA-N					
3-(chloromethyl)-heptane	4.5×10^{-4}		Hilal et al. (2008)	Q	
$C_8H_{17}Cl$	4.9×10^{-4}		Modarresi et al. (2007)	Q	67
[123-04-6]					
WLVCBAMXYMWGLJ-UHFFFAOYSA-N					
1,8-dichlorooctane	7.1×10^{-3}	7100	Sarraute et al. (2006)	M	678
$C_8H_{16}Cl_2$					
[2162-99-4]					
WXYMNDFVLNUAIA-UHFFFAOYSA-N					
1-chlorononane	1.6×10^{-4}		Yaws et al. (2005)	X	446
$C_9H_{19}Cl$	3.5×10^{-4}		Hilal et al. (2008)	Q	
[2473-01-0]					
RKAMCQVGHFRILV-UHFFFAOYSA-N					

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-chlorononane $C_9H_{19}Cl$ [2216-36-6] DTWJISBCMBWFNY-UHFFFAOYSA-N	2.7×10^{-4} 3.0×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	446
5-chlorononane $C_9H_{19}Cl$ [28123-70-8] GHLDSOWZIOPMTC-UHFFFAOYSA-N	2.2×10^{-4} 2.6×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	446
1-chlorodecane $C_{10}H_{21}Cl$ [1002-69-3] ZTEHOZMYMCEYRM-UHFFFAOYSA-N	1.6×10^{-4} 2.5×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	446
1,10-dichlorodecane $C_{10}H_{20}Cl_2$ [2162-98-3] RBBNTRDPSVZESY-UHFFFAOYSA-N	2.0×10^{-3} 5.3×10^{-3}		Drouillard et al. (1998) Hilal et al. (2008)	V Q	
1,2,9,10-tetrachlorodecane $C_{10}H_{18}Cl_4$ [205646-11-3] VXBHNYIEBLRXAW-UHFFFAOYSA-N	5.6×10^{-2} 6.2×10^{-2} 3.9×10^{-2} 6.2×10^{-4} 1.4×10^{-2}		Drouillard et al. (1998) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Hilal et al. (2008)	M Q Q Q Q	 242, 243 244 245
pentachlorodecane isomers $C_{10}H_{17}Cl_5$ [175801-37-3] AMKBEJYNNQNKGD-UHFFFAOYSA-N	2.0×10^{-1} 3.8×10^{-1}		Drouillard et al. (1998) Drouillard et al. (1998)	M M	
1-chloroundecane $C_{11}H_{23}Cl$ [2473-03-2] ZHKKNUKCXPWZOP-UHFFFAOYSA-N	1.7×10^{-4} 2.3×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	446
1,2,10,11-tetrachloroundecane $C_{11}H_{20}Cl_4$ [210049-49-3] VVAAXDBMZVCVPA-UHFFFAOYSA-N	1.6×10^{-1} 4.9×10^{-2} 3.1×10^{-2} 4.9×10^{-4} 1.1×10^{-2}		Drouillard et al. (1998) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010) Hilal et al. (2008)	M Q Q Q Q	 242, 243 244 245
pentachloroundecane isomers $C_{11}H_{19}Cl_5$ [210175-48-7] BBCUCNDIXLWBNQ-UHFFFAOYSA-N	6.8×10^{-1} 1.5		Drouillard et al. (1998) Drouillard et al. (1998)	M M	
1-chlorododecane $C_{12}H_{25}Cl$ [112-52-7] YAYNEUUHHLGGAH-UHFFFAOYSA-N	2.3×10^{-4} 1.9×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	446

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,12-dichlorododecane $C_{12}H_{24}Cl_2$ [3922-28-9] RNXPZVYZVHJVHM-UHFFFAOYSA-N	1.5×10^{-3} 3.1×10^{-3}		Drouillard et al. (1998) Hilal et al. (2008)	V Q	
1-chlorotridecane $C_{13}H_{27}Cl$ [822-13-9] ASZMYJSJEOGSBR-UHFFFAOYSA-N	2.9×10^{-4} 1.4×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	446
1-chlorotetradecane $C_{14}H_{29}Cl$ [2425-54-9] RNHWYOLIEJIAMV-UHFFFAOYSA-N	3.9×10^{-4} 1.2×10^{-4}		Yaws et al. (2005) Hilal et al. (2008)	X Q	446
tetrachlorocyclopentane $C_5H_6Cl_4$ [59808-78-5] ZFMWDTNZPKDVBU-UHFFFAOYSA-N	6.4×10^{-3} 4.1×10^{-1} 1.5 2.9×10^{-2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
1,1,2,3,3,4- hexachlorocyclopentane $C_5H_4Cl_6$ [68258-91-3] RPUFWOAXMFQSDJ-UHFFFAOYSA-N	5.1×10^{-2} 1.9×10^{-1} 1.6 2.2×10^{-2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
1,1,2,3,3,4,5- heptachlorocyclopentane $C_5H_3Cl_7$ [68258-90-2] XCEUTYGYMGYCBG-UHFFFAOYSA-N	1.5×10^{-1} 7.9×10^{-1} 1.6 8.6×10^{-2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
1,2,3,3,4,5- hexachlorocyclopentene $C_5H_2Cl_6$ OSRFTCIVMWPVNP-UHFFFAOYSA-N	1.4×10^{-2} 4.4×10^{-2} 4.4×10^{-1} 6.4×10^{-2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
heptachlorocyclopentene C_5HCl_7 [62111-47-1] AJUXFTIOMRYFRL-UHFFFAOYSA-N	3.9×10^{-2} 3.5×10^{-2} 8.4×10^{-2} 5.4×10^{-2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
chlorocyclohexane $C_6H_{11}Cl$ [542-18-7] UNFUYWDGSFDHCW-UHFFFAOYSA-N	2.8×10^{-3} 3.2×10^{-3}	3300 4200 3200	Bakierowska and Trzeszczyński (2003) Hilal et al. (2008) Kühne et al. (2005) Kühne et al. (2005)	M Q Q ?	

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Table A6.1: Chlorocarbons (C, H, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
α-1,2,3,4,5,6-hexachlorocyclohexane	1.5		Xiao et al. (2004)	L	366
$C_6H_6Cl_6$	1.4		Xiao et al. (2004)	L	367
(α-lindane; α-HCH)	3.0	5500	Cetin et al. (2006)	M	
[319-84-6]	1.7	7500	Sahsuvar et al. (2003)	M	
JLYXXMFPNIAWKQ-SHFUYGGZSA-N	8.1×10^{-1}		Altschuh et al. (1999)	M	
	1.3	6500	Kucklick et al. (1991)	M	
	4.2×10^{-1}		Atlas et al. (1982)	M	679
	1.1		Mackay et al. (2006d)	V	
	9.1×10^{-1}		Ballschmiter and Wittlinger (1991)	V	
	2.3		Calamari et al. (1991)	V	12
	1.1		Suntio et al. (1988)	V	12
	5.9×10^{-3}	3900	Paasivirta et al. (1999)	T	
	1.8		Suntio et al. (1988)	C	680
	3.9×10^{-2}		Zhang et al. (2010)	Q	287, 288
	7.7		Zhang et al. (2010)	Q	287, 289
	4.0×10^{1}		Zhang et al. (2010)	Q	287, 290
	3.8×10^{-1}		Zhang et al. (2010)	Q	287, 291
	1.1		Modarresi et al. (2007)	Q	67
		7100	Kühne et al. (2005)	Q	
		7100	Kühne et al. (2005)	?	
β-1,2,3,4,5,6-hexachlorocyclohexane	2.7×10^{1}		Xiao et al. (2004)	L	366
$C_6H_6Cl_6$	2.7×10^{1}		Xiao et al. (2004)	L	367
(β-lindane; β-HCH)	2.8×10^{1}	7800	Sahsuvar et al. (2003)	M	
[319-85-7]	2.2×10^{1}		Altschuh et al. (1999)	M	
JLYXXMFPNIAWKQ-CDRYSYESSA-N	8.6		Mackay et al. (2006d)	V	
	1.4×10^{1}		Ballschmiter and Wittlinger (1991)	V	
	8.3		Suntio et al. (1988)	V	12
	5.6×10^{1}		Suntio et al. (1988)	C	681
	6.7×10^{-1}		Ryan et al. (1988)	C	
	5.8		Keshavarz et al. (2022)	Q	
	3.0×10^{-2}		Duchowicz et al. (2020)	Q	184
	1.1		Modarresi et al. (2007)	Q	67
		7100	Kühne et al. (2005)	Q	
	2.2×10^{1}		Duchowicz et al. (2020)	?	185, 21
		7800	Kühne et al. (2005)	?	
γ-1,2,3,4,5,6-hexachlorocyclohexane	3.7		Xiao et al. (2004)	L	366
$C_6H_6Cl_6$	3.3		Xiao et al. (2004)	L	367
(γ-lindane; lindane; γ-HCH)	3.1		Mackay and Shiu (1981)	L	
[58-89-9]	3.1		Chao et al. (2017)	M	
JLYXXMFPNIAWKQ-GNIYUCBRSA-N	3.9	3300	Cetin et al. (2006)	M	
	6.0	6200	Xie et al. (2004)	M	
	4.3	7500	Sahsuvar et al. (2003)	M	
	1.9		Altschuh et al. (1999)	M	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.8	5500	Kucklick et al. (1991)	M	
	4.9		Fendinger et al. (1989)	M	72
	5.0		Fendinger and Glotfelty (1988)	M	72
	6.7		Mackay et al. (2006d)	V	
	3.3		Siebers et al. (1994)	V	
	1.0×10^{1}		Ballschmiter and Wittlinger (1991)	V	
	5.9		Calamari et al. (1991)	V	12
	3.7		McLachlan et al. (1990)	V	373
	7.7		Suntio et al. (1988)	V	12
	6.7×10^{-1}		Caron et al. (1985)	V	
	7.9		Burkhard and Guth (1981)	V	
	3.1		Chiou et al. (1980)	V	
	2.0×10^{1}		Mackay and Leinonen (1975)	V	
	6.2×10^{-2}	7100	Paasivirta et al. (1999)	T	
	3.1×10^{1}		McCarty (1980)	X	368
	2.0×10^{1}		Suntio et al. (1988)	C	12
	5.0		Suntio et al. (1988)	C	681
	1.4		Suntio et al. (1988)	C	
	5.8		Keshavarz et al. (2022)	Q	
	3.0×10^{-2}		Duchowicz et al. (2020)	Q	
	3.9×10^{-2}		Zhang et al. (2010)	Q	287, 288
	7.7		Zhang et al. (2010)	Q	287, 289
	4.7×10^{1}		Zhang et al. (2010)	Q	287, 290
	3.8×10^{-1}		Zhang et al. (2010)	Q	287, 291
	5.3		Hilal et al. (2008)	Q	
	1.1		Modarresi et al. (2007)	Q	67
		7100	Kühne et al. (2005)	Q	
	1.9		Duchowicz et al. (2020)	?	185, 21
		6200	Kühne et al. (2005)	?	
	2.2×10^{1}		Brimblecombe (1986)	?	80
δ-1,2,3,4,5,6-hexachlorocyclohexane	2.3×10^{1}		Duchowicz et al. (2020)	V	186
$C_6H_6Cl_6$	2.3×10^{1}		HSDB (2015)	V	
(δ-lindane; δ-HCH)	1.4×10^{1}		Mackay et al. (2006d)	V	
[319-86-8]	1.4×10^{1}		Suntio et al. (1988)	V	12
JLYXXMFPNIAWKQ-GPIVLXJGSA-N	5.6×10^{1}		Suntio et al. (1988)	C	681
	3.0×10^{-2}		Duchowicz et al. (2020)	Q	
	1.1		Modarresi et al. (2007)	Q	67
4,5,6,7,8,8-hexachloro-3a,4,7,7a-tetrahydro-4,7-methano-1H-indene	2.0×10^{-2}		HSDB (2015)	Q	99
$C_{10}H_6Cl_6$	2.0×10^{-2}		Zhang et al. (2010)	Q	287, 288
[3734-48-3]	6.2×10^{-3}		Zhang et al. (2010)	Q	287, 289
XCJXQCUJXDUNDN-UHFFFAOYSA-N	2.2		Zhang et al. (2010)	Q	287, 290
	4.2×10^{-1}		Zhang et al. (2010)	Q	287, 291

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Table A6.1: Chlorocarbons (C, H, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dienochlor	1.8×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{10}Cl_{10}$	1.2×10^{-2}		Duchowicz et al. (2020)	Q	
[2227-17-0]					
LWLJUMBEZJHXHV-UHFFFAOYSA-N					
mirex	1.2×10^{-2}	11000	Yin and Hassett (1986)	M	
$C_{10}Cl_{12}$	1.2×10^{-3}		Mackay et al. (2006d)	V	
(dodecachloropentacyclodecane)	5.8×10^{-2}		McLachlan et al. (1990)	V	373
[2385-85-5]	1.2×10^{-3}		Suntio et al. (1988)	V	12
GVYLCNUFSHDAAW-UHFFFAOYSA-N	5.2×10^{-2}		Smith and Bomberger (1980)	V	24
	9.9×10^{-4}		Suntio et al. (1988)	C	12
	1.3×10^{-1}		Keshavarz et al. (2022)	Q	
	4.3		Duchowicz et al. (2020)	Q	
	3.9×10^{-3}		Hilal et al. (2008)	Q	
		10000	Kühne et al. (2005)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		11000	Kühne et al. (2005)	?	
dechlorane plus	1.3		HSDB (2015)	Q	99
$C_{18}H_{12}Cl_{12}$	1.3		Zhang et al. (2010)	Q	287, 288
[13560-89-9]	7.0×10^{-2}		Zhang et al. (2010)	Q	287, 289
UGQQAJOWXNCOPY-UHFFFAOYSA-N	2.1×10^{3}		Zhang et al. (2010)	Q	287, 290
	4.6×10^{1}		Zhang et al. (2010)	Q	287, 291
chloroethene	4.1×10^{-4}	2500	Schwardt et al. (2021)	L	1
CH_2CHCl	3.8×10^{-4}	3100	Burkholder et al. (2019)	L	
(vinyl chloride)	3.8×10^{-4}	3100	Burkholder et al. (2015)	L	
[75-01-4]	4.3×10^{-4}	3000	Brockbank (2013)	L	1
BZHJMEDXRYGGRV-UHFFFAOYSA-N	3.8×10^{-4}	3100	Warneck (2007)	L	
	3.9×10^{-4}	3100	Staudinger and Roberts (2001)	L	
	3.9×10^{-4}	3100	Staudinger and Roberts (1996)	L	
	4.5×10^{-4}	3000	Wilhelm et al. (1977)	L	
	3.9×10^{-4}	2400	Schwardt et al. (2021)	M	682, 11
	3.9×10^{-4}	3200	Hiatt (2013)	M	
	4.1×10^{-4}	2300	Chen et al. (2012)	M	
			Chiang et al. (1998)	M	652
	4.0×10^{-4}	2900	Ashworth et al. (1988)	M	278
	3.7×10^{-4}	3300	Gossett (1987)	M	
	8.5×10^{-6}		Pearson and McConnell (1975)	M	649, 373
			Mackay et al. (2006b)	V	683
	9.1×10^{-4}		Lide and Frederikse (1995)	V	
	1.2×10^{-4}		Mackay et al. (1993)	V	
	1.1×10^{-4}		Hwang et al. (1992)	V	
	5.4×10^{-4}		Smith and Bomberger (1980)	V	24
	9.4×10^{-6}		Dilling (1977)	V	
	4.2×10^{-4}		Dilling (1977)	V	
	1.8×10^{-4}		Hine and Mookerjee (1975)	V	
	4.4×10^{-4}		Yaws (2003)	X	237
	6.5×10^{-4}		Ryan et al. (1988)	C	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.0×10^{-4}		Wang et al. (2017)	Q	80, 238
	2.4×10^{-4}		Wang et al. (2017)	Q	80, 239
	6.3×10^{-4}		Wang et al. (2017)	Q	80, 240
	3.4×10^{-3}		Li et al. (2014)	Q	241
	4.9×10^{-4}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	2.6×10^{-4}		Gharagheizi et al. (2010)	Q	246
	2.1×10^{-4}		Hilal et al. (2008)	Q	
	1.2×10^{-3}		Modarresi et al. (2007)	Q	67
	4.2×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	1.4×10^{-3}		Yao et al. (2002)	Q	229
	2.4×10^{-3}		Suzuki et al. (1992)	Q	232
	2.0×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	8.1×10^{-4}		Irmann (1965)	Q	
	3.7×10^{-4}		Mackay et al. (2006b)	?	
	4.4×10^{-4}		Yaws (1999)	?	21
	3.9×10^{-4}	2700	Yaws et al. (1999)	?	21
	3.7×10^{-4}		Mackay et al. (1993)	?	
	4.4×10^{-4}		Yaws and Yang (1992)	?	21
	4.5×10^{-4}		Abraham et al. (1990)	?	
chloroethene-d3 CD_2CDCl (vinyl chloride-d3) [6745-35-3] BZHJMEDXRYGGRV-FUDHJZNOSA-N	3.8×10^{-4}	3100	Hiatt (2013)	M	
1,1-dichloroethene CH_2CCl_2 [75-35-4] LGXVIGDEPROXKC-UHFFFAOYSA-N	3.7×10^{-4}	3500	Schwardt et al. (2021)	L	1
	3.7×10^{-4}	3400	Burkholder et al. (2019)	L	
	3.7×10^{-4}	3400	Burkholder et al. (2015)	L	
	3.1×10^{-4}	3900	Brockbank (2013)	L	1, 684
	3.7×10^{-4}	3400	Warneck (2007)	L	
	4.0×10^{-4}	3800	Fogg and Sangster (2003)	L	
	3.4×10^{-4}	4000	Staudinger and Roberts (2001)	L	
	3.4×10^{-4}	3900	Staudinger and Roberts (1996)	L	
	4.0×10^{-4}	3400	Schwardt et al. (2021)	M	685
	4.1×10^{-4}	4600	Hiatt (2013)	M	
	3.7×10^{-4}	4200	Dewulf et al. (1999)	M	
	4.4×10^{-4}		Chiang et al. (1998)	M	12
	4.6×10^{-4}	1600	Kondoh and Nakajima (1997)	M	
	3.5×10^{-4}	3300	Tse et al. (1992)	M	
	3.4×10^{-4}	4500	Bissonette et al. (1990)	M	
	3.7×10^{-4}	2900	Ashworth et al. (1988)	M	278, 686
	3.8×10^{-4}	3700	Gossett (1987)	M	
	1.3×10^{-4}		Yurteri et al. (1987)	M	12
	2.6×10^{-4}	4600	Leighton and Calo (1981)	M	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.4×10^{-4}	6600	Ervin et al. (1980)	M	
	6.6×10^{-4}		Warner et al. (1980)	M	
	6.6×10^{-5}		Pearson and McConnell (1975)	M	649, 12
	4.3×10^{-4}		Mackay et al. (2006b)	V	
	3.3×10^{-4}		Lide and Frederikse (1995)	V	
	4.3×10^{-4}		Mackay et al. (1993)	V	
	7.5×10^{-5}		Mackay and Shiu (1981)	V	
	6.5×10^{-4}		Warner et al. (1980)	V	
	5.2×10^{-5}		Dilling (1977)	V	651
	6.1×10^{-5}		Dilling (1977)	V	12
	4.3×10^{-4}		Yaws (2003)	X	237
	6.4×10^{-4}	1200	Goldstein (1982)	X	298
	2.2×10^{-3}		Ryan et al. (1988)	C	
	6.6×10^{-4}		Shen (1982)	C	
	1.0×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.3×10^{-4}		Wang et al. (2017)	Q	80, 239
	4.5×10^{-4}		Wang et al. (2017)	Q	80, 240
	1.3×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.3×10^{-4}		Hilal et al. (2008)	Q	
	8.9×10^{-4}		Modarresi et al. (2007)	Q	67
		3300	Kühne et al. (2005)	Q	
	3.8×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	2.6×10^{-3}		Yao et al. (2002)	Q	229, 267
	2.7×10^{-4}		Katritzky et al. (1998)	Q	
	3.8×10^{-4}		Mackay et al. (2006b)	?	
		3700	Kühne et al. (2005)	?	
	4.3×10^{-4}		Yaws (1999)	?	21
	3.8×10^{-4}		Mackay et al. (1993)	?	
	4.3×10^{-4}		Yaws and Yang (1992)	?	21
	2.7×10^{-4}		Abraham et al. (1990)	?	
1,2-dichloroethene $C_2H_2Cl_2$ [540-59-0] KFUSEUYYWQURPO-UHFFFAOYSA-N	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	5.1×10^{-3}		Duchowicz et al. (2020)	Q	299
	3.7×10^{-4}		Hilal et al. (2008)	Q	
	2.3×10^{-3}		Modarresi et al. (2007)	Q	67
	1.4×10^{-3}		Yaffe et al. (2003)	Q	248, 272
	6.2×10^{-4}		Katritzky et al. (1998)	Q	
	4.5×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	2.4×10^{-3}		Duchowicz et al. (2020)	?	185, 21

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(*Z*)-1,2-dichloroethene	2.3×10^{-3}	3400	Schwardt et al. (2021)	L	1
CHClCHCl	2.6×10^{-3}	3700	Burkholder et al. (2019)	L	
(*cis*-1,2-dichloroethene)	2.6×10^{-3}	3700	Burkholder et al. (2015)	L	
[156-59-2]	2.4×10^{-3}	4000	Brockbank (2013)	L	1
KFUSEUYYWQURPO-UPHRSURJSA-N	2.6×10^{-3}	3700	Warneck (2007)	L	
	2.5×10^{-3}	4000	Fogg and Sangster (2003)	L	
	2.3×10^{-3}	3900	Staudinger and Roberts (2001)	L	
	2.3×10^{-3}	3900	Staudinger and Roberts (1996)	L	
	2.7×10^{-3}	3800	Hiatt (2013)	M	
	2.5×10^{-3}	3900	Chen et al. (2012)	M	
	2.2×10^{-3}	3100	Shimotori and Arnold (2003)	M	
	1.5×10^{-3}		Ryu and Park (1999)	M	
	3.2×10^{-3}		Hovorka and Dohnal (1997)	M	12
	2.5×10^{-3}	3000	Kondoh and Nakajima (1997)	M	
	1.3×10^{-3}	3100	Park et al. (1997)	M	
	2.4×10^{-3}	4000	Wright et al. (1992)	M	687
	2.5×10^{-3}	3800	Tse et al. (1992)	M	
	2.5×10^{-3}	4200	Bissonette et al. (1990)	M	
	2.1×10^{-3}	3200	Ashworth et al. (1988)	M	278
	2.6×10^{-3}	4200	Gossett (1987)	M	
	2.2×10^{-3}		Yurteri et al. (1987)	M	12
	2.2×10^{-3}	4100	Ervin et al. (1980)	M	
	1.1×10^{-3}		Sato and Nakajima (1979b)	M	14
	1.3×10^{-3}		Mackay et al. (2006b)	V	
	1.3×10^{-3}		Park et al. (1997)	V	
	1.3×10^{-3}		Mackay et al. (1993)	V	
	1.3×10^{-3}		Mackay and Shiu (1981)	V	
	1.3×10^{-3}		Dilling (1977)	V	
	2.9×10^{-3}		Hine and Mookerjee (1975)	V	
	1.3×10^{-3}		Yaws (2003)	X	237
	1.8×10^{-3}		Wang et al. (2017)	Q	314, 80, 238
	4.9×10^{-4}		Wang et al. (2017)	Q	314, 80, 239
	1.1×10^{-3}		Wang et al. (2017)	Q	314, 80, 240
	3.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.3×10^{-3}		Modarresi et al. (2007)	Q	67
		3300	Kühne et al. (2005)	Q	
	1.4×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	5.2×10^{-3}		Yao et al. (2002)	Q	229
	2.7×10^{-3}		English and Carroll (2001)	Q	230, 231
	2.2×10^{-3}		Mackay et al. (2006b)	?	
		4200	Kühne et al. (2005)	?	
	1.3×10^{-3}		Yaws (1999)	?	21
	1.2×10^{-3}		Abraham and Weathersby (1994)	?	21

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{-3}		Mackay et al. (1993)	?	
	1.3×10^{-3}		Yaws and Yang (1992)	?	21
	1.3×10^{-3}		Abraham et al. (1990)	?	
(*E*)-1,2-dichloroethene	9.9×10^{-4}	3600	Schwardt et al. (2021)	L	1
CHClCHCl	1.0×10^{-3}	3600	Burkholder et al. (2019)	L	
(*trans*-1,2-dichloroethene)	1.0×10^{-3}	3600	Burkholder et al. (2015)	L	
[156-60-5]	1.0×10^{-3}	3900	Brockbank (2013)	L	1
KFUSEUYYWQURPO-OWOJBTEDSA-N	1.0×10^{-3}	3500	Warneck (2007)	L	
	1.1×10^{-3}	4200	Fogg and Sangster (2003)	L	
	9.0×10^{-4}	4100	Staudinger and Roberts (2001)	L	
	9.0×10^{-4}	4100	Staudinger and Roberts (1996)	L	
	9.2×10^{-4}	2600	Schwardt et al. (2021)	M	688, 11
	1.0×10^{-3}	4000	Hiatt (2013)	M	
	1.0×10^{-3}	3500	Shimotori and Arnold (2003)	M	
	1.6×10^{-3}		Ryu and Park (1999)	M	
	1.3×10^{-3}		Hovorka and Dohnal (1997)	M	12
	1.1×10^{-3}	2200	Kondoh and Nakajima (1997)	M	
	1.8×10^{-3}	6200	Park et al. (1997)	M	
	9.3×10^{-4}	4900	Khalfaoui and Newsham (1994b)	M	689
	9.8×10^{-4}	3400	Hansen et al. (1993)	M	281
	1.0×10^{-3}	4200	Wright et al. (1992)	M	690
	1.0×10^{-3}	3700	Tse et al. (1992)	M	
	9.7×10^{-4}	5000	Cooling et al. (1992)	M	691
	8.4×10^{-4}	4800	Bissonette et al. (1990)	M	
	9.9×10^{-4}	3000	Ashworth et al. (1988)	M	278, 686
	1.1×10^{-3}	4200	Gossett (1987)	M	
	1.1×10^{-3}		Yurteri et al. (1987)	M	12
	7.0×10^{-4}	5400	Ervin et al. (1980)	M	
	1.9×10^{-3}		Warner et al. (1980)	M	
	8.1×10^{-4}		Sato and Nakajima (1979b)	M	14
	1.5×10^{-3}		Mackay et al. (2006b)	V	
	1.5×10^{-3}		Park et al. (1997)	V	
	1.5×10^{-3}		Mackay et al. (1993)	V	
	1.5×10^{-3}		Hwang et al. (1992)	V	
	1.5×10^{-3}		Mackay and Shiu (1981)	V	
	2.4×10^{-3}		Warner et al. (1980)	V	
	1.5×10^{-3}		Dilling (1977)	V	
	1.5×10^{-3}		Hine and Mookerjee (1975)	V	
	1.5×10^{-3}		Yaws (2003)	X	237
	1.9×10^{-3}	1700	Goldstein (1982)	X	298
	1.5×10^{-3}		Ryan et al. (1988)	C	
	1.9×10^{-3}		Shen (1982)	C	
	1.8×10^{-3}		Wang et al. (2017)	Q	314, 80, 238
	4.9×10^{-4}		Wang et al. (2017)	Q	314, 80, 239

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^{-3}		Wang et al. (2017)	Q	314, 80, 240
	2.1×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.3×10^{-3}		Modarresi et al. (2007)	Q	67
		3300	Kühne et al. (2005)	Q	
	2.2×10^{-3}		Yao et al. (2002)	Q	229
	2.3×10^{-3}		English and Carroll (2001)	Q	230, 231
	1.0×10^{-3}		Mackay et al. (2006b)	?	
		4300	Kühne et al. (2005)	?	
	1.5×10^{-3}		Yaws (1999)	?	21
	8.4×10^{-4}		Abraham and Weathersby (1994)	?	21
	1.0×10^{-3}		Mackay et al. (1993)	?	
	1.5×10^{-3}		Yaws and Yang (1992)	?	21
	1.5×10^{-3}		Abraham et al. (1990)	?	
trichloroethene C_2HCl_3 (trichloroethylene) [79-01-6] XSTXAVWGXDQKEL-UHFFFAOYSA-N	1.1×10^{-3}	4100	Schwardt et al. (2021)	L	1
	1.1×10^{-3}	4300	Burkholder et al. (2019)	L	
	8.6×10^{-4}	4200	Burkholder et al. (2019)	L	70
	1.1×10^{-3}	4300	Burkholder et al. (2015)	L	
	8.6×10^{-4}	4200	Burkholder et al. (2015)	L	70
	1.0×10^{-3}	4200	Brockbank (2013)	L	1
	1.1×10^{-3}	4300	Warneck (2007)	L	
	1.0×10^{-3}	4300	Fogg and Sangster (2003)	L	
	1.0×10^{-3}	4600	Staudinger and Roberts (2001)	L	
	9.9×10^{-4}	4600	Staudinger and Roberts (1996)	L	
	6.6×10^{-4}		Steward et al. (1973)	L	14
	1.1×10^{-3}	4100	Allott et al. (1973)	L	
	1.0×10^{-3}	4200	Schwardt et al. (2021)	M	692
	1.2×10^{-3}	4700	Hiatt (2013)	M	
	1.6×10^{-3}	2800	Zhang et al. (2013)	M	324
	1.3×10^{-3}		Zhang et al. (2013)	M	325
	1.0×10^{-3}	3900	Chen et al. (2012)	M	
	9.4×10^{-4}		Helburn et al. (2008)	M	
	1.0×10^{-3}	3900	Shimotori and Arnold (2003)	M	
	9.5×10^{-4}	4300	Görgényi et al. (2002)	M	693
	1.2×10^{-3}	3600	Bierwagen and Keller (2001)	M	
	7.6×10^{-4}	4900	Moore (2000)	M	70
	1.0×10^{-3}		David et al. (2000)	M	72
	1.1×10^{-3}	3900	Vane and Giroux (2000)	M	
	1.1×10^{-3}	4800	Knauss et al. (2000)	M	694
	9.5×10^{-4}	4900	Dewulf et al. (1999)	M	
	9.5×10^{-4}		Ryu and Park (1999)	M	
	9.3×10^{-4}	3700	Heron et al. (1998)	M	
	1.1×10^{-3}		Chiang et al. (1998)	M	12
	1.4×10^{-3}		Peng and Wan (1998)	M	
	8.7×10^{-4}	4000	Peng and Wan (1998)	M	70
	1.1×10^{-3}	3800	Peng and Wan (1997)	M	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.3×10^{-3}		Hovorka and Dohnal (1997)	M	12
	1.1×10^{-3}	2200	Kondoh and Nakajima (1997)	M	
	8.8×10^{-4}	3600	Park et al. (1997)	M	
	8.5×10^{-4}		Turner et al. (1996)	M	
	8.3×10^{-4}		Ramachandran et al. (1996)	M	
	1.2×10^{-3}	3900	Dewulf et al. (1995)	M	
	1.3×10^{-3}		Nielsen et al. (1994)	M	
	9.5×10^{-4}	5000	Khalfaoui and Newsham (1994b)	M	695
	9.4×10^{-4}	3100	Robbins et al. (1993)	M	696
	1.1×10^{-3}		Hoff et al. (1993)	M	
	1.0×10^{-3}		Li et al. (1993)	M	
	1.1×10^{-3}	3700	Wright et al. (1992)	M	697
	1.1×10^{-3}	4200	Tse et al. (1992)	M	
	9.7×10^{-4}	4900	Cooling et al. (1992)	M	698
	1.3×10^{-3}	5200	Tancrède and Yanagisawa (1990)	M	
	1.0×10^{-3}	5200	Bissonette et al. (1990)	M	
	9.7×10^{-4}	2000	Lamarche and Droste (1989)	M	345
	5.5×10^{-4}		Guitart et al. (1989)	M	14
	9.5×10^{-4}	3700	Ashworth et al. (1988)	M	278
	1.0×10^{-3}	4800	Gossett (1987)	M	
	9.6×10^{-4}	4700	Munz and Roberts (1987)	M	
	9.8×10^{-4}		Hellmann (1987)	M	87
	9.4×10^{-4}		Yurteri et al. (1987)	M	12
	9.0×10^{-4}	5400	Schoene and Steinhanses (1985)	M	
	1.1×10^{-3}	4300	Gossett et al. (1985)	M	
	1.0×10^{-3}		Garbarini and Lion (1985)	M	
	9.7×10^{-4}	4900	Lincoff and Gossett (1984)	M	
	1.0×10^{-3}	4600	Leighton and Calo (1981)	M	
	7.4×10^{-4}	4800	Ervin et al. (1980)	M	
	8.4×10^{-4}		Warner et al. (1980)	M	
	5.0×10^{-4}		Sato and Nakajima (1979b)	M	14
	1.1×10^{-3}		Pearson and McConnell (1975)	M	649, 12
	8.5×10^{-4}		Mackay et al. (2006b)	V	
	9.9×10^{-4}		Park et al. (1997)	V	
	8.4×10^{-4}		Mackay et al. (1993)	V	
	1.1×10^{-3}		Hwang et al. (1992)	V	
	8.1×10^{-4}		Mackay and Shiu (1981)	V	
	8.4×10^{-4}		Warner et al. (1980)	V	
	8.2×10^{-4}		Dilling (1977)	V	651
	1.0×10^{-3}		Dilling (1977)	V	12
	2.4×10^{-3}		Dilling (1977)	V	153
	8.4×10^{-4}		Hine and Mookerjee (1975)	V	
	8.4×10^{-4}		Dilling et al. (1975)	V	
	8.6×10^{-4}		Yaws (2003)	X	258
	8.5×10^{-4}		Yaws (2003)	X	237
	8.8×10^{-4}	1600	Goldstein (1982)	X	298
	1.1×10^{-3}		Ryan et al. (1988)	C	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.4×10^{-4}		Shen (1982)	C	
	6.2×10^{-4}		Dupeux et al. (2022)	Q	259
	2.2×10^{-3}		Keshavarz et al. (2022)	Q	
	2.9×10^{-3}		Duchowicz et al. (2020)	Q	184
	2.9×10^{-3}		Wang et al. (2017)	Q	80, 238
	2.2×10^{-4}		Wang et al. (2017)	Q	80, 239
	6.9×10^{-4}		Wang et al. (2017)	Q	80, 240
	8.4×10^{-4}		Li et al. (2014)	Q	241
	5.5×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	8.7×10^{-4}		Gharagheizi et al. (2010)	Q	246
	3.0×10^{-4}		Hilal et al. (2008)	Q	
	1.8×10^{-3}		Modarresi et al. (2007)	Q	67
		3600	Kühne et al. (2005)	Q	
	1.1×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.1×10^{-3}		English and Carroll (2001)	Q	230, 274
	4.0×10^{-4}		Katritzky et al. (1998)	Q	
	8.4×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.0×10^{-3}		Duchowicz et al. (2020)	?	185, 21
	9.7×10^{-4}		Mackay et al. (2006b)	?	
		4200	Kühne et al. (2005)	?	
	8.5×10^{-4}		Yaws (1999)	?	21
	5.2×10^{-4}		Abraham and Weathersby (1994)	?	21
	9.7×10^{-4}		Mackay et al. (1993)	?	
	8.4×10^{-4}		Yaws and Yang (1992)	?	21
	8.4×10^{-4}		Abraham et al. (1990)	?	
tetrachloroethene	5.7×10^{-4}	4700	Schwardt et al. (2021)	L	1
C_2Cl_4	5.5×10^{-4}	4500	Burkholder et al. (2019)	L	
(tetrachloroethylene)	4.6×10^{-4}	4400	Burkholder et al. (2019)	L	70
[127-18-4]	5.5×10^{-4}	4500	Burkholder et al. (2015)	L	
CYTYCFOTNPOANT-UHFFFAOYSA-N	4.6×10^{-4}	4400	Burkholder et al. (2015)	L	70
	5.6×10^{-4}	4700	Brockbank (2013)	L	1
	6.2×10^{-4}	4500	Warneck (2007)	L	
	6.0×10^{-4}	4200	Fogg and Sangster (2003)	L	
	5.9×10^{-4}	4800	Staudinger and Roberts (2001)	L	
	5.8×10^{-4}	4800	Staudinger and Roberts (1996)	L	
	4.3×10^{-4}		Mackay and Shiu (1981)	L	
	5.8×10^{-4}	4500	Schwardt et al. (2021)	M	699
	9.9×10^{-4}	4600	Hiatt (2013)	M	
	6.2×10^{-4}	4200	Chen et al. (2012)	M	
	5.8×10^{-4}	4200	Shimotori and Arnold (2003)	M	
	4.1×10^{-4}	5300	Moore (2000)	M	70
	6.0×10^{-4}	4100	Vane and Giroux (2000)	M	
	4.8×10^{-4}	4400	Knauss et al. (2000)	M	700
	5.3×10^{-4}		Ryu and Park (1999)	M	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.6×10^{-4}		Dohnal and Hovorka (1999)	M	12
	6.2×10^{-4}		Chiang et al. (1998)	M	12
	7.8×10^{-4}		Peng and Wan (1998)	M	
	4.7×10^{-4}	4100	Peng and Wan (1998)	M	70
	6.1×10^{-4}	4200	Peng and Wan (1997)	M	
	8.4×10^{-4}		Hovorka and Dohnal (1997)	M	12
	6.9×10^{-4}	2200	Kondoh and Nakajima (1997)	M	
	5.5×10^{-4}	4200	Park et al. (1997)	M	
	6.9×10^{-4}	4800	Dewulf et al. (1995)	M	
	5.8×10^{-4}	5200	Robbins et al. (1993)	M	701
	6.3×10^{-4}		Hoff et al. (1993)	M	
	6.3×10^{-4}		Li et al. (1993)	M	
	8.1×10^{-4}	2100	Kolb et al. (1992)	M	33, 277
	5.9×10^{-4}	5500	Tancrède and Yanagisawa (1990)	M	
	6.2×10^{-4}	5300	Bissonette et al. (1990)	M	
	5.4×10^{-4}	4400	Ashworth et al. (1988)	M	278
	5.6×10^{-4}	4900	Gossett (1987)	M	
	5.4×10^{-4}	4400	Munz and Roberts (1987)	M	
	7.7×10^{-4}		Hellmann (1987)	M	87
	7.5×10^{-4}		Yurteri et al. (1987)	M	12
	6.5×10^{-4}	4600	Gossett et al. (1985)	M	
	5.7×10^{-4}	5100	Lincoff and Gossett (1984)	M	
	6.1×10^{-4}	4700	Leighton and Calo (1981)	M	
	5.7×10^{-4}	5200	Ervin et al. (1980)	M	
	3.4×10^{-4}		Warner et al. (1980)	M	
	1.1×10^{-3}	4300	Gossett (1980)	M	
	1.7×10^{-4}		Sato and Nakajima (1979b)	M	14
	5.0×10^{-4}		Pearson and McConnell (1975)	M	649, 12
	3.7×10^{-4}		Mackay et al. (2006b)	V	
	3.4×10^{-4}		Park et al. (1997)	V	
	3.7×10^{-4}		Mackay et al. (1993)	V	
	3.6×10^{-4}		Hwang et al. (1992)	V	
	9.1×10^{-4}		Addison et al. (1983)	V	
	3.5×10^{-4}		Warner et al. (1980)	V	
	3.4×10^{-4}		Dilling (1977)	V	651
	4.0×10^{-4}		Dilling (1977)	V	12
	1.2×10^{-3}		Dilling (1977)	V	153
	3.7×10^{-4}		Hine and Mookerjee (1975)	V	
	9.8×10^{-4}		Dilling et al. (1975)	V	
	3.6×10^{-4}		Yaws (2003)	X	237
	3.6×10^{-4}	1500	Goldstein (1982)	X	298
	6.3×10^{-4}		Ryan et al. (1988)	C	
	3.4×10^{-4}		Shen (1982)	C	
	8.1×10^{-4}		Dilling (1977)	C	
	8.1×10^{-4}		Dilling et al. (1975)	C	
	4.4×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.2×10^{-4}		Wang et al. (2017)	Q	80, 239

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.5×10^{-4}		Wang et al. (2017)	Q	80, 240
	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.7×10^{-4}		Hilal et al. (2008)	Q	
	1.2×10^{-3}		Modarresi et al. (2007)	Q	67
		3900	Kühne et al. (2005)	Q	
	5.6×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	3.1×10^{-4}		English and Carroll (2001)	Q	230, 231
	9.9×10^{-5}		Katritzky et al. (1998)	Q	
	8.8×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	5.8×10^{-4}		Mackay et al. (2006b)	?	
		5100	Kühne et al. (2005)	?	
	3.7×10^{-4}		Yaws (1999)	?	21
	1.7×10^{-4}		Abraham and Weathersby (1994)	?	21
	5.8×10^{-4}		Mackay et al. (1993)	?	
	3.7×10^{-4}		Yaws and Yang (1992)	?	21
	3.4×10^{-4}		Abraham et al. (1990)	?	
	2.9×10^{-3}		Chiou et al. (1980)	?	79
dichloroethyne C_2Cl_2 [7572-29-4] ZMJOVJSTYLQINE-UHFFFAOYSA-N	4.9×10^{-4}		HSDB (2015)	Q	99
1-chloro-1-propene C_3H_5Cl [590-21-6] OWXJKYNZGFSVRC-UHFFFAOYSA-N	1.8×10^{-4}		HSDB (2015)	Q	99
2-chloro-1-propene C_3H_5Cl [557-98-2] PNLQPWWBHXMFCA-UHFFFAOYSA-N	1.4×10^{-4}		HSDB (2015)	Q	99
3-chloro-1-propene	9.1×10^{-4}		Mackay and Shiu (1981)	L	
C_3H_5Cl	1.3×10^{-3}	4500	Hiatt (2013)	M	
(allyl chloride)	3.7×10^{-3}		Welke et al. (1998)	M	
[107-05-1]	9.0×10^{-4}		Duchowicz et al. (2020)	V	186
OSDWBNJEKMUWAV-UHFFFAOYSA-N	9.0×10^{-4}		HSDB (2015)	V	
	4.6×10^{-4}		Mackay et al. (1993)	V	
	9.2×10^{-4}		Dilling (1977)	V	
	1.1×10^{-3}		Hine and Mookerjee (1975)	V	
	1.1×10^{-3}		Yaws (2003)	X	237
	4.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.1×10^{-3}		Li et al. (2014)	Q	241
	1.4×10^{-3}		Gharagheizi et al. (2012)	Q	
	8.4×10^{-4}		Gharagheizi et al. (2010)	Q	246
	4.0×10^{-3}		Hilal et al. (2008)	Q	
	2.8×10^{-3}		Modarresi et al. (2007)	Q	67

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	5.9×10^{-4}		Yao et al. (2002)	Q	229
	1.1×10^{-3}		English and Carroll (2001)	Q	230, 231
	1.8×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	1.9×10^{-3}		Suzuki et al. (1992)	Q	232
	1.7×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.1×10^{-3}		Yaws (1999)	?	21
	1.1×10^{-3}		Yaws and Yang (1992)	?	21
	1.1×10^{-3}		Abraham et al. (1990)	?	
1,1-dichloropropene $C_3H_4Cl_2$ [563-58-6] ZAIDIVBQUMFXEC-UHFFFAOYSA-N	6.1×10^{-4}	4200	Hiatt (2013)	M	
	5.4×10^{-4}	1900	Kondoh and Nakajima (1997)	M	
1,2-dichloropropene $C_3H_4Cl_2$ [563-54-2] PPKPKFIWDXDAGC-UHFFFAOYSA-N	2.0×10^{-3}		HSDB (2015)	V	
	3.1×10^{-4}		Hilal et al. (2008)	Q	
	1.8×10^{-3}		Modarresi et al. (2007)	Q	67
1,3-dichloropropene $C_3H_4Cl_2$ [542-75-6] UOORRWUZONOOLO-UHFFFAOYSA-N	6.4×10^{-3}	4300	Wright et al. (1992)	M	702
	2.8×10^{-3}		Warner et al. (1980)	M	
	7.3×10^{-3}		Warner et al. (1980)	V	
	2.4×10^{-5}		Barcelo and Hennion (1997)	X	567
	2.8×10^{-3}	1500	Goldstein (1982)	X	298
	5.8×10^{-3}		Hilal et al. (2008)	C	
	2.8×10^{-3}		Horvath and Getzen (1999)	C	
	8.1×10^{-3}		Ryan et al. (1988)	C	
	2.8×10^{-3}		Shen (1982)	C	
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	5.1×10^{-5}		Goodarzi et al. (2010)	Q	568
	5.7×10^{-3}		Hilal et al. (2008)	Q	
	5.1×10^{-3}		Modarresi et al. (2007)	Q	67
cis-1,3-dichloropropene $C_3H_4Cl_2$ [10061-01-5] UOORRWUZONOOLO-UPHRSURJSA-N	4.2×10^{-3}		Mackay and Shiu (1981)	L	
	9.5×10^{-3}	5500	Hiatt (2013)	M	
	1.0×10^{-2}		Thomas et al. (2006)	M	154, 703
	6.3×10^{-3}	4300	Kondoh and Nakajima (1997)	M	
	4.2×10^{-3}		Albanese et al. (1987)	M	
	5.0×10^{-3}	5800	Leistra (1970)	M	
	4.2×10^{-3}		Dilling (1977)	V	
	8.7×10^{-3}		Thomas et al. (2006)	?	154, 704
	5.5×10^{-3}		Yates and Gan (1998)	?	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
trans-1,3-dichloropropene	5.6×10^{-3}		Mackay and Shiu (1981)	L	
$C_3H_4Cl_2$	5.8×10^{-3}	4800	Hiatt (2013)	M	
[10061-02-6]	1.5×10^{-2}		Thomas et al. (2006)	M	154, 703
UOORRWUZONOOLO-OWOJBTEDSA-N	1.0×10^{-2}	5000	Kondoh and Nakajima (1997)	M	
	5.6×10^{-3}		Albanese et al. (1987)	M	
	8.1×10^{-3}	5700	Leistra (1970)	M	
	5.6×10^{-3}		Dilling (1977)	V	
	1.5×10^{-2}		Thomas et al. (2006)	?	154, 704
	9.4×10^{-3}		Yates and Gan (1998)	?	
2,3-dichloropropene	2.8×10^{-3}		Mackay and Shiu (1981)	L	
$C_3H_4Cl_2$	3.5×10^{-3}		Albanese et al. (1987)	M	
[78-88-6]	2.4×10^{-3}		Duchowicz et al. (2020)	V	186
FALCMQXTWHPRIH-UHFFFAOYSA-N	2.7×10^{-3}		Dilling (1977)	V	
	2.4×10^{-3}		Yaws (2003)	X	237
	4.0×10^{-3}		Duchowicz et al. (2020)	Q	
	4.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	2.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
	4.8×10^{-3}		Hilal et al. (2008)	Q	
	3.8×10^{-3}		Modarresi et al. (2007)	Q	67
	2.9×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.8×10^{-3}		Yao et al. (2002)	Q	229, 267
	2.0×10^{-3}		Katritzky et al. (1998)	Q	
	2.4×10^{-3}		Yaws (1999)	?	21
1,2,3-trichloro-1-propene	5.5×10^{-4}		HSDB (2015)	Q	99
$C_3H_3Cl_3$					
[96-19-5]					
HIILBTHBHCLUER-UHFFFAOYSA-N					
1,1,2,3,3,3-hexachloro-1-propene	2.1×10^{-3}		Duchowicz et al. (2020)	V	186
C_3Cl_6	1.3×10^{-3}		Duchowicz et al. (2020)	Q	
[1888-71-7]	6.2×10^{-3}		HSDB (2015)	Q	99
VFDYKPARTDCDCU-UHFFFAOYSA-N	9.9×10^{-4}		Hilal et al. (2008)	Q	
	3.8×10^{-3}		Modarresi et al. (2007)	Q	67
	2.1×10^{-3}		Yaffe et al. (2003)	Q	248, 249
3-chloro-1-butene	5.6×10^{-4}		Ebert et al. (2023)	?	316
C_4H_7Cl					
[563-52-0]					
VZGLVCFVUREVDP-UHFFFAOYSA-N					
3-chloro-2-methyl-1-propene	1.1×10^{-3}		Duchowicz et al. (2020)	V	186
C_4H_7Cl	1.1×10^{-3}		HSDB (2015)	V	
[563-47-3]	1.5×10^{-3}		Duchowicz et al. (2020)	Q	
OHXAOPZTJOUYKM-UHFFFAOYSA-N					

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Table A6.1: Chlorocarbons (C, H, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloro-2-butene C_4H_7Cl (crotyl chloride) [591-97-9] YTKRILODNOEEPX-UHFFFAOYSA-N	9.5×10^{-4}		Ebert et al. (2023)	?	318
(Z)-1-chloro-2-butene	1.2×10^{-3}	2800	Bakierowska and Trzeszczyński (2003)	M	
C_4H_7Cl		3800	Kühne et al. (2005)	Q	
(*cis*-1-chloro-2-butene)		2800	Kühne et al. (2005)	?	
[4628-21-1]					
YTKRILODNOEEPX-IHWYPQMZSA-N					
(E)-1-chloro-2-butene	3.1×10^{-3}	3000	Bakierowska and Trzeszczyński (2003)	M	
C_4H_7Cl		3800	Kühne et al. (2005)	Q	
(*trans*-1-chloro-2-butene)		3000	Kühne et al. (2005)	?	
[4894-61-5]					
YTKRILODNOEEPX-NSCUHMNNSA-N					
1,3-dichloro-2-butene $C_4H_6Cl_2$ [926-57-8] WLIADPFXSACYLS-UHFFFAOYSA-N	2.6×10^{-4}		HSDB (2015)	Q	99
1,4-dichloro-2-butene	1.2×10^{-3}		Duchowicz et al. (2020)	V	186
$C_4H_6Cl_2$	1.7×10^{-2}		HSDB (2015)	V	
[764-41-0]	4.2×10^{-3}		Duchowicz et al. (2020)	Q	
FQDIANVAWVHZIR-UHFFFAOYSA-N	8.9×10^{-3}		Modarresi et al. (2007)	Q	67
(Z)-1,4-dichloro-2-butene	3.0×10^{-2}	9400	Hiatt (2013)	M	
$C_4H_6Cl_2$	1.0×10^{-2}		Albanese et al. (1987)	M	
[1476-11-5]	8.5×10^{-3}		Duchowicz et al. (2020)	V	186
FQDIANVAWVHZIR-UPHRSURJSA-N	8.2×10^{-3}		HSDB (2015)	V	
	4.2×10^{-3}		Duchowicz et al. (2020)	Q	
(E)-1,4-dichloro-2-butene	3.5×10^{-2}	6600	Hiatt (2013)	M	
$C_4H_6Cl_2$	1.7×10^{-2}		Albanese et al. (1987)	M	
[110-57-6]	1.5×10^{-2}		Duchowicz et al. (2020)	V	186
FQDIANVAWVHZIR-OWOJBTEDSA-N	1.5×10^{-2}		HSDB (2015)	V	
	4.2×10^{-3}		Duchowicz et al. (2020)	Q	
	7.2×10^{-2}		Hilal et al. (2008)	Q	
	8.9×10^{-3}		Modarresi et al. (2007)	Q	67
3,4-dichloro-1-butene	1.2×10^{-3}		Duchowicz et al. (2020)	V	186
$C_4H_6Cl_2$	1.1×10^{-3}		HSDB (2015)	V	
[760-23-6]	6.4×10^{-3}		Duchowicz et al. (2020)	Q	
XVEASTGLHPVZNA-UHFFFAOYSA-N					

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloro-2-methylpropene C_4H_7Cl (dimethylvinyl chloride) [513-37-1] KWISWUFGPUHDRY-UHFFFAOYSA-N	5.2×10^{-4}		HSDB (2015) Haynes (2014)	V W	 705
2-chloro-1,3-butadiene C_4H_5Cl [126-99-8] YACLQRRMGMJLJV-UHFFFAOYSA-N	4.7×10^{-2} 1.8×10^{-4}		Mackay et al. (1993) HSDB (2015)	V Q	 99
hexachlorobutadiene $CCl_2CClCClCCl_2$ [87-68-3] RWNKSTSCBHKHTB-UHFFFAOYSA-N	5.6×10^{-4} 8.3×10^{-4} 2.3×10^{-3} 6.2×10^{-4} 7.0×10^{-4} 2.3×10^{-3} 9.6×10^{-4} 4.0×10^{-4} 6.1×10^{-4} 6.5×10^{-4} 9.1×10^{-4} 3.8×10^{-4} 4.2×10^{-4} 9.8×10^{-4} 9.7×10^{-4} 9.6×10^{-4} 9.4×10^{-4} 9.6×10^{-4} 9.0×10^{-4} 5.0×10^{-4} 2.3×10^{-3} 1.7×10^{-2} 4.3×10^{-4} 6.2×10^{-4} 7.6×10^{-3} 2.7×10^{-4} 4.2×10^{-4}	5500 3100 6200 4900 2500 4600 5300 3500 	Brockbank (2013) Fogg and Sangster (2003) Hiatt (2013) Dewulf et al. (1999) Kondoh and Nakajima (1997) Oliver (1985) Warner et al. (1980) Pearson and McConnell (1975) Mackay et al. (2006b) Mackay et al. (1993) Ballschmiter and Wittlinger (1991) Warner et al. (1980) Yaws (2003) Goldstein (1982) Hilal et al. (2008) Horvath and Getzen (1999) Ryan et al. (1988) Shen (1982) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Gharagheizi et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Kühne et al. (2005) Yao et al. (2002) Kühne et al. (2005) Yaws (1999)	L L M M M M M M V V V V X X C C C C Q Q Q Q Q Q Q Q ? ?	1 649, 12 237 298 287, 288 287, 289 287, 290 287, 291 246 67 229 21
hexachlorocyclopentadiene C_5Cl_6 [77-47-4] VUNCWTMEJYMOOR-UHFFFAOYSA-N	3.7×10^{-4} 6.0×10^{-4} 6.1×10^{-4} 6.0×10^{-4} 6.2×10^{-4} 2.7×10^{-4} 6.0×10^{-4} 2.7×10^{-4}	 1500 	Wolfe et al. (1982) Warner et al. (1980) Mackay et al. (2006b) Mackay et al. (1993) Wolfe et al. (1982) Warner et al. (1980) Goldstein (1982) Ryan et al. (1988)	M M V V V V X C	 298

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.0×10^{-4}		Shen (1982)	C	
	4.6×10^{-3}		Zhang et al. (2010)	Q	287, 288
	5.3×10^{-3}		Zhang et al. (2010)	Q	287, 289
	1.4×10^{-2}		Zhang et al. (2010)	Q	287, 290
	1.6×10^{-2}		Zhang et al. (2010)	Q	287, 291
	2.3×10^{-3}		Hilal et al. (2008)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	67
	3.7×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	2.4×10^{-3}		Katritzky et al. (1998)	Q	
chlordane	1.8×10^{-1}		Fendinger et al. (1989)	M	72
$C_{10}H_6Cl_8$	1.2×10^{-1}		Fendinger et al. (1989)	M	645
[57-74-9]	2.1×10^{-1}		Warner et al. (1980)	M	
BIWJNBZANLAXMG-UHFFFAOYSA-N	1.1×10^{-1}		Suntio et al. (1988)	V	12
	1.1×10^{-3}		Barcelo and Hennion (1997)	X	567
	2.0×10^{-1}		Suntio et al. (1988)	C	
	1.1×10^{-1}		Suntio et al. (1988)	C	
	1.0×10^{-1}		Ryan et al. (1988)	C	
	2.1×10^{-1}		Shen (1982)	C	
	1.3×10^{-1}		Keshavarz et al. (2022)	Q	
	3.6×10^{-2}		Duchowicz et al. (2020)	Q	184
	1.4×10^{-1}		Zhang et al. (2010)	Q	287, 288
	4.8×10^{-2}		Zhang et al. (2010)	Q	287, 289
	2.4×10^{1}		Zhang et al. (2010)	Q	287, 290
	1.5		Zhang et al. (2010)	Q	287, 291
	2.1×10^{-4}		Goodarzi et al. (2010)	Q	568, 569
	5.3×10^{-2}		Hilal et al. (2008)	Q	
	2.0×10^{-1}		Duchowicz et al. (2020)	?	185, 21
cis-chlordane	1.7×10^{-1}		Shen and Wania (2005)	L	366
$C_{10}H_6Cl_8$	1.8×10^{-1}		Shen and Wania (2005)	L	367
(α-chlordane)	3.7×10^{-2}	4100	Jantunen and Bidleman (2006)	M	
[5103-71-9]	1.5×10^{-1}	6100	Cetin et al. (2006)	M	
BIWJNBZANLAXMG-KMMBHOGFSA-N	1.1×10^{-2}		Atlas et al. (1982)	M	679
	2.8×10^{-2}		Duchowicz et al. (2020)	V	186
			Mackay et al. (2006d)	V	558
	4.8×10^{-3}	7300	Paasivirta et al. (1999)	T	
	3.6×10^{-2}		Duchowicz et al. (2020)	Q	
trans-chlordane	1.7×10^{-1}		Shen and Wania (2005)	L	366
$C_{10}H_6Cl_8$	1.5×10^{-1}		Shen and Wania (2005)	L	367
(β-chlordane)	3.4×10^{-2}	3500	Jantunen and Bidleman (2006)	M	
[5103-74-2]	6.3×10^{-2}	7600	Cetin et al. (2006)	M	
BIWJNBZANLAXMG-OESJLNMISA-N	7.4×10^{-3}		Atlas et al. (1982)	M	679
	2.0×10^{-2}		Duchowicz et al. (2020)	V	186
			Mackay et al. (2006d)	V	558
	3.6×10^{-3}	7100	Paasivirta et al. (1999)	T	
	3.6×10^{-2}		Duchowicz et al. (2020)	Q	
	1.0		Modarresi et al. (2007)	Q	67

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
γ-chlordane $C_{10}H_6Cl_8$ [5566-34-7] JBZJEPYXXVKOKF-UHFFFAOYSA-N	6.3×10^{-2}		Ebert et al. (2023)	?	579
cis-nonachlor $C_{10}H_5Cl_9$ [5103-73-1] OCHOKXCPKDPNQU-BBXWSCHTSA-N	1.4	5100	Cetin et al. (2006)	M	
trans-nonachlor $C_{10}H_5Cl_9$ [39765-80-5] OCHOKXCPKDPNQU-FLVMBEMLSA-N	3.1×10^{-2} 8.8×10^{-2} 7.9×10^{-4}	4800 8000 7600	Jantunen and Bidleman (2006) Cetin et al. (2006) Paasivirta et al. (1999)	M M T	
chlorobenzene C_6H_5Cl [108-90-7] MVPPADPHJFYWMZ-UHFFFAOYSA-N	2.4×10^{-3} 2.6×10^{-3} 2.7×10^{-3} 2.7×10^{-3} 2.9×10^{-3} 2.0×10^{-3} 3.7×10^{-3} 1.7×10^{-3} 2.4×10^{-3} 1.5×10^{-3} 2.5×10^{-3} 1.9×10^{-3} 3.6×10^{-3} 3.4×10^{-3} 2.7×10^{-3} 3.2×10^{-3} 3.5×10^{-3} 3.0×10^{-3} 1.9×10^{-3} 2.9×10^{-3} 3.0×10^{-3} 2.6×10^{-3} 3.1×10^{-3} 2.5×10^{-3} 3.0×10^{-3} 2.4×10^{-3} 2.5×10^{-3} 2.9×10^{-3} 3.1×10^{-3} 3.2×10^{-3} 3.0×10^{-3} 2.9×10^{-3} 2.5×10^{-3}	3700 3600 3800 3800 3800 4400 1300 2300 4300 3600 1700 2900 2900 3100 4700 2700 3500 4200 	Schwardt et al. (2021) Brockbank (2013) Staudinger and Roberts (2001) Staudinger and Roberts (1996) Mackay and Shiu (1981) Schwardt et al. (2021) Hiatt (2013) Lau et al. (2010) Li et al. (2008) Lei et al. (2004) Dewulf et al. (1999) Ryu and Park (1999) Dohnal and Hovorka (1999) de Wolf and Lieder (1998) Welke et al. (1998) Shiu and Mackay (1997) Hovorka and Dohnal (1997) Kondoh and Nakajima (1997) Park et al. (1997) Ramachandran et al. (1996) Khalfaoui and Newsham (1994b) Hoff et al. (1993) Ettre et al. (1993) Li and Carr (1993) Cooling et al. (1992) Bissonette et al. (1990) Ashworth et al. (1988) Hellmann (1987) Yurteri et al. (1987) Mackay and Shiu (1981) Leighton and Calo (1981) Ervin et al. (1980) Warner et al. (1980)	L L L L L M M M M M M M M M M M M M M M M M M M M M M M M M M M M M M M M	1, 706 1 707 33, 11 327 12 87 12 708 11 709 278 87 12

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.6×10^{-3}		Mackay et al. (1979)	M	
	1.6×10^{-3}		Sato and Nakajima (1979b)	M	14
	2.8×10^{-3}	4900	Hartkopf and Karger (1973)	M	
	2.7×10^{-3}		Mackay et al. (2006b)	V	
	2.9×10^{-3}	2400	Fogg and Sangster (2003)	V	
	2.7×10^{-3}		Shiu and Mackay (1997)	V	
	2.8×10^{-3}		Park et al. (1997)	V	
	2.9×10^{-3}		Lide and Frederikse (1995)	V	
	2.7×10^{-3}		Mackay et al. (1993)	V	
	2.7×10^{-3}		Mackay et al. (1992a)	V	
	2.5×10^{-3}		Hwang et al. (1992)	V	
	2.7×10^{-3}		Bobra et al. (1985)	V	
	2.7×10^{-3}		Yoshida et al. (1983)	V	
	2.7×10^{-3}		Cabani et al. (1981)	V	
	2.7×10^{-3}		Warner et al. (1980)	V	
	2.2×10^{-3}		Hine and Mookerjee (1975)	V	
	2.7×10^{-3}		Mackay et al. (1979)	T	
	2.2×10^{-3}		Yaws (2003)	X	237
	2.5×10^{-3}	2100	Goldstein (1982)	X	298
	2.7×10^{-3}		Schüürmann (2000)	C	21
	2.7×10^{-3}		Ryan et al. (1988)	C	
	2.5×10^{-3}		Shen (1982)	C	
	2.4×10^{-2}		Hayer et al. (2022)	Q	20
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	8.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.5×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
	4.0×10^{-3}		Hilal et al. (2008)	Q	
	8.6×10^{-3}		Modarresi et al. (2007)	Q	67
		4000	Kühne et al. (2005)	Q	
	2.9×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	2.8×10^{-3}		Delgado and Alderete (2002)	Q	
	3.6×10^{-3}		Yao et al. (2002)	Q	229
	4.0×10^{-3}		English and Carroll (2001)	Q	230, 231
	1.7×10^{-3}		Katritzky et al. (1998)	Q	
	1.5×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	2.2×10^{-3}		Suzuki et al. (1992)	Q	232
	4.2×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.8×10^{-3}		Arbuckle (1983)	Q	
	3.2×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4000	Kühne et al. (2005)	?	
	2.2×10^{-3}		Yaws (1999)	?	21
	1.6×10^{-3}		Abraham and Weathersby (1994)	?	21
	2.6×10^{-3}		Mackay et al. (1993)	?	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{-3}		Yaws and Yang (1992)	?	21
	2.8×10^{-3}		Abraham et al. (1990)	?	
	3.8×10^{-3}		Mackay and Yeun (1983)	?	
chlorobenzene-d5 C_6D_5Cl [3114-55-4] MVPPADPHJFYWMZ-RALIUCGRSA-N	3.6×10^{-3}	4500	Hiatt (2013)	M	
1,2-dichlorobenzene $C_6H_4Cl_2$ (*o*-dichlorobenzene) [95-50-1] RFFLAFLAYFXFSW-UHFFFAOYSA-N	5.6×10^{-3}	3700	Schwardt et al. (2021)	L	1
	5.9×10^{-3}	5200	Brockbank (2013)	L	1, 710
	6.8×10^{-3}	5300	Fogg and Sangster (2003)	L	711
	5.4×10^{-3}	5900	Staudinger and Roberts (2001)	L	
	5.4×10^{-3}	5900	Staudinger and Roberts (1996)	L	
	5.3×10^{-3}		Mackay and Shiu (1981)	L	
	8.0×10^{-3}	4200	Hiatt (2013)	M	
	6.3×10^{-3}		Li et al. (2008)	M	
	4.7×10^{-3}		Ryu and Park (1999)	M	
	5.1×10^{-3}		Shiu and Mackay (1997)	M	
	7.2×10^{-3}		Hovorka and Dohnal (1997)	M	12
	6.2×10^{-3}	5000	Kondoh and Nakajima (1997)	M	
	4.9×10^{-3}	4400	Park et al. (1997)	M	
	4.8×10^{-3}		Li and Carr (1993)	M	
	3.5×10^{-3}		Yu (1992)	M	12
	4.9×10^{-3}	5100	Bissonette et al. (1990)	M	
	5.3×10^{-3}	1400	Ashworth et al. (1988)	M	42, 278
	8.2×10^{-3}		Oliver (1985)	M	
	5.9×10^{-3}	6700	Gossett et al. (1985)	M	
	5.2×10^{-3}		Mackay and Shiu (1981)	M	
	5.1×10^{-3}		Warner et al. (1980)	M	
	3.5×10^{-3}		Sato and Nakajima (1979b)	M	14
	5.6×10^{-3}		Mackay et al. (2006b)	V	
	4.1×10^{-3}		Shiu and Mackay (1997)	V	
	8.6×10^{-3}		Park et al. (1997)	V	
	8.3×10^{-3}		Lide and Frederikse (1995)	V	
	4.1×10^{-3}		Mackay et al. (1992a)	V	
	6.0×10^{-3}		Hwang et al. (1992)	V	
	4.1×10^{-3}		Bobra et al. (1985)	V	
	4.9×10^{-3}		Warner et al. (1980)	V	
	4.0×10^{-3}		Hine and Mookerjee (1975)	V	
	3.5×10^{-3}		Yaws (2003)	X	237
	5.2×10^{-3}	2800	Goldstein (1982)	X	298
	5.2×10^{-3}		Schüürmann (2000)	C	21
	2.7×10^{-3}		Ryan et al. (1988)	C	
	5.1×10^{-3}		Shen (1982)	C	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	1.5×10^{-2}		Duchowicz et al. (2020)	Q	184
	4.0×10^{-3}		Li et al. (2014)	Q	241

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.7×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
	8.2×10^{-3}		Hilal et al. (2008)	Q	
	4.5×10^{-3}		Modarresi et al. (2007)	Q	67
		4400	Kühne et al. (2005)	Q	
	5.6×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	7.1×10^{-3}		Delgado and Alderete (2002)	Q	
	8.0×10^{-3}		Yao et al. (2002)	Q	229
	4.7×10^{-3}		English and Carroll (2001)	Q	230, 231
	3.3×10^{-3}		Katritzky et al. (1998)	Q	
	2.3×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	8.4×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	5.1×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4800	Kühne et al. (2005)	?	
	3.5×10^{-3}		Yaws (1999)	?	21
	3.6×10^{-3}		Abraham and Weathersby (1994)	?	21
	3.3×10^{-3}		Yaws and Yang (1992)	?	21
	5.1×10^{-3}		Abraham et al. (1990)	?	
	6.2×10^{-3}		Chiou et al. (1980)	?	79
1,2-dichlorobenzene-d4 $C_6D_4Cl_2$ (*o*-dichlorobenzene-d4) [2199-69-1] RFFLAFLAYFXFSW-RHQRLBAQSA-N	8.2×10^{-3}	4200	Hiatt (2013)	M	
1,3-dichlorobenzene $C_6H_4Cl_2$ (*m*-dichlorobenzene) [541-73-1] ZPQOPVIELGIULI-UHFFFAOYSA-N	3.1×10^{-3}	3700	Schwardt et al. (2021)	L	1
	3.1×10^{-3}	4400	Brockbank (2013)	L	1
	3.4×10^{-3}	4300	Fogg and Sangster (2003)	L	
	2.8×10^{-3}		Mackay and Shiu (1981)	L	
	5.2×10^{-3}	4800	Hiatt (2013)	M	
	2.9×10^{-3}		Li et al. (2008)	M	
	3.7×10^{-3}		de Wolf and Lieder (1998)	M	87
	4.7×10^{-3}		Hovorka and Dohnal (1997)	M	12
	3.8×10^{-3}	4400	Kondoh and Nakajima (1997)	M	
	3.4×10^{-3}		Hoff et al. (1993)	M	
	3.0×10^{-3}	2600	Ashworth et al. (1988)	M	33, 278
	5.5×10^{-3}		Oliver (1985)	M	
	3.8×10^{-3}		Warner et al. (1980)	M	
	2.1×10^{-3}		Sato and Nakajima (1979b)	M	14
	3.1×10^{-3}		Mackay et al. (2006b)	V	
	2.7×10^{-3}		Shiu and Mackay (1997)	V	
	5.6×10^{-3}		Lide and Frederikse (1995)	V	
	2.7×10^{-3}		Mackay et al. (1992a)	V	
	2.7×10^{-3}		Bobra et al. (1985)	V	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.3×10^{-3}		Warner et al. (1980)	V	
	2.1×10^{-3}		Hine and Mookerjee (1975)	V	
	2.9×10^{-3}		Yaws (2003)	X	237
	3.9×10^{-3}	2400	Goldstein (1982)	X	298
	3.7×10^{-3}		Ryan et al. (1988)	C	
	3.8×10^{-3}		Shen (1982)	C	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	9.2×10^{-3}		Duchowicz et al. (2020)	Q	299
	3.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
	4.7×10^{-3}		Hilal et al. (2008)	Q	
	3.2×10^{-3}		Modarresi et al. (2007)	Q	67
		4100	Kühne et al. (2005)	Q	
	3.8×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	4.5×10^{-3}		Delgado and Alderete (2002)	Q	
	5.0×10^{-3}		Yao et al. (2002)	Q	229, 267
	3.7×10^{-3}		English and Carroll (2001)	Q	230, 274
	4.2×10^{-3}		Katritzky et al. (1998)	Q	
	2.3×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	8.4×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	3.8×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4500	Kühne et al. (2005)	?	
	2.9×10^{-3}		Yaws (1999)	?	21
	2.2×10^{-3}		Abraham and Weathersby (1994)	?	21
	3.0×10^{-3}		Yaws and Yang (1992)	?	21
	2.7×10^{-3}		Abraham et al. (1990)	?	
1,4-dichlorobenzene	3.2×10^{-3}	3800	Schwardt et al. (2021)	L	1
$C_6H_4Cl_2$	3.8×10^{-3}	6000	Brockbank (2013)	L	1
(p-dichlorobenzene)	4.5×10^{-3}	4400	Fogg and Sangster (2003)	L	
[106-46-7]	6.3×10^{-3}		Mackay and Shiu (1981)	L	
OCJBOOLMMGQPQU-UHFFFAOYSA-N	5.8×10^{-3}	4600	Hiatt (2013)	M	
	3.3×10^{-3}		Li et al. (2008)	M	
	2.5×10^{-3}		Chiang et al. (1998)	M	12
	4.1×10^{-3}		Shiu and Mackay (1997)	M	
	5.4×10^{-3}		Hovorka and Dohnal (1997)	M	12
	4.7×10^{-3}	4800	Kondoh and Nakajima (1997)	M	
	3.1×10^{-3}	2700	Ashworth et al. (1988)	M	278
	5.2×10^{-3}		Yurteri et al. (1987)	M	12
	6.6×10^{-3}		Oliver (1985)	M	
	4.2×10^{-3}		Mackay and Shiu (1981)	M	
	3.6×10^{-3}		Warner et al. (1980)	M	
	4.1×10^{-3}		Mackay et al. (2006b)	V	
	6.3×10^{-3}		Shiu and Mackay (1997)	V	
	6.7×10^{-3}		Lide and Frederikse (1995)	V	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.3×10^{-3}		Mackay et al. (1992a)	V	
	3.8×10^{-3}		Suntio et al. (1988)	V	12
	5.8×10^{-3}		Bobra et al. (1985)	V	
	2.2×10^{-3}		Hine and Mookerjee (1975)	V	
	2.3×10^{-3}		Yaws (2003)	X	237
	3.7×10^{-3}	2700	Goldstein (1982)	X	298
	4.1×10^{-3}		Schüürmann (2000)	C	21
	4.1×10^{-3}		Ryan et al. (1988)	C	
	3.6×10^{-3}		Shen (1982)	C	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	8.4×10^{-3}		Duchowicz et al. (2020)	Q	184
	3.9×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
	6.5×10^{-3}		Hilal et al. (2008)	Q	
	3.0×10^{-3}		Modarresi et al. (2007)	Q	67
		4100	Kühne et al. (2005)	Q	
	4.1×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	4.1×10^{-3}		Delgado and Alderete (2002)	Q	
	4.3×10^{-3}		Katritzky et al. (1998)	Q	
	2.3×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	8.4×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	2.1×10^{-3}		Arbuckle (1983)	Q	
	4.1×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		3700	Kühne et al. (2005)	?	
	2.3×10^{-3}		Yaws and Yang (1992)	?	21
	3.8×10^{-3}		Abraham et al. (1990)	?	
1,2,3-trichlorobenzene	6.2×10^{-3}	4600	Brockbank (2013)	L	1
$C_6H_3Cl_3$	1.5×10^{-2}	4800	Hiatt (2013)	M	
[87-61-6]	6.3×10^{-3}	4600	Brockbank et al. (2013)	M	
RELMFMZEBKVZJC-UHFFFAOYSA-N	8.0×10^{-3}		Lee et al. (2012)	M	
	3.6×10^{-3}	4200	Dewulf et al. (1999)	M	
	7.9×10^{-3}		Shiu and Mackay (1997)	M	
	1.5×10^{-2}	7300	Kondoh and Nakajima (1997)	M	
	1.4×10^{-2}		ten Hulscher et al. (1992)	M	12
	1.1×10^{-2}		Oliver (1985)	M	
	7.9×10^{-3}		Mackay and Shiu (1981)	M	
	4.1×10^{-3}		Mackay et al. (2006b)	V	
	5.8×10^{-3}		Fogg and Sangster (2003)	V	
	2.1×10^{-3}		Fogg and Sangster (2003)	V	
	4.1×10^{-3}		Shiu and Mackay (1997)	V	
	3.3×10^{-3}		Abraham et al. (1994a)	V	
	4.1×10^{-3}		Mackay et al. (1992a)	V	
	4.2×10^{-3}		Bobra et al. (1985)	V	
	4.3×10^{-3}		Mackay and Shiu (1981)	V	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	2.1×10^{-2}		Duchowicz et al. (2020)	Q	299
	5.0×10^{-3}		Abraham et al. (2019)	Q	
	8.0×10^{-3}		Li et al. (2014)	Q	241
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	4.5×10^{-3}		Zhang et al. (2010)	Q	287, 288
	6.9×10^{-3}		Zhang et al. (2010)	Q	287, 289
	1.6×10^{-2}		Zhang et al. (2010)	Q	287, 290
	5.2×10^{-3}		Zhang et al. (2010)	Q	287, 291
	8.0×10^{-3}		Hilal et al. (2008)	Q	
	4.6×10^{-3}		Modarresi et al. (2007)	Q	67
		4800	Kühne et al. (2005)	Q	
	1.1×10^{-2}		Delgado and Alderete (2002)	Q	
	3.4×10^{-3}		English and Carroll (2001)	Q	230, 231
	4.4×10^{-3}		Katritzky et al. (1998)	Q	
	3.5×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	1.8×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	7.9×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4200	Kühne et al. (2005)	?	
1,2,3-trichlorobenzene-d3 $C_6D_3Cl_3$ [3907-98-0] SMNOERSLNYGGOU-UHFFFAOYSA-N	1.5×10^{-2}	4600	Hiatt (2013)	M	
1,2,4-trichlorobenzene $C_6H_3Cl_3$ [120-82-1] PBKONEOXTCPAFI-UHFFFAOYSA-N	3.9×10^{-3}	3100	Schwardt et al. (2021)	L	1
	4.2×10^{-3}	6400	Brockbank (2013)	L	1
	1.1×10^{-2}	5100	Hiatt (2013)	M	
	5.8×10^{-3}		Lee et al. (2012)	M	
	2.4×10^{-3}	3500	Dewulf et al. (1999)	M	712
	2.7×10^{-3}		Ryu and Park (1999)	M	
	6.5×10^{-3}	5500	Kondoh and Nakajima (1997)	M	
	9.9×10^{-3}		ten Hulscher et al. (1992)	M	12
	4.6×10^{-3}	3900	Ashworth et al. (1988)	M	33, 278
	8.2×10^{-3}		Oliver (1985)	M	
	7.0×10^{-3}		Warner et al. (1980)	M	
			Mackay et al. (2006b)	V	683
	7.1×10^{-3}		Fogg and Sangster (2003)	V	
	8.6×10^{-3}		Fogg and Sangster (2003)	V	
	3.6×10^{-3}		Shiu and Mackay (1997)	V	
	7.1×10^{-3}		Lide and Frederikse (1995)	V	
	3.6×10^{-3}		Mackay et al. (1992a)	V	
	4.8×10^{-3}		McLachlan et al. (1990)	V	373
	3.6×10^{-3}		Bobra et al. (1985)	V	
	2.5×10^{-3}		Yoshida et al. (1983)	V	
	2.6×10^{-3}		Mackay and Shiu (1981)	V	

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Table A6.1: Chlorocarbons (C, H, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.3×10^{-3}		Warner et al. (1980)	V	
	3.3×10^{-3}		Yaws (2003)	X	237
	7.0×10^{-3}		Goldstein (1982)	X	446
	7.0×10^{-3}	2500	Goldstein (1982)	X	298
	6.9×10^{-3}		Meylan and Howard (1991)	C	
	4.2×10^{-4}		Ryan et al. (1988)	C	
	7.0×10^{-3}		Shen (1982)	C	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	Q	
	2.5×10^{-3}		Abraham et al. (2019)	Q	
	4.5×10^{-3}		Zhang et al. (2010)	Q	287, 288
	7.7×10^{-3}		Zhang et al. (2010)	Q	287, 289
	1.5×10^{-2}		Zhang et al. (2010)	Q	287, 290
	4.6×10^{-3}		Zhang et al. (2010)	Q	287, 291
	2.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
	9.9×10^{-3}		Hilal et al. (2008)	Q	
	4.2×10^{-3}		Modarresi et al. (2007)	Q	67
		4500	Kühne et al. (2005)	Q	
	2.4×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	6.7×10^{-3}		Delgado and Alderete (2002)	Q	
	7.4×10^{-3}		Yao et al. (2002)	Q	229
	3.4×10^{-3}		English and Carroll (2001)	Q	230, 260
	6.4×10^{-3}		Katritzky et al. (1998)	Q	
	1.6×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	3.5×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	4.5×10^{-3}		Meylan and Howard (1991)	Q	
	6.9×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		3200	Kühne et al. (2005)	?	
	3.3×10^{-3}		Yaws (1999)	?	21
1,2,4-trichlorobenzene-d3 $C_6D_3Cl_3$ [2199-72-6] PBKONEOXTCPAFI-CBYSEHNBSA-N	9.8×10^{-3}	4600	Hiatt (2013)	M	
1,3,5-trichlorobenzene $C_6H_3Cl_3$ [108-70-3] XKEFYDZQGKAQCN-UHFFFAOYSA-N	1.8×10^{-3}	4100	Dewulf et al. (1999)	M	713
	5.2×10^{-3}		ten Hulscher et al. (1992)	M	12
	3.5×10^{-2}		Hellmann (1987)	M	87
	5.2×10^{-3}		Oliver (1985)	M	
			Mackay et al. (2006b)	V	683
	1.4×10^{-3}		Fogg and Sangster (2003)	V	
	8.5×10^{-4}		Fogg and Sangster (2003)	V	
	9.1×10^{-4}		Shiu and Mackay (1997)	V	
	1.0×10^{-2}		Lide and Frederikse (1995)	V	
	1.5×10^{-3}		Abraham et al. (1994a)	V	
	9.1×10^{-4}		Mackay et al. (1992a)	V	
	9.1×10^{-4}		Bobra et al. (1985)	V	
	6.2×10^{-3}		Mackay and Shiu (1981)	V	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	7.5×10^{-3}		Duchowicz et al. (2020)	Q	184
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	4.6×10^{-3}		Hilal et al. (2008)	Q	
	4.2×10^{-3}		Modarresi et al. (2007)	Q	67
		4200	Kühne et al. (2005)	Q	
	4.5×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	4.6×10^{-3}		Delgado and Alderete (2002)	Q	
	1.6×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	3.5×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	4.5×10^{-3}		Meylan and Howard (1991)	Q	
	1.8×10^{-3}		Rumble (2021)	?	714
	5.2×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4400	Kühne et al. (2005)	?	
1,2,3,4-tetrachlorobenzene	3.5×10^{-3}		Ryu and Park (1999)	M	
$C_6H_2Cl_4$	1.3×10^{-2}	4800	ten Hulscher et al. (1992)	M	
[634-66-2]	5.7×10^{-2}		Hellmann (1987)	M	87
GBDZXPJXOMHESU-UHFFFAOYSA-N	1.4×10^{-2}		Oliver (1985)	M	
	9.0×10^{-3}		Mackay et al. (2006b)	V	
	6.9×10^{-3}		Shiu and Mackay (1997)	V	
	6.9×10^{-3}		Mackay et al. (1992a)	V	
	5.8×10^{-3}		McLachlan et al. (1990)	V	373
	6.9×10^{-3}		Bobra et al. (1985)	V	
	3.8×10^{-3}		Mackay and Shiu (1981)	V	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	2.0×10^{-2}		Duchowicz et al. (2020)	Q	299
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	6.1×10^{-3}		Zhang et al. (2010)	Q	287, 288
	7.7×10^{-3}		Zhang et al. (2010)	Q	287, 289
	2.1×10^{-2}		Zhang et al. (2010)	Q	287, 290
	4.6×10^{-3}		Zhang et al. (2010)	Q	287, 291
	8.6×10^{-3}		Hilal et al. (2008)	Q	
	5.7×10^{-3}		Modarresi et al. (2007)	Q	67
		5200	Kühne et al. (2005)	Q	
	1.1×10^{-2}		Delgado and Alderete (2002)	Q	
	4.2×10^{-3}		English and Carroll (2001)	Q	230, 231
	5.7×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	6.1×10^{-3}		Meylan and Howard (1991)	Q	
	1.3×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		4500	Kühne et al. (2005)	?	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,5-tetrachlorobenzene	6.3×10^{-3}		Shiu and Mackay (1997)	M	
$C_6H_2Cl_4$	1.0×10^{-2}		ten Hulscher et al. (1992)	M	12
[634-90-2]	6.3×10^{-3}		Mackay and Shiu (1981)	M	
QZYNWJQFTJXIRN-UHFFFAOYSA-N	1.7×10^{-3}		Mackay et al. (2006b)	V	
	2.1×10^{-3}		Fogg and Sangster (2003)	V	
	1.8×10^{-3}		Fogg and Sangster (2003)	V	
	1.7×10^{-3}		Shiu and Mackay (1997)	V	
	1.7×10^{-3}		Mackay et al. (1992a)	V	
	1.7×10^{-3}		Bobra et al. (1985)	V	
	1.7×10^{-3}		Mackay and Shiu (1981)	V	
	6.3×10^{-3}		Meylan and Howard (1991)	C	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	1.2×10^{-2}		Duchowicz et al. (2020)	Q	
	1.7×10^{-3}		Li et al. (2014)	Q	241
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	7.7×10^{-3}		Hilal et al. (2008)	Q	
	5.4×10^{-3}		Modarresi et al. (2007)	Q	67
	7.1×10^{-3}		Delgado and Alderete (2002)	Q	
	4.2×10^{-3}		English and Carroll (2001)	Q	230, 274
	3.2×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	5.7×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	6.1×10^{-3}		Meylan and Howard (1991)	Q	
	2.4×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	6.2×10^{-3}		Duchowicz et al. (2020)	?	185, 21
1,2,4,5-tetrachlorobenzene	1.8×10^{-2}		McPhedran et al. (2013)	M	
$C_6H_2Cl_4$	6.6×10^{-3}		Lee et al. (2012)	M	
[95-94-3]	9.9×10^{-3}		Oliver (1985)	M	
JHBKHLUZVFWLAG-UHFFFAOYSA-N	8.2×10^{-3}		Mackay et al. (2006b)	V	
	2.8×10^{-4}		Fogg and Sangster (2003)	V	
	1.1×10^{-3}		Fogg and Sangster (2003)	V	
	8.2×10^{-3}		Shiu and Mackay (1997)	V	
	8.2×10^{-3}		Mackay et al. (1992a)	V	
	8.2×10^{-3}		Bobra et al. (1985)	V	
	3.8×10^{-3}		Mackay and Shiu (1981)	V	
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	6.1×10^{-3}		Zhang et al. (2010)	Q	287, 288
	8.4×10^{-3}		Zhang et al. (2010)	Q	287, 289
	1.8×10^{-2}		Zhang et al. (2010)	Q	287, 290
	4.8×10^{-3}		Zhang et al. (2010)	Q	287, 291
	9.2×10^{-3}		Hilal et al. (2008)	Q	
	6.1×10^{-3}		Modarresi et al. (2007)	Q	67
	6.8×10^{-3}		Delgado and Alderete (2002)	Q	
	4.2×10^{-3}		English and Carroll (2001)	Q	230, 231

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.2×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	5.7×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	6.1×10^{-3}		Meylan and Howard (1991)	Q	
pentachlorobenzene	1.4×10^{-2}	5400	Schwardt et al. (2021)	L	1
C_6HCl_5	1.4×10^{-2}	5200	Shen and Wania (2005)	L	366
[608-93-5]	1.4×10^{-2}	5600	Shen and Wania (2005)	L	367
CEOCDNVZRAIOQZ-UHFFFAOYSA-N	3.0×10^{-2}		McPhedran et al. (2013)	M	
	5.6×10^{-3}		Lee et al. (2012)	M	
	1.4×10^{-2}	5200	ten Hulscher et al. (1992)	M	
	2.0×10^{-1}		Hellmann (1987)	M	87
	1.4×10^{-2}		Oliver (1985)	M	
	1.2×10^{-2}		Mackay et al. (2006b)	V	
	3.5×10^{-2}		Fogg and Sangster (2003)	V	
	2.4×10^{-2}		Fogg and Sangster (2003)	V	
	1.2×10^{-2}		Shiu and Mackay (1997)	V	
	1.2×10^{-2}		Mackay et al. (1992a)	V	
	1.2×10^{-2}		Bobra et al. (1985)	V	
	1.0×10^{-3}		Mackay and Shiu (1981)	V	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	1.5×10^{-2}		Duchowicz et al. (2020)	Q	299
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	8.2×10^{-3}		Zhang et al. (2010)	Q	287, 288
	6.9×10^{-3}		Zhang et al. (2010)	Q	287, 289
	1.8×10^{-2}		Zhang et al. (2010)	Q	287, 290
	7.0×10^{-3}		Zhang et al. (2010)	Q	287, 291
	7.2×10^{-3}		Hilal et al. (2008)	Q	
	1.1×10^{-2}		Modarresi et al. (2007)	Q	67
		5700	Kühne et al. (2005)	Q	
	1.0×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	7.9×10^{-3}		Delgado and Alderete (2002)	Q	
	9.4×10^{-3}		Myrdal and Yalkowsky (1994)	Q	
	1.4×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		5100	Kühne et al. (2005)	?	
hexachlorobenzene	6.5×10^{-3}	6600	Brockbank (2013)	L	1
C_6Cl_6	1.9×10^{-2}	6000	Shen and Wania (2005)	L	366
[118-74-1]	1.5×10^{-2}	6400	Shen and Wania (2005)	L	367
CKAPSXZOOQJIBF-UHFFFAOYSA-N	3.3×10^{-2}		McPhedran et al. (2013)	M	
	7.6×10^{-3}		Lee et al. (2012)	M	
	3.0×10^{-2}	6900	Jantunen and Bidleman (2006)	M	
	4.2×10^{-2}		Altschuh et al. (1999)	M	
	3.8×10^{-5}	570	Hansen et al. (1993)	M	281
	2.0×10^{-2}	5700	ten Hulscher et al. (1992)	M	
	2.6		Hellmann (1987)	M	87
	2.1×10^{-2}		Oliver (1985)	M	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.4×10^{-2}		Atlas et al. (1983)	M	72
	7.5×10^{-3}		Atlas et al. (1982)	M	679
	5.8×10^{-3}		Warner et al. (1980)	M	
	7.6×10^{-3}		Mackay et al. (2006b)	V	
	7.6×10^{-3}		Shiu and Mackay (1997)	V	
	7.7×10^{-3}		Lide and Frederikse (1995)	V	
	7.6×10^{-3}		Mackay et al. (1992a)	V	
	7.1×10^{-3}		Ballschmiter and Wittlinger (1991)	V	
	1.1×10^{-2}		Calamari et al. (1991)	V	12
	1.4×10^{-1}		Riederer (1990)	V	
	2.5×10^{-2}		McLachlan et al. (1990)	V	373
	1.4×10^{-1}		Suntio et al. (1988)	V	12
	7.2×10^{-3}		Bobra et al. (1985)	V	
	1.6×10^{-2}		Yoshida et al. (1983)	V	
	2.0×10^{-1}		Mackay and Shiu (1981)	V	
	3.0×10^{-3}	3700	Paasivirta et al. (1999)	T	
	2.6×10^{-3}		Yaws (2003)	X	237
	5.8×10^{-3}	1600	Goldstein (1982)	X	298
	1.0×10^{-2}		Hilal et al. (2008)	C	
	1.5×10^{-2}		Suntio et al. (1988)	C	12
	5.8×10^{-3}		Ryan et al. (1988)	C	
	5.8×10^{-3}		Shen (1982)	C	
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	1.4×10^{-2}		Duchowicz et al. (2020)	Q	184
	1.1×10^{-2}		Zhang et al. (2010)	Q	287, 288
	6.1×10^{-3}		Zhang et al. (2010)	Q	287, 289
	1.6×10^{-2}		Zhang et al. (2010)	Q	287, 290
	1.0×10^{-2}		Zhang et al. (2010)	Q	287, 291
	2.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.0×10^{-2}		Hilal et al. (2008)	Q	
	1.4×10^{-2}		Modarresi et al. (2007)	Q	67
		6400	Kühne et al. (2005)	Q	
	2.1×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	6.5×10^{-3}		Delgado and Alderete (2002)	Q	
	1.6×10^{-2}		Myrdal and Yalkowsky (1994)	Q	
	8.6×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	5.8×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		7200	Kühne et al. (2005)	?	
	2.4×10^{-5}		Yaws and Yang (1992)	?	21
(chloromethyl)-benzene	2.2×10^{-2}	4400	Brockbank (2013)	L	1
$C_6H_5CH_2Cl$	2.0×10^{-2}	7200	Hiatt (2013)	M	
(benzylchloride)	2.8×10^{-2}		Hovorka and Dohnal (1997)	M	12
[100-44-7]	1.2×10^{-2}		Li and Carr (1993)	M	
KCXMKQUNVWSEMD-UHFFFAOYSA-N	2.4×10^{-2}		Duchowicz et al. (2020)	V	186
	2.4×10^{-2}		HSDB (2015)	V	
	2.9×10^{-2}		Lide and Frederikse (1995)	V	
	1.6×10^{-2}		Mackay and Shiu (1981)	V	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.6×10^{-3}		Duchowicz et al. (2020)	Q	
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	271, 243
	3.1×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.0×10^{-2}		Hilal et al. (2008)	Q	
	1.9×10^{-2}		Modarresi et al. (2007)	Q	67
	1.6×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.3×10^{-2}		Katritzky et al. (1998)	Q	
	1.0×10^{-2}		Abraham et al. (1990)	?	
1-chloro-2-methylbenzene	2.2×10^{-3}	4500	Brockbank (2013)	L	1
C_7H_7Cl	3.2×10^{-3}	4100	Hiatt (2013)	M	
(o-chlorotoluene)	2.4×10^{-3}	3400	Kondoh and Nakajima (1997)	M	
[95-49-8]	2.8×10^{-3}	3500	Leighton and Calo (1981)	M	
IBSQPLPBRSHTTG-UHFFFAOYSA-N	1.9×10^{-2}	3000	Goldstein (1982)	X	298
	2.8×10^{-3}		Schüürmann (2000)	C	21
	5.3×10^{-2}		Keshavarz et al. (2022)	Q	
	4.3×10^{-3}		Duchowicz et al. (2020)	Q	299
	4.3×10^{-3}		Hilal et al. (2008)	Q	
	5.4×10^{-3}		Modarresi et al. (2007)	Q	67
		4400	Kühne et al. (2005)	Q	
	5.7×10^{-3}		Katritzky et al. (1998)	Q	
	3.1×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	2.8×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4900	Kühne et al. (2005)	?	
	2.8×10^{-3}		Abraham et al. (1990)	?	
1-chloro-3-methylbenzene	6.1×10^{-4}		Duchowicz et al. (2020)	V	186
C_7H_7Cl	6.2×10^{-4}		Schüürmann (2000)	V	
(m-chlorotoluene)	4.3×10^{-3}		Duchowicz et al. (2020)	Q	
[108-41-8]	3.8×10^{-3}		Hilal et al. (2008)	Q	
OSOUNOBYRMOXQQ-UHFFFAOYSA-N	6.4×10^{-3}		Modarresi et al. (2007)	Q	67
		4400	Kühne et al. (2005)	Q	
	6.1×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	4.8×10^{-3}		Katritzky et al. (1998)	Q	
		4800	Kühne et al. (2005)	?	
1-chloro-4-methylbenzene	2.7×10^{-3}	4900	Brockbank (2013)	L	1
C_7H_7Cl	4.1×10^{-3}	4200	Hiatt (2013)	M	
(p-chlorotoluene)	2.9×10^{-3}	3900	Kondoh and Nakajima (1997)	M	
[106-43-4]	2.3×10^{-3}		Duchowicz et al. (2020)	V	186
NPDACUSDTOMAMK-UHFFFAOYSA-N	2.2×10^{-3}		HSDB (2015)	V	
	3.1×10^{-3}		Yaws (2003)	X	237, 12
	4.3×10^{-3}		Duchowicz et al. (2020)	Q	
	8.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
	4.0×10^{-3}		Hilal et al. (2008)	Q	
	6.8×10^{-3}		Modarresi et al. (2007)	Q	67
		4400	Kühne et al. (2005)	Q	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.1×10^{-3}		Yao et al. (2002)	Q	229
	4.8×10^{-3}		Katritzky et al. (1998)	Q	
		4300	Kühne et al. (2005)	?	
	2.3×10^{-3}		Yaws (1999)	?	21, 12
(dichloromethyl)-benzene	2.5×10^{-2}		Duchowicz et al. (2020)	V	186
$C_7H_6Cl_2$	1.8×10^{-2}		Duchowicz et al. (2020)	Q	
[98-87-3]	1.3×10^{-2}		Zhang et al. (2010)	Q	287, 288
CAHQGWAXKLQREW-UHFFFAOYSA-N	3.4×10^{-2}		Zhang et al. (2010)	Q	287, 289
	1.1×10^{-1}		Zhang et al. (2010)	Q	287, 290
	1.0×10^{-2}		Zhang et al. (2010)	Q	287, 291
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	2.0×10^{-2}		Modarresi et al. (2007)	Q	67
1,2-dichloro-4-methylbenzene	3.8×10^{-3}		Duchowicz et al. (2020)	V	186
$C_7H_6Cl_2$	7.9×10^{-3}		Duchowicz et al. (2020)	Q	
(3,4-dichlorotoluene)	7.9×10^{-3}		Hilal et al. (2008)	Q	
[95-75-0]	4.1×10^{-3}		Modarresi et al. (2007)	Q	67
WYUIWKFIFOJVKW-UHFFFAOYSA-N	4.1×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	9.0×10^{-3}		Katritzky et al. (1998)	Q	
1,3-dichloro-2-methylbenzene	2.3×10^{-3}		HSDB (2015)	Q	99
$C_7H_6Cl_2$	3.1×10^{-3}		Zhang et al. (2010)	Q	287, 288
(2,6-dichlorotoluene)	8.6×10^{-3}		Zhang et al. (2010)	Q	287, 289
[118-69-4]	4.2×10^{-3}		Zhang et al. (2010)	Q	287, 290
DMEDNTFWIHCBRK-UHFFFAOYSA-N	1.8×10^{-3}		Zhang et al. (2010)	Q	287, 291
2,4-dichloro-1-methylbenzene	2.7×10^{-3}	5000	Schwardt et al. (2021)	L	1
$C_7H_6Cl_2$	2.7×10^{-3}	5000	Brockbank (2013)	L	1
(2,4-dichlorotoluene)	2.7×10^{-3}	4900	Brockbank et al. (2013)	M	
[95-73-8]	2.3×10^{-3}		HSDB (2015)	Q	99
FUNUTBJJKQIVSY-UHFFFAOYSA-N	3.1×10^{-3}		Zhang et al. (2010)	Q	287, 288
	5.4×10^{-3}		Zhang et al. (2010)	Q	287, 289
	6.7×10^{-3}		Zhang et al. (2010)	Q	287, 290
	1.8×10^{-3}		Zhang et al. (2010)	Q	287, 291
		4400	Kühne et al. (2005)	Q	
		5500	Kühne et al. (2005)	?	
2,3,6-trichloromethylbenzene	6.6×10^{-3}		Oliver (1985)	M	
$C_7H_5Cl_3$	1.4×10^{-2}		Hilal et al. (2008)	Q	
(2,3,6-trichlorotoluene)	6.0×10^{-3}		Modarresi et al. (2007)	Q	67
[2077-46-5]	4.1×10^{-3}		Meylan and Howard (1991)	Q	
UZYYBZNZSSNYSA-UHFFFAOYSA-N					
2,4,5-trichloromethylbenzene	6.6×10^{-3}		Oliver (1985)	M	
$C_7H_5Cl_3$	1.2×10^{-2}		Hilal et al. (2008)	Q	
(2,4,5-trichlorotoluene)	6.2×10^{-3}		Modarresi et al. (2007)	Q	67
[6639-30-1]	4.1×10^{-3}		Meylan and Howard (1991)	Q	
ZCXHZKNWIYVQNC-UHFFFAOYSA-N					

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4,6-trichloromethylbenzene $C_7H_5Cl_3$ (2,4,6-trichlorotoluene) [23749-65-7] RCTKUIOMKBEGTG-UHFFFAOYSA-N	6.5×10^{-3}		Ebert et al. (2023)	?	365
pentachloromethylbenzene	1.3×10^{-2}		Oliver (1985)	M	
$C_7H_3Cl_5$	1.6×10^{-2}		Hilal et al. (2008)	Q	
(2,3,4,5,6-pentachlorotoluene)	1.7×10^{-2}		Modarresi et al. (2007)	Q	67
[877-11-2]	7.4×10^{-3}		Meylan and Howard (1991)	Q	
AVSIMRGRHWKCAY-UHFFFAOYSA-N					
1-chloro-2-(chloromethyl)benzene	6.4×10^{-3}		Zhang et al. (2010)	Q	287, 288
$C_7H_6Cl_2$	7.2×10^{-2}		Zhang et al. (2010)	Q	287, 289
[611-19-8]	2.1×10^{-1}		Zhang et al. (2010)	Q	287, 290
BASMANVIUSSIIM-UHFFFAOYSA-N	6.1×10^{-3}		Zhang et al. (2010)	Q	287, 291
1-chloro-4-(chloromethyl)benzene	2.9×10^{-2}		HSDB (2015)	Q	99
$C_7H_6Cl_2$	6.4×10^{-3}		Zhang et al. (2010)	Q	287, 288
[104-83-6]	7.5×10^{-2}		Zhang et al. (2010)	Q	287, 289
JQZAEUFPPSRDOP-UHFFFAOYSA-N	8.2×10^{-2}		Zhang et al. (2010)	Q	287, 290
	6.1×10^{-3}		Zhang et al. (2010)	Q	287, 291
chloro(dichloromethyl)benzene	1.8×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_7H_5Cl_3$	7.3×10^{-2}		Zhang et al. (2010)	Q	287, 289
[88-66-4]	5.4×10^{-2}		Zhang et al. (2010)	Q	287, 290
BXSVYGKOUULJCL-UHFFFAOYSA-N	1.3×10^{-2}		Zhang et al. (2010)	Q	287, 291
(trichloromethyl)-benzene	3.8×10^{-2}		HSDB (2015)	Q	99
$C_7H_5Cl_3$	3.8×10^{-2}		Zhang et al. (2010)	Q	287, 288
[98-07-7]	7.2×10^{-3}		Zhang et al. (2010)	Q	287, 289
XEMRAKSQROQPBR-UHFFFAOYSA-N	2.0×10^{-2}		Zhang et al. (2010)	Q	287, 290
	4.7×10^{-3}		Zhang et al. (2010)	Q	287, 291
1-chloro-4- (trichloromethyl)benzene	5.1×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_7H_4Cl_4$	1.8×10^{-2}		Zhang et al. (2010)	Q	287, 289
[5216-25-1]	3.4×10^{-2}		Zhang et al. (2010)	Q	287, 290
LVZPKYYPPLUECL-UHFFFAOYSA-N	6.9×10^{-3}		Zhang et al. (2010)	Q	287, 291
1-chloro-3-ethenylbenzene C_8H_7Cl [2039-85-2] BOVQCIDBZXNFEJ-UHFFFAOYSA-N	4.7×10^{-3}		HSDB (2015)	Q	99
1-chloro-4-ethenylbenzene C_8H_7Cl [1073-67-2] KTZVZZJJVJQZHV-UHFFFAOYSA-N	4.7×10^{-3}		HSDB (2015)	Q	99

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Table A6.1: Chlorocarbons (C, H, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,4-dichloro-2,5-dimethylbenzene	2.7×10^{-3}		Zhang et al. (2010)	Q	287, 288
$C_8H_8Cl_2$	1.2×10^{-2}		Zhang et al. (2010)	Q	287, 289
[1124-05-6]	4.6×10^{-3}		Zhang et al. (2010)	Q	287, 290
UTGSRNVBAFCOEU-UHFFFAOYSA-N	2.3×10^{-3}		Zhang et al. (2010)	Q	287, 291
1,4-bis(trichloromethyl)benzene	7.9×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_8H_4Cl_6$	3.7×10^{-2}		Zhang et al. (2010)	Q	287, 289
[68-36-0]	1.1×10^{-1}		Zhang et al. (2010)	Q	287, 290
OTEKOJQFKOIXMU-UHFFFAOYSA-N	5.8×10^{-3}		Zhang et al. (2010)	Q	287, 291
α,α-dichloro-o-xylene	1.0×10^{-1}	11000	Hiatt (2013)	M	
$C_8H_8Cl_2$					
[612-12-4]					
FMGGHNGKHRCJLL-UHFFFAOYSA-N					
2-chlorostyrene	4.7×10^{-3}		HSDB (2015)	Q	99
C_8H_7Cl	6.2×10^{-3}		Hilal et al. (2008)	Q	
[2039-87-4]					
ISRGONDNXBCDBM-UHFFFAOYSA-N					
octachlorostyrene	7.6×10^{-2}		Oliver (1985)	M	
C_8Cl_8	4.3×10^{-2}		HSDB (2015)	Q	99
[29082-74-4]	1.6×10^{-2}		Hilal et al. (2008)	Q	
RUYUCCQRWINUHE-UHFFFAOYSA-N	4.3×10^{-2}		Meylan and Howard (1991)	Q	
heptachlor	3.3×10^{-2}		Shen and Wania (2005)	L	366
$C_{10}H_5Cl_7$	2.6×10^{-2}		Shen and Wania (2005)	L	367
[76-44-8]	1.9×10^{-2}	4300	Cetin et al. (2006)	M	
FRCCEHPWNOQAEU-UHFFFAOYSA-N	3.4×10^{-2}		Altschuh et al. (1999)	M	
	6.7×10^{-3}		Warner et al. (1980)	M	
	2.8×10^{-3}		Mackay et al. (2006d)	V	
	8.9×10^{-3}		Suntio et al. (1988)	V	12
	8.8×10^{-5}		Barcelo and Hennion (1997)	X	567
	4.3×10^{-3}		McCarty (1980)	X	368
	6.7×10^{-3}		Meylan and Howard (1991)	C	
	6.5×10^{-3}		Ryan et al. (1988)	C	
	6.7×10^{-3}		Shen (1982)	C	
	1.3×10^{-1}		Keshavarz et al. (2022)	Q	
	2.9×10^{-2}		Duchowicz et al. (2020)	Q	
	2.0×10^{-4}		Goodarzi et al. (2010)	Q	568
	2.4×10^{-2}		Hilal et al. (2008)	Q	
	5.8×10^{-1}		Modarresi et al. (2007)	Q	67
	5.6×10^{-2}		Meylan and Howard (1991)	Q	
	3.4×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	2.8×10^{-3}		MacBean (2012a)	?	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloro-2-methyl-2-phenylpropane $C_{10}H_{13}Cl$ [515-40-2] DNXXUUPUQXSUFH-UHFFFAOYSA-N	2.0×10^{-3}		Zhang et al. (2010)	Q	287, 288
	9.5×10^{-3}		Zhang et al. (2010)	Q	287, 289
	1.6×10^{-2}		Zhang et al. (2010)	Q	287, 290
	1.6×10^{-3}		Zhang et al. (2010)	Q	287, 291
1,3-dichloro-5-[(2*S*)-2,4,4,4-tetrachlorobutan-2-yl]benzene $C_{10}H_8Cl_6$ [73588-42-8] DELZPCKTBPIBEE-VIFPVBQESA-N	8.4×10^{-2}		Zhang et al. (2010)	Q	287, 288
	6.1×10^{-2}		Zhang et al. (2010)	Q	287, 289
	1.5		Zhang et al. (2010)	Q	287, 290
	2.9×10^{-3}		Zhang et al. (2010)	Q	287, 291
1,2,3,4,5,6,7,8,8-nonachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H-indene $C_{10}H_5Cl_9$ (nonachlor) [3734-49-4] OCHOKXCPKDPNQU-UHFFFAOYSA-N	3.9×10^{-1}		HSDB (2015)	Q	99
1,1-dichloro-2,2-bis-(4-chlorophenyl)-ethane $C_{14}H_{10}Cl_4$ (p,p'-DDD) [72-54-8] AHJKRLASYNVKDZ-UHFFFAOYSA-N	1.5		Shen and Wania (2005)	L	366
	2.0		Shen and Wania (2005)	L	367
	7.6×10^{-1}		Chao et al. (2017)	M	
	9.1×10^{-1}	5100	Cetin et al. (2006)	M	
	1.5		Altschuh et al. (1999)	M	
			Mackay et al. (2006d)	V	558
	1.1×10^{-1}		Ballschmiter and Wittlinger (1991)	V	
	1.6		Suntio et al. (1988)	V	12
	4.6×10^{-1}		Yoshida et al. (1983)	V	
	2.9×10^{-2}	7300	Paasivirta et al. (1999)	T	
	8.1×10^{-4}		Ryan et al. (1988)	C	
	4.3×10^{-1}		Keshavarz et al. (2022)	Q	
	9.5×10^{-2}		Duchowicz et al. (2020)	Q	184
	2.1		Hilal et al. (2008)	Q	
	3.1×10^{-1}		Modarresi et al. (2007)	Q	67
	1.5		Duchowicz et al. (2020)	?	185, 21
mitotane $C_{14}H_{10}Cl_4$ (o,p'-DDD) [53-19-0] JWBOIMRXGHLCPP-UHFFFAOYSA-N	1.2		Duchowicz et al. (2020)	V	186
	1.2		HSDB (2015)	V	
	1.6		Suntio et al. (1988)	V	12
	5.6×10^{2}		Suntio et al. (1988)	C	715
	9.5×10^{-2}		Duchowicz et al. (2020)	Q	
	2.3×10^{-1}		Zhang et al. (2010)	Q	287, 288
	1.6		Zhang et al. (2010)	Q	287, 289
	1.1×10^{1}		Zhang et al. (2010)	Q	287, 290
	3.9×10^{-1}		Zhang et al. (2010)	Q	287, 291

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1-dichloro-2,2-bis-(4-chlorophenyl)-ethene	2.4×10^{-1}		Shen and Wania (2005)	L	366
$C_{14}H_8Cl_4$	2.4×10^{-1}		Shen and Wania (2005)	L	367
(p,p'-DDE)	2.9×10^{-2}	4700	Jantunen and Bidleman (2006)	M	
[72-55-9]	1.6×10^{-1}	7700	Cetin et al. (2006)	M	
UCNVFOCBFJOQAL-UHFFFAOYSA-N	2.4×10^{-1}		Altschuh et al. (1999)	M	
	8.1×10^{-3}		Atlas et al. (1982)	M	679
			Mackay et al. (2006d)	V	558
	2.9×10^{-2}		Ballschmiter and Wittlinger (1991)	V	
	1.6×10^{-1}		Calamari et al. (1991)	V	12
	7.6×10^{-1}		McLachlan et al. (1990)	V	373
	1.3×10^{-1}		Suntio et al. (1988)	V	12
	5.1×10^{-2}		Yoshida et al. (1983)	V	
	1.2×10^{-1}		Addison et al. (1983)	V	
	2.6×10^{-2}	7600	Paasivirta et al. (1999)	T	
	4.5×10^{-1}		Suntio et al. (1988)	C	681
	4.5×10^{-1}		Ryan et al. (1988)	C	
	8.1×10^{-2}		Keshavarz et al. (2022)	Q	
	4.2×10^{-2}		Duchowicz et al. (2020)	Q	
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	67
	2.4×10^{-1}		Duchowicz et al. (2020)	?	185, 21
o,p'-DDE	5.3×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{14}H_8Cl_4$	3.9×10^{-1}		Mackay et al. (2006d)	V	
[3424-82-6]	3.9×10^{-1}		Suntio et al. (1988)	V	12
ZDYJWDIWLRZXDB-UHFFFAOYSA-N	1.4×10^{-1}		Suntio et al. (1988)	C	12
	4.2×10^{-2}		Duchowicz et al. (2020)	Q	
1,1,1-trichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane	1.3		Duchowicz et al. (2020)	V	186
$C_{14}H_9Cl_5$	2.9		Mackay et al. (2006d)	V	
(o,p'-DDT)	1.9×10^{-2}		Calamari et al. (1991)	V	12
[789-02-6]	4.4×10^{-2}		Duchowicz et al. (2020)	Q	
CVUGPAFCQJIYDT-UHFFFAOYSA-N					
1,1,1-trichloro-2,2-bis-(4-chlorophenyl)-ethane	9.1×10^{-1}		Shen and Wania (2005)	L	366
$C_{14}H_9Cl_5$	9.1×10^{-1}		Shen and Wania (2005)	L	367
(DDT; p,p'-DDT)	1.9×10^{-1}		Mackay and Shiu (1981)	L	
[50-29-3]	9.0×10^{-1}	7500	Cetin et al. (2006)	M	
YVGGHNCTFXOJCH-UHFFFAOYSA-N	1.2		Altschuh et al. (1999)	M	
	7.7×10^{-1}		Fendinger et al. (1989)	M	72
	1.2		Fendinger et al. (1989)	M	645
			Mackay et al. (2006d)	V	558
	1.7×10^{-1}		Ballschmiter and Wittlinger (1991)	V	
	3.4×10^{-1}		Calamari et al. (1991)	V	12
	4.2×10^{-1}		Suntio et al. (1988)	V	12
	6.1×10^{-1}		Caron et al. (1985)	V	

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.7×10^{-1}		Yoshida et al. (1983)	V	
	1.3×10^{-1}		Burkhard and Guth (1981)	V	
	2.5×10^{-1}		Mackay and Leinonen (1975)	V	
	1.9×10^{-2}	7800	Paasivirta et al. (1999)	T	
	4.2×10^{-3}		Barcelo and Hennion (1997)	X	567
	1.7×10^{-1}		Suntio et al. (1988)	C	681
	2.0×10^{-1}		Ryan et al. (1988)	C	
	4.3×10^{-1}		Keshavarz et al. (2022)	Q	
	4.4×10^{-2}		Duchowicz et al. (2020)	Q	299
	6.4×10^{-1}		Zhang et al. (2010)	Q	287, 288
	6.2×10^{-1}		Zhang et al. (2010)	Q	287, 289
	1.6×10^{1}		Zhang et al. (2010)	Q	287, 290
	2.0×10^{-1}		Zhang et al. (2010)	Q	287, 291
	7.7×10^{-3}		Goodarzi et al. (2010)	Q	568
	6.7×10^{-1}		Hilal et al. (2008)	Q	
	3.5×10^{-1}		Modarresi et al. (2007)	Q	67
	1.2		Duchowicz et al. (2020)	?	185, 21
	2.8×10^{-1}		Brimblecombe (1986)	?	80
aldrin $C_{12}H_8Cl_6$ [309-00-2] QBYJBZPUGVGKQQ-SJJAEHHWSA-N	6.7×10^{-2}		Shen and Wania (2005)	L	366
	4.3×10^{-2}		Shen and Wania (2005)	L	367
	3.6×10^{-1}		Mackay and Shiu (1981)	L	
	2.6×10^{-1}		Chao et al. (2017)	M	
	2.2×10^{-2}	3900	Cetin et al. (2006)	M	
	2.2×10^{-1}		Altschuh et al. (1999)	M	
	2.0×10^{-2}		Warner et al. (1980)	M	
	1.1×10^{-2}		Mackay et al. (2006d)	V	
	1.1×10^{-2}		Suntio et al. (1988)	V	12
	6.9×10^{-1}		Mackay and Leinonen (1975)	V	
	1.1×10^{-4}		Barcelo and Hennion (1997)	X	567
	2.0×10^{-2}		Hilal et al. (2008)	C	
	2.0×10^{-2}		Meylan and Howard (1991)	C	
	7.0×10^{-1}		Suntio et al. (1988)	C	12
	6.1×10^{-1}		Suntio et al. (1988)	C	
	2.6×10^{-2}		Suntio et al. (1988)	C	681
	2.0×10^{-2}		Suntio et al. (1988)	C	12
	8.2×10^{-1}		Ryan et al. (1988)	C	
	2.0×10^{-2}		Shen (1982)	C	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	2.3×10^{-2}		Duchowicz et al. (2020)	Q	184
	6.4×10^{-4}		Goodarzi et al. (2010)	Q	568, 569
	8.6×10^{-3}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Modarresi et al. (2007)	Q	67
	2.6×10^{-2}		Meylan and Howard (1991)	Q	
	2.2×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	8.4×10^{-1}		Brimblecombe (1986)	?	80

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Table A6.1: Chlorocarbons (C, H, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
isodrin $C_{12}H_8Cl_6$ [465-73-6] QBYJBZPUGVGKQQ-DIFDVCDBSA-N	2.5×10^{-2}		HSDB (2015)	Q	99
1,1'-(2,2-dichloroethylidene)bis[4- ethylbenzene $C_{18}H_{20}Cl_2$ (perthane) [72-56-0] QFMDFTQOJHFVNR-UHFFFAOYSA-N	5.8×10^{-2}		HSDB (2015)	Q	99

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A6.2 Polychlorinated naphthalenes (PCNs)

Table A6.2: Polychlorinated naphthalenes (PCNs)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloronaphthalene	2.8×10^{-2}		Shiu and Mackay (1997)	M	
$C_{10}H_7Cl$	2.8×10^{-3}		Mackay and Shiu (1981)	M	
(PCN-1)	5.0×10^{-2}		Yaws (2003)	X	237
[90-13-1]	4.7×10^{-2}		Yaws et al. (2005)	X	446
JTPNRXUCIXHOKM-UHFFFAOYSA-N	2.4×10^{-2}		Keshavarz et al. (2022)	Q	
	3.3×10^{-2}		Duchowicz et al. (2020)	Q	
	1.1×10^{-2}		Li et al. (2014)	Q	241
	3.1×10^{-1}		Gharagheizi et al. (2012)	Q	
	5.3×10^{-2}		Gharagheizi et al. (2010)	Q	246
	5.7×10^{-2}		Hilal et al. (2008)	Q	
	7.3×10^{-2}		Modarresi et al. (2007)	Q	67
	3.1×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	1.1×10^{-2}		Katritzky et al. (1998)	Q	
	6.5×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	2.8×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	5.1×10^{-2}		Yaws (1999)	?	21
2-chloronaphthalene	3.0×10^{-2}		Shiu and Mackay (1997)	M	
$C_{10}H_7Cl$	3.1×10^{-2}		Mackay and Shiu (1981)	M	
(PCN-2)	1.5×10^{-2}		Hwang et al. (1992)	V	
[91-58-7]	1.6×10^{-2}	3800	Goldstein (1982)	X	298
CGYGETOMCSJHJU-UHFFFAOYSA-N	3.1×10^{-2}		Ryan et al. (1988)	C	
	2.4×10^{-2}		Keshavarz et al. (2022)	Q	
	3.3×10^{-2}		Duchowicz et al. (2020)	Q	184
	6.0×10^{-2}		Hilal et al. (2008)	Q	
	1.0×10^{-1}		Modarresi et al. (2007)	Q	67
	3.1×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	6.5×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	3.1×10^{-2}		Duchowicz et al. (2020)	?	185, 21
1,2-dichloronaphthalene $C_{10}H_6Cl_2$ (PCN-3) [2050-69-3] MOXLHAPKZWTHEX-UHFFFAOYSA-N	1.2×10^{-1}		Ebert et al. (2023)	?	716
1,3-dichloronaphthalene	3.4×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{10}H_6Cl_2$	7.0×10^{-2}		Zhang et al. (2010)	Q	287, 289
(PCN-4)	4.2×10^{-2}		Zhang et al. (2010)	Q	287, 290
[2198-75-6]	4.7×10^{-2}		Zhang et al. (2010)	Q	287, 291
AMCBMCWLCDERHY-UHFFFAOYSA-N					

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Table A6.2: Polychlorinated naphthalenes (PCNs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,4-dichloronaphthalene $C_{10}H_6Cl_2$ (PCN-5) [1825-31-6] JDPKCYMVSKDOGS-UHFFFAOYSA-N	2.4×10^{-2} 3.2×10^{-2}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
1,5-dichloronaphthalene $C_{10}H_6Cl_2$ (PCN-6) [1825-30-5] ZBQZXTBAGBTUAD-UHFFFAOYSA-N	4.0×10^{-2}		Ebert et al. (2023)	?	716
2,7-dichloronaphthalene $C_{10}H_6Cl_2$ (PCN-12) [2198-77-8] DWBQZSYTSNYEEJ-UHFFFAOYSA-N	3.1×10^{-2}		Ebert et al. (2023)	?	717
1,2,4-trichloronaphthalene $C_{10}H_5Cl_3$ (PCN-14) [50402-51-2] MRJBOPVWPORBKZ-UHFFFAOYSA-N	8.3×10^{-2}		Ebert et al. (2023)	?	365
1,2,5-trichloronaphthalene $C_{10}H_5Cl_3$ (PCN-15) [55720-33-7] MMHZKSMAFILONG-UHFFFAOYSA-N	1.1×10^{-1}	5300	Odabasi and Adali (2016)	M	718
1,2,6-trichloronaphthalene $C_{10}H_5Cl_3$ (PCN-16) [51570-44-6] AAUJSCRITBXDJH-UHFFFAOYSA-N	1.7×10^{-1}	6500	Odabasi and Adali (2016)	M	718
1,2,7-trichloronaphthalene $C_{10}H_5Cl_3$ (PCN-17) [55720-34-8] QYYUVUXSJZJCLQ-UHFFFAOYSA-N	1.5×10^{-1}		Ebert et al. (2023)	?	365
1,3,5-trichloronaphthalene $C_{10}H_5Cl_3$ (PCN-19) [51570-43-5] DZHZYPCCEISGSQ-UHFFFAOYSA-N	7.1×10^{-2}	5500	Odabasi and Adali (2016)	M	718

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Table A6.2: Polychlorinated naphthalenes (PCNs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
1,4,5-trichloronaphthalene $C_{10}H_5Cl_3$ (PCN-23) [2437-55-0] VQSNXLCFFHGXTI-UHFFFAOYSA-N	2.2×10^{-1}	5400	Odabasi and Adali (2016)	M	718
1,4,6-trichloronaphthalene $C_{10}H_5Cl_3$ (PCN-24) [2437-54-9] RLTTZFDRZKJVKJ-UHFFFAOYSA-N	8.3×10^{-2}		Ebert et al. (2023)	?	365
1,6,7-trichloronaphthalene $C_{10}H_5Cl_3$ (PCN-25) [55720-39-3] FUEZTEBYLIMNHN-UHFFFAOYSA-N	1.5×10^{-1}		Ebert et al. (2023)	?	365
1,2,3,4-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-27) [20020-02-4] NAQWICRLNQSPPW-UHFFFAOYSA-N	4.1×10^{-2} 4.1×10^{-2} 8.3×10^{-2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
1,2,3,5-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-28) [53555-63-8] HJJKSUVYCQAMBG-UHFFFAOYSA-N	1.3×10^{-1}		Ebert et al. (2023)	?	716
1,2,4,5-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-32) [6733-54-6] BIVDISPRSYAHQQ-UHFFFAOYSA-N	1.5×10^{-1}	5900	Odabasi and Adali (2016)	M	718
1,2,4,6-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-33) [51570-45-7] GLVVZPZGCNEVEM-UHFFFAOYSA-N	7.8×10^{-2}		Ebert et al. (2023)	?	365
1,2,4,7-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-34) [67922-21-8] PWXOBMRJWBBEED-UHFFFAOYSA-N	7.8×10^{-2}		Ebert et al. (2023)	?	365

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Table A6.2: Polychlorinated naphthalenes (PCNs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
1,2,4,8-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-35) [6529-87-9] WCMSFBRREKZZFL-UHFFFAOYSA-N	1.8×10^{-1}	6000	Odabasi and Adali (2016)	M	718
1,2,5,6-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-36) [67922-22-9] ZPUUGNBIWHBXBM-UHFFFAOYSA-N	1.0×10^{-1}		Ebert et al. (2023)	?	365
1,2,5,7-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-37) [67922-23-0] KQZUIOXHRIVQGR-UHFFFAOYSA-N	7.8×10^{-2}		Ebert et al. (2023)	?	365
1,2,5,8-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-38) [149864-80-2] DLTBLLHAQLBHDR-UHFFFAOYSA-N	2.2×10^{-1}		Ebert et al. (2023)	?	365
1,2,6,8-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-40) [67922-24-1] OVAYDYKVLHHIDQ-UHFFFAOYSA-N	2.2×10^{-1}		Ebert et al. (2023)	?	365
1,3,5,7-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-42) [53555-64-9] OTTCXKPQKOLSJN-UHFFFAOYSA-N	5.6×10^{-2}	5600	Odabasi and Adali (2016)	M	718
1,3,5,8-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-43) [31604-28-1] VFTLNRFRXWCJJK-UHFFFAOYSA-N	1.3×10^{-1}		Ebert et al. (2023)	?	717
1,3,6,8-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-45) [150224-15-0] XXWQPOHDPJIYIN-UHFFFAOYSA-N	1.0×10^{-1}		Ebert et al. (2023)	?	365

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Table A6.2: Polychlorinated naphthalenes (PCNs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
1,4,5,8-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-46) [3432-57-3] LITCKAVLJAKHOE-UHFFFAOYSA-N	3.5×10^{-1}	5700	Odabasi and Adali (2016)	M	718
1,4,6,7-tetrachloronaphthalene $C_{10}H_4Cl_4$ (PCN-47) [55720-43-9] VJZRCIYSYVGDMU-UHFFFAOYSA-N	9.2×10^{-2}	5800	Odabasi and Adali (2016)	M	718
1,2,3,4,6-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-50) [67922-26-3] BAOLNVSMVTYGDA-UHFFFAOYSA-N	7.8×10^{-2}	9000	Odabasi and Adali (2016)	M	718
1,2,3,5,7-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-52) [53555-65-0] OVSKLQPHXHPXDR-UHFFFAOYSA-N	6.9×10^{-2}		Ebert et al. (2023)	?	365
1,2,3,5,8-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-53) [150224-24-1] HVYRFNJXZVEGFK-UHFFFAOYSA-N	1.7×10^{-1}	9700	Odabasi and Adali (2016)	M	718
1,2,4,5,6-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-57) [150224-20-7] KPOZENRUJCHWOA-UHFFFAOYSA-N	1.4×10^{-1}	9500	Odabasi and Adali (2016)	M	718
1,2,4,5,7-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-58) [150224-19-4] WYLDWCYZCFRVRH-UHFFFAOYSA-N	8.9×10^{-2}	8700	Odabasi and Adali (2016)	M	718
1,2,4,5,8-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-59) [150224-25-2] FEIKEVSWLMYFFF-UHFFFAOYSA-N	2.6×10^{-1}	9100	Odabasi and Adali (2016)	M	718

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Table A6.2: Polychlorinated naphthalenes (PCNs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
1,2,4,6,7-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-60) [150224-17-2] GXQUDLBNLKOIQB-UHFFFAOYSA-N	6.9×10^{-2}		Ebert et al. (2023)	?	365
1,2,4,6,8-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-61) [150224-22-9] HGSDQSUMXKHGTH-UHFFFAOYSA-N	1.0×10^{-1}	8800	Odabasi and Adali (2016)	M	718
1,2,4,7,8-pentachloronaphthalene $C_{10}H_3Cl_5$ (PCN-62) [150224-21-8] LBCOXKFWBDTJTF-UHFFFAOYSA-N	1.7×10^{-1}	9200	Odabasi and Adali (2016)	M	718
1,2,3,4,5,6-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-63) [58877-88-6] CTLMCQOGOWNFHA-UHFFFAOYSA-N	7.8×10^{-1}	12000	Odabasi and Adali (2016)	M	718
1,2,3,4,5,7-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-64) [67922-27-4] SWRNUKWDDYPZGV-UHFFFAOYSA-N	3.7×10^{-1}		Ebert et al. (2023)	?	365
1,2,3,4,5,8-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-65) [103426-93-3] PGCDNPCENWGYMA-UHFFFAOYSA-N	9.3×10^{-1}	10000	Odabasi and Adali (2016)	M	718
1,2,3,4,6,7-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-66) [103426-96-6] ZRNSVEOEIWQEMU-UHFFFAOYSA-N	4.3×10^{-1}		Ebert et al. (2023)	?	716
1,2,3,5,6,7-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-67) [103426-97-7] XZLJCGGEQLNWDT-UHFFFAOYSA-N	2.5×10^{-1}		Ebert et al. (2023)	?	365

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Table A6.2: Polychlorinated naphthalenes (PCNs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,5,6,8-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-68) [103426-95-5] FQELOCOACCYGLL-UHFFFAOYSA-N	3.7×10^{-1}		Ebert et al. (2023)	?	365
1,2,3,5,7,8-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-69) [103426-94-4] JPQLLIUTUFJWMH-UHFFFAOYSA-N	4.3×10^{-1}	12000	Odabasi and Adali (2016)	M	718
1,2,4,5,6,8-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-71) [90948-28-0] JHKLUUFTHIWTKX-UHFFFAOYSA-N	4.5×10^{-1}		Ebert et al. (2023)	?	365
1,2,4,5,7,8-hexachloronaphthalene $C_{10}H_2Cl_6$ (PCN-72) [103426-92-2] SFZREMCYQNYZMZ-UHFFFAOYSA-N	4.5×10^{-1}		Ebert et al. (2023)	?	365
1,2,3,4,5,6,7-heptachloronaphthalene $C_{10}HCl_7$ (PCN-73) [58863-14-2] NDZIBNJHNBUHKW-UHFFFAOYSA-N	3.6	10000	Odabasi and Adali (2016)	M	718
1,2,3,4,5,6,8-heptachloronaphthalene $C_{10}HCl_7$ (PCN-74) [58863-15-3] QYEGXUUXWMKHHS-UHFFFAOYSA-N	2.4	10000	Odabasi and Adali (2016)	M	718
octachloronaphthalene $C_{10}Cl_8$ (PCN-75) [2234-13-1] RTNLUFLDZOAXIC-UHFFFAOYSA-N	1.2 1.4×10^{-2} 1.4×10^{-2} 7.8×10^{-2}	7800	Odabasi and Adali (2016) Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	M V V Q	718 186

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A6.3 Polychlorinated biphenyls (PCBs)

Table A6.3: Polychlorinated biphenyls (PCBs)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-chlorobiphenyl	3.0×10^{-2}		Lau et al. (2006)	M	719
$C_{12}H_9Cl$	2.3×10^{-2}		Lau et al. (2006)	M	720
(PCB-1)	3.0×10^{-2}	5300	Charles and Destaillats (2005)	M	
[2051-60-7]	4.9×10^{-2}	5100	Bamford et al. (2000)	M	
LAXBNTIAOJWAOP-UHFFFAOYSA-N	1.7×10^{-2}	5300	Paasivirta and Sinkkonen (2009)	V	
	1.4×10^{-2}		Mackay et al. (2006b)	V	
	1.4×10^{-2}		Mackay et al. (1992a)	V	
	2.7×10^{-3}		Hwang et al. (1992)	V	
	1.4×10^{-2}		Shiu and Mackay (1986)	V	
	3.5×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	3.9×10^{-2}		Duchowicz et al. (2020)	Q	184
	2.3×10^{-2}		Hilal et al. (2008)	Q	
	7.0×10^{-2}		Modarresi et al. (2007)	Q	67
	1.7×10^{-2}		Fang Lee (2007)	Q	721
	2.2×10^{-2}		Fang Lee (2007)	Q	722
		4600	Kühne et al. (2005)	Q	
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	1.3×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		5400	Kühne et al. (2005)	?	
3-chlorobiphenyl	3.2×10^{-2}	5400	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_9Cl$	1.3×10^{-2}		Mackay et al. (2006b)	V	
(PCB-2)	1.3×10^{-2}		Mackay et al. (1992a)	V	
[2051-61-8]	1.3×10^{-2}		Shiu and Mackay (1986)	V	
NMWSKOLWZZWHPL-UHFFFAOYSA-N	6.9×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	3.9×10^{-2}		Duchowicz et al. (2020)	Q	299
	3.7×10^{-2}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	67
	3.7×10^{-2}		Fang Lee (2007)	Q	721
	3.1×10^{-2}		Fang Lee (2007)	Q	722
	3.5×10^{-2}		Dunnivant et al. (1992)	Q	
	1.6×10^{-2}		Duchowicz et al. (2020)	?	185, 21
4-chlorobiphenyl	2.8×10^{-2}	5700	Li et al. (2003)	L	366
$C_{12}H_9Cl$	4.2×10^{-2}	6100	Li et al. (2003)	L	367
(PCB-3)	3.6×10^{-2}		Lau et al. (2006)	M	719
[2051-62-9]	2.9×10^{-2}		Lau et al. (2006)	M	720
FPWNLURCHDRMHC-UHFFFAOYSA-N	3.5×10^{-2}	6700	Charles and Destaillats (2005)	M	
	5.6×10^{-2}	6700	Bamford et al. (2002)	M	
	1.4×10^{-2}	5100	Paasivirta and Sinkkonen (2009)	V	
	2.3×10^{-2}		Mackay et al. (2006b)	V	
	2.3×10^{-2}		Mackay et al. (1992a)	V	
	2.3×10^{-2}		Shiu and Mackay (1986)	V	
	7.7×10^{-2}		Burkhard et al. (1985)	V	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	3.9×10^{-2}		Duchowicz et al. (2020)	Q	299
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Modarresi et al. (2007)	Q	67
	2.1×10^{-2}		Fang Lee (2007)	Q	721
	3.4×10^{-2}		Fang Lee (2007)	Q	722
	3.6×10^{-2}		Dunnivant et al. (1992)	Q	
	1.7×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,2'-dichlorobiphenyl	4.6×10^{-2}	6000	Bamford et al. (2002)	M	
$C_{12}H_8Cl_2$	4.0×10^{-2}		Fendinger and Glotfelty (1990)	M	
(PCB-4)	2.9×10^{-2}		Dunnivant et al. (1988)	M	
[13029-08-8]	2.9×10^{-2}		Dunnivant and Elzerman (1988)	M	723
JAYCNKDKIKZTAF-UHFFFAOYSA-N	3.3×10^{-2}		Murphy et al. (1987)	M	12
	4.5×10^{-2}		Murphy et al. (1983a)	M	24
	7.1×10^{-3}	5500	Paasivirta and Sinkkonen (2009)	V	
	1.7×10^{-2}		Mackay et al. (2006b)	V	
	1.7×10^{-2}		Mackay et al. (1992a)	V	
	1.7×10^{-2}		Shiu and Mackay (1986)	V	
	1.8×10^{-2}		Burkhard et al. (1985)	V	
	2.6×10^{-2}		Chiou et al. (1980)	V	
	4.5×10^{-2}		Murphy et al. (1983b)	X	724, 24
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.5×10^{-2}		Duchowicz et al. (2020)	Q	299
	2.5×10^{-2}		Hilal et al. (2008)	Q	
	6.9×10^{-2}		Modarresi et al. (2007)	Q	67
	2.7×10^{-2}		Fang Lee (2007)	Q	721
	2.1×10^{-2}		Fang Lee (2007)	Q	722
	4.8×10^{-2}		English and Carroll (2001)	Q	230, 231
	3.0×10^{-2}		Dunnivant et al. (1992)	Q	
	4.3×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,3-dichlorobiphenyl	4.3×10^{-2}	5800	Bamford et al. (2002)	M	
$C_{12}H_8Cl_2$	2.1×10^{-2}	5500	Paasivirta and Sinkkonen (2009)	V	
(PCB-5)	5.1×10^{-2}		Burkhard et al. (1985)	V	
[16605-91-7]	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
XOMKZKJEJBZBJJ-UHFFFAOYSA-N	7.1×10^{-2}		Duchowicz et al. (2020)	Q	184
	4.7×10^{-2}		Hilal et al. (2008)	Q	
	8.2×10^{-2}		Modarresi et al. (2007)	Q	67
	3.8×10^{-2}		Fang Lee (2007)	Q	721
	4.1×10^{-2}		Fang Lee (2007)	Q	722
		5000	Kühne et al. (2005)	Q	
	4.3×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
	3.5×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.3×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		5800	Kühne et al. (2005)	?	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3'-dichlorobiphenyl	4.3×10^{-2}	5700	Bamford et al. (2002)	M	
$C_{12}H_8Cl_2$	3.9×10^{-2}		Brunner et al. (1990)	M	
(PCB-6)	3.2×10^{-2}		Murphy et al. (1987)	M	12
[25569-80-6]	4.7×10^{-2}		Murphy et al. (1983a)	M	24
ZHBBDTRJIVXKEX-UHFFFAOYSA-N	3.9×10^{-2}	5900	Paasivirta and Sinkkonen (2009)	V	
	2.5×10^{-2}		Shiu and Mackay (1986)	V	
	3.6×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.5×10^{-2}		Duchowicz et al. (2020)	Q	184
	5.6×10^{-2}		Hilal et al. (2008)	Q	
	7.2×10^{-2}		Modarresi et al. (2007)	Q	67
	3.4×10^{-2}		Fang Lee (2007)	Q	721
	3.3×10^{-2}		Fang Lee (2007)	Q	722
	4.3×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	3.0×10^{-2}		Dunnivant et al. (1992)	Q	
	2.5×10^{-2}		Sabljić and Güsten (1989)	Q	
	3.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,4-dichlorobiphenyl	3.7×10^{-2}	5200	Bamford et al. (2002)	M	
$C_{12}H_8Cl_2$	2.8×10^{-2}		Dunnivant and Elzerman (1988)	M	
(PCB-7)	2.7×10^{-2}		Murphy et al. (1987)	M	12
[33284-50-3]	3.0×10^{-2}	5700	Paasivirta and Sinkkonen (2009)	V	
WEJZHZJJXPXXMU-UHFFFAOYSA-N	2.2×10^{-2}		Mackay et al. (2006b)	V	
	2.2×10^{-2}		Mackay et al. (1992a)	V	
	2.2×10^{-2}		Shiu and Mackay (1986)	V	
	3.4×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	4.2×10^{-2}		Duchowicz et al. (2020)	Q	
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	8.6×10^{-2}		Modarresi et al. (2007)	Q	67
	2.2×10^{-2}		Fang Lee (2007)	Q	721
	3.0×10^{-2}		Fang Lee (2007)	Q	722
		4700	Kühne et al. (2005)	Q	
	3.4×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.6×10^{-2}		Dunnivant et al. (1992)	Q	
	3.5×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		5500	Kühne et al. (2005)	?	
2,4'-dichlorobiphenyl	3.8×10^{-2}	6000	Li et al. (2003)	L	366
$C_{12}H_8Cl_2$	4.4×10^{-2}	6300	Li et al. (2003)	L	367
(PCB-8)	2.6×10^{-2}		Lau et al. (2006)	M	719
[34883-43-7]	1.9×10^{-2}		Lau et al. (2006)	M	720
UFNIBRDIUNVOMX-UHFFFAOYSA-N	2.3×10^{-2}	5300	Charles and Destaillats (2005)	M	
	4.0×10^{-2}	5300	Bamford et al. (2000)	M	
	3.5×10^{-2}		Murphy et al. (1987)	M	12
	5.7×10^{-2}		Brownawell (1986)	M	294
	4.5×10^{-2}		Murphy et al. (1983a)	M	24
	1.0×10^{-2}		Atlas et al. (1982)	M	679

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{-2}	5600	Paasivirta and Sinkkonen (2009)	V	
	1.1×10^{-2}		Shiu and Mackay (1986)	V	
	4.0×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.5×10^{-2}		Duchowicz et al. (2020)	Q	299
	5.7×10^{-2}		Hilal et al. (2008)	Q	
	8.4×10^{-2}		Modarresi et al. (2007)	Q	67
	1.7×10^{-2}		Fang Lee (2007)	Q	721
	3.4×10^{-2}		Fang Lee (2007)	Q	722
		4700	Kühne et al. (2005)	Q	
	4.3×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	3.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.3×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		5600	Kühne et al. (2005)	?	
2,5-dichlorobiphenyl	2.3×10^{-2}	5700	ten Hulscher et al. (1992)	M	
$C_{12}H_8Cl_2$	2.5×10^{-2}		Dunnivant et al. (1988)	M	
(PCB-9)	2.5×10^{-2}		Dunnivant and Elzerman (1988)	M	723
[34883-39-1]	2.0×10^{-2}	5600	Paasivirta and Sinkkonen (2009)	V	
KKQWHYGECTYFIA-UHFFFAOYSA-N	5.0×10^{-2}		Mackay et al. (2006b)	V	
	5.0×10^{-2}		Mackay et al. (1992a)	V	
	5.0×10^{-2}		Shiu and Mackay (1986)	V	
	3.0×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	3.8×10^{-2}		Duchowicz et al. (2020)	Q	184
	4.1×10^{-2}		Hilal et al. (2008)	Q	
	7.0×10^{-2}		Modarresi et al. (2007)	Q	67
	3.1×10^{-2}		Fang Lee (2007)	Q	721
	2.6×10^{-2}		Fang Lee (2007)	Q	722
		4700	Kühne et al. (2005)	Q	
	3.4×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	3.0×10^{-2}		Dunnivant et al. (1992)	Q	
	3.5×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		5800	Kühne et al. (2005)	?	
2,6-dichlorobiphenyl	1.2×10^{-2}	5700	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_8Cl_2$	2.1×10^{-2}		Burkhard et al. (1985)	V	
(PCB-10)	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
[33146-45-1]	4.2×10^{-2}		Duchowicz et al. (2020)	Q	299
IYZWUWBAFUBNCH-UHFFFAOYSA-N	3.0×10^{-2}		Hilal et al. (2008)	Q	
	5.8×10^{-2}		Modarresi et al. (2007)	Q	67
	1.9×10^{-2}		Fang Lee (2007)	Q	721
	2.3×10^{-2}		Fang Lee (2007)	Q	722
	4.3×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	2.3×10^{-2}		Dunnivant et al. (1992)	Q	
	2.1×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.3×10^{-2}		Duchowicz et al. (2020)	?	185, 21

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3'-dichlorobiphenyl	4.2×10^{-2}		Dunnivant et al. (1988)	M	
$C_{12}H_8Cl_2$	4.2×10^{-2}		Dunnivant and Elzerman (1988)	M	723
(PCB-11)	3.4×10^{-2}	5700	Paasivirta and Sinkkonen (2009)	V	
[2050-67-1]	5.9×10^{-2}		Mackay et al. (2006b)	V	
KTXUOWUHFLBZPW-UHFFFAOYSA-N	5.8×10^{-2}		Mackay et al. (1992a)	V	
	7.4×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.5×10^{-2}		Duchowicz et al. (2020)	Q	184
	9.0×10^{-2}		Hilal et al. (2008)	Q	
	2.0×10^{-1}		Modarresi et al. (2007)	Q	67
	7.4×10^{-2}		Fang Lee (2007)	Q	721
	4.3×10^{-2}		Fang Lee (2007)	Q	722
	3.4×10^{-2}		Dunnivant et al. (1992)	Q	
	4.3×10^{-2}		Meylan and Howard (1991)	Q	
	4.2×10^{-2}		Duchowicz et al. (2020)	?	185, 21
3,4-dichlorobiphenyl	7.0×10^{-2}		Brunner et al. (1990)	M	
$C_{12}H_8Cl_2$	4.8×10^{-2}		Dunnivant et al. (1988)	M	
(PCB-12)	4.8×10^{-2}		Dunnivant and Elzerman (1988)	M	723
[2974-92-7]	2.0×10^{-2}	5300	Paasivirta and Sinkkonen (2009)	V	
ZGHQUYZPMWMLBM-UHFFFAOYSA-N	1.0×10^{-1}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	7.1×10^{-2}		Duchowicz et al. (2020)	Q	184
	7.7×10^{-2}		Hilal et al. (2008)	Q	
	1.1×10^{-1}		Modarresi et al. (2007)	Q	67
	4.8×10^{-2}		Fang Lee (2007)	Q	721
	4.3×10^{-2}		Fang Lee (2007)	Q	722
	7.3×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	4.2×10^{-2}		Dunnivant et al. (1992)	Q	
	7.0×10^{-2}		Duchowicz et al. (2020)	?	185, 21
3,4'-dichlorobiphenyl	4.9×10^{-2}	6100	Bamford et al. (2002)	M	
$C_{12}H_8Cl_2$	8.5×10^{-2}	5900	Paasivirta and Sinkkonen (2009)	V	
(PCB-13)	8.1×10^{-2}		Burkhard et al. (1985)	V	
[2974-90-5]	9.5×10^{-2}		Hilal et al. (2008)	Q	
CJDNEKOMKXLSBN-UHFFFAOYSA-N	3.7×10^{-2}		Fang Lee (2007)	Q	721
	4.4×10^{-2}		Fang Lee (2007)	Q	722
	3.9×10^{-2}		Dunnivant et al. (1992)	Q	
	3.1×10^{-2}		Sabljić and Güsten (1989)	Q	
3,5-dichlorobiphenyl	2.7×10^{-2}	5500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_8Cl_2$	6.0×10^{-2}		Burkhard et al. (1985)	V	
(PCB-14)	5.0×10^{-2}		Hilal et al. (2008)	Q	
[34883-41-5]	9.4×10^{-2}		Modarresi et al. (2007)	Q	67
QHZSDTDMQZPUKC-UHFFFAOYSA-N	6.7×10^{-2}		Fang Lee (2007)	Q	721
	3.2×10^{-2}		Fang Lee (2007)	Q	722
	2.3×10^{-2}		Dunnivant et al. (1992)	Q	
	2.0×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,4'-dichlorobiphenyl	7.0×10^{-2}	6000	Li et al. (2003)	L	366
$C_{12}H_8Cl_2$	7.5×10^{-2}	6700	Li et al. (2003)	L	367
(PCB-15)	5.0×10^{-2}		Lau et al. (2006)	M	719
[2050-68-2]	3.3×10^{-2}		Lau et al. (2006)	M	720
YTBRNEUEFCNVHC-UHFFFAOYSA-N	3.5×10^{-2}	5300	Charles and Destaillats (2005)	M	33
	1.0×10^{-1}		Fendinger and Glotfelty (1990)	M	
	5.0×10^{-2}		Dunnivant et al. (1988)	M	
	5.0×10^{-2}		Dunnivant and Elzerman (1988)	M	723
	3.3×10^{-3}	4900	Paasivirta and Sinkkonen (2009)	V	
	5.6×10^{-2}		Mackay et al. (2006b)	V	
	5.9×10^{-2}		Mackay et al. (1992a)	V	
	5.9×10^{-2}		Shiu and Mackay (1986)	V	
	9.1×10^{-2}		Burkhard et al. (1985)	V	
	1.0×10^{-1}		Chiou et al. (1980)	V	
	3.3×10^{-2}		Murphy et al. (1983b)	X	724, 24
	6.8×10^{-2}		Dunnivant et al. (1988)	C	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.5×10^{-2}		Duchowicz et al. (2020)	Q	184
	9.7×10^{-2}		Hilal et al. (2008)	Q	
	1.8×10^{-1}		Modarresi et al. (2007)	Q	67
	2.1×10^{-2}		Fang Lee (2007)	Q	721
	4.8×10^{-2}		Fang Lee (2007)	Q	722
	4.4×10^{-2}		Dunnivant et al. (1992)	Q	
	4.3×10^{-2}		Meylan and Howard (1991)	Q	
	5.0×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,2',3-trichlorobiphenyl	4.2×10^{-2}	5700	Bamford et al. (2002)	M	
$C_{12}H_7Cl_3$	4.1×10^{-2}		Murphy et al. (1987)	M	12
(PCB-16)	1.2×10^{-2}		Atlas et al. (1982)	M	679
[38444-78-9]	1.5×10^{-2}	5800	Paasivirta and Sinkkonen (2009)	V	
XVIZMMSINIOIQP-UHFFFAOYSA-N	1.3×10^{-2}		Shiu and Mackay (1986)	V	
	2.8×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	299
	5.6×10^{-2}		Hilal et al. (2008)	Q	
	6.9×10^{-2}		Modarresi et al. (2007)	Q	67
	6.1×10^{-2}		Fang Lee (2007)	Q	721
	4.4×10^{-2}		Fang Lee (2007)	Q	722
		4500	Kühne et al. (2005)	Q	
	3.9×10^{-2}		Dunnivant et al. (1992)	Q	
	3.6×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		4700	Kühne et al. (2005)	?	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',4-trichlorobiphenyl	3.3×10^{-2}	4700	Bamford et al. (2002)	M	
$C_{12}H_7Cl_3$	3.0×10^{-2}		Murphy et al. (1987)	M	12
(PCB-17)	4.0×10^{-2}	6200	Paasivirta and Sinkkonen (2009)	V	
[37680-66-3]	1.9×10^{-2}		Burkhard et al. (1985)	V	
YKKYCYQDUUXNLN-UHFFFAOYSA-N	3.7×10^{-2}		Hilal et al. (2008)	Q	
	3.5×10^{-2}		Fang Lee (2007)	Q	721
	3.2×10^{-2}		Fang Lee (2007)	Q	722
	2.6×10^{-2}		Dunnivant et al. (1992)	Q	
	2.5×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',5-trichlorobiphenyl	2.9×10^{-1}		Bhangare et al. (2019)	M	725
$C_{12}H_7Cl_3$	9.0×10^{-2}		Bhangare et al. (2019)	M	726
(PCB-18)	3.9×10^{-2}	4200	Bamford et al. (2000)	M	
[37680-65-2]	3.9×10^{-2}		Brunner et al. (1990)	M	
DCMURXAZTZQAFB-UHFFFAOYSA-N	2.6×10^{-2}		Dunnivant and Elzerman (1988)	M	
	3.3×10^{-2}		Murphy et al. (1987)	M	12
	4.9×10^{-2}		Oliver (1985)	M	
	4.9×10^{-2}		Murphy et al. (1983a)	M	24
	9.9×10^{-3}		Atlas et al. (1982)	M	679
	9.8×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
	1.1×10^{-2}		Mackay et al. (2006b)	V	
	1.1×10^{-2}		Mackay et al. (1992a)	V	
	1.1×10^{-2}		Shiu and Mackay (1986)	V	
	1.7×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.5×10^{-2}		Duchowicz et al. (2020)	Q	299
	4.6×10^{-2}		Hilal et al. (2008)	Q	
	6.4×10^{-2}		Modarresi et al. (2007)	Q	67
	4.9×10^{-2}		Fang Lee (2007)	Q	721
	3.0×10^{-2}		Fang Lee (2007)	Q	722
		4200	Kühne et al. (2005)	Q	
	5.8×10^{-2}		Yaffe et al. (2003)	Q	248, 272
	6.0×10^{-2}		English and Carroll (2001)	Q	230, 274
	3.1×10^{-2}		Dunnivant et al. (1992)	Q	
	3.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		4500	Kühne et al. (2005)	?	
2,2',6-trichlorobiphenyl	3.3×10^{-2}	4700	Bamford et al. (2002)	M	
$C_{12}H_7Cl_3$	4.3×10^{-2}		Brunner et al. (1990)	M	
(PCB-19)	3.3×10^{-2}		Murphy et al. (1987)	M	12
[38444-73-4]	4.7×10^{-2}		Murphy et al. (1983a)	M	24
MVXIJRBBCDLNLX-UHFFFAOYSA-N	2.5×10^{-3}	5400	Paasivirta and Sinkkonen (2009)	V	
	8.0×10^{-3}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	6.0×10^{-2}		Duchowicz et al. (2020)	Q	
	5.4×10^{-2}		Hilal et al. (2008)	Q	
	6.0×10^{-2}		Modarresi et al. (2007)	Q	67
	3.0×10^{-2}		Fang Lee (2007)	Q	721

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.4×10^{-2}		Fang Lee (2007)	Q	722
		3600	Kühne et al. (2005)	Q	
	2.2×10^{-2}		Dunnivant et al. (1992)	Q	
	2.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.3×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		3100	Kühne et al. (2005)	?	
2,3,3'-trichlorobiphenyl	1.2×10^{-2}		Atlas et al. (1982)	M	679
$C_{12}H_7Cl_3$	2.0×10^{-2}	5800	Paasivirta and Sinkkonen (2009)	V	
(PCB-20)	1.2×10^{-2}		Shiu and Mackay (1986)	V	
[38444-84-7]	5.8×10^{-2}		Burkhard et al. (1985)	V	
SXHLTVKPNQVZGL-UHFFFAOYSA-N	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	299
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	8.4×10^{-2}		Modarresi et al. (2007)	Q	67
	7.6×10^{-2}		Fang Lee (2007)	Q	721
	6.5×10^{-2}		Fang Lee (2007)	Q	722
	4.5×10^{-2}		Dunnivant et al. (1992)	Q	
	3.3×10^{-2}		Sabljić and Güsten (1989)	Q	
	6.2×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,3,4-trichlorobiphenyl	4.3×10^{-3}	5200	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_7Cl_3$	6.8×10^{-2}		Burkhard et al. (1985)	V	
(PCB-21)	7.9×10^{-2}		Hilal et al. (2008)	Q	
[55702-46-0]	5.0×10^{-2}		Fang Lee (2007)	Q	721
IUYHQGMDSZOPDZ-UHFFFAOYSA-N	5.9×10^{-2}		Fang Lee (2007)	Q	722
	4.3×10^{-2}		Dunnivant et al. (1992)	Q	
	4.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,4'-trichlorobiphenyl	3.4×10^{-2}	4800	Bamford et al. (2002)	M	
$C_{12}H_7Cl_3$	5.0×10^{-2}		Murphy et al. (1987)	M	12
(PCB-22)	5.5×10^{-2}		Murphy et al. (1983a)	M	24
[38444-85-8]	1.3×10^{-2}	5600	Paasivirta and Sinkkonen (2009)	V	
ZMHWQAHZKUPENF-UHFFFAOYSA-N	6.5×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	1.0×10^{-1}		Modarresi et al. (2007)	Q	67
	3.8×10^{-2}		Fang Lee (2007)	Q	721
	6.4×10^{-2}		Fang Lee (2007)	Q	722
	5.2×10^{-2}		Dunnivant et al. (1992)	Q	
	4.4×10^{-2}		Sabljić and Güsten (1989)	Q	
	7.0×10^{-2}		Duchowicz et al. (2020)	?	185, 21

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,5-trichlorobiphenyl	1.5×10^{-2}	5700	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_7Cl_3$	3.9×10^{-2}		Burkhard et al. (1985)	V	
(PCB-23)	6.9×10^{-2}		Fang Lee (2007)	Q	721
[55720-44-0]	4.7×10^{-2}		Fang Lee (2007)	Q	722
GBUCDGDROYMOAN-UHFFFAOYSA-N	3.1×10^{-2}		Dunnivant et al. (1992)	Q	
	2.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,6-trichlorobiphenyl	3.3×10^{-2}	4700	Bamford et al. (2002)	M	
$C_{12}H_7Cl_3$	4.5×10^{-2}		Brunner et al. (1990)	M	
(PCB-24)	3.1×10^{-2}		Murphy et al. (1987)	M	12
[55702-45-9]	7.7×10^{-3}	5600	Paasivirta and Sinkkonen (2009)	V	
LVROLHVSYNLFBE-UHFFFAOYSA-N	2.3×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.3×10^{-2}		Duchowicz et al. (2020)	Q	299
	4.7×10^{-2}		Hilal et al. (2008)	Q	
	8.5×10^{-2}		Modarresi et al. (2007)	Q	67
	4.2×10^{-2}		Fang Lee (2007)	Q	721
	4.4×10^{-2}		Fang Lee (2007)	Q	722
		4500	Kühne et al. (2005)	Q	
	3.2×10^{-2}		Dunnivant et al. (1992)	Q	
	2.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.5×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		2800	Kühne et al. (2005)	?	
2,3',4-trichlorobiphenyl	3.3×10^{-2}	4700	Bamford et al. (2002)	M	
$C_{12}H_7Cl_3$	2.4×10^{-2}		Murphy et al. (1987)	M	12
(PCB-25)	6.2×10^{-2}		Murphy et al. (1983a)	M	24
[55712-37-3]	2.8×10^{-2}	5900	Paasivirta and Sinkkonen (2009)	V	
XBBZAULFUPBZSP-UHFFFAOYSA-N	3.9×10^{-2}		Burkhard et al. (1985)	V	
	4.4×10^{-2}		Fang Lee (2007)	Q	721
	4.5×10^{-2}		Fang Lee (2007)	Q	722
		4800	Kühne et al. (2005)	Q	
	3.1×10^{-2}		Dunnivant et al. (1992)	Q	
	2.3×10^{-2}		Sabljić and Güsten (1989)	Q	
		5700	Kühne et al. (2005)	?	
2,3',5-trichlorobiphenyl	3.5×10^{-2}	4900	Bamford et al. (2002)	M	
$C_{12}H_7Cl_3$	3.0×10^{-2}		Dunnivant et al. (1988)	M	
(PCB-26)	3.0×10^{-2}		Dunnivant and Elzerman (1988)	M	723
[38444-81-4]	2.9×10^{-2}		Murphy et al. (1987)	M	12
ONNCPBRWFSKDMQ-UHFFFAOYSA-N	2.2×10^{-2}	5900	Paasivirta and Sinkkonen (2009)	V	
	3.5×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.5×10^{-2}		Duchowicz et al. (2020)	Q	299
	9.9×10^{-2}		Hilal et al. (2008)	Q	
	7.3×10^{-2}		Modarresi et al. (2007)	Q	67
	6.1×10^{-2}		Fang Lee (2007)	Q	721
	4.3×10^{-2}		Fang Lee (2007)	Q	722
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.9×10^{-2}		Meylan and Howard (1991)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,3',6-trichlorobiphenyl	3.5×10^{-2}		Murphy et al. (1987)	M	12
$C_{12}H_7Cl_3$	3.1×10^{-2}	6100	Paasivirta and Sinkkonen (2009)	V	
(PCB-27)	2.4×10^{-2}		Burkhard et al. (1985)	V	
[38444-76-7]	3.7×10^{-2}		Fang Lee (2007)	Q	721
VQOFJPFYTCHPTR-UHFFFAOYSA-N	4.2×10^{-2}		Fang Lee (2007)	Q	722
	2.4×10^{-2}		Dunnivant et al. (1992)	Q	
	2.0×10^{-2}		Sabljić and Güsten (1989)	Q	
2,4,4'-trichlorobiphenyl	3.0×10^{-2}	6300	Li et al. (2003)	L	366
$C_{12}H_7Cl_3$	3.3×10^{-2}	6600	Li et al. (2003)	L	367
(PCB-28)	5.9×10^{-3}		Bhangare et al. (2019)	M	725
[7012-37-5]	5.0×10^{-2}		Bhangare et al. (2019)	M	726
BZTYNSQSZHARAZ-UHFFFAOYSA-N	2.3×10^{-2}		Lau et al. (2006)	M	719
	1.4×10^{-2}		Lau et al. (2006)	M	720
	1.8×10^{-2}	2300	Charles and Destaillats (2005)	M	33
	2.6×10^{-2}	3900	Bamford et al. (2000)	M	
	3.6×10^{-2}	6100	ten Hulscher et al. (1992)	M	
	4.9×10^{-2}		Brunner et al. (1990)	M	
	3.1×10^{-2}		Dunnivant and Elzerman (1988)	M	
	3.7×10^{-2}		Murphy et al. (1987)	M	12
	6.9×10^{-2}		Brownawell (1986)	M	294
	2.7×10^{-2}	5900	Paasivirta and Sinkkonen (2009)	V	
	4.4×10^{-2}		Burkhard et al. (1985)	V	
	2.7×10^{-2}	7100	Paasivirta et al. (1999)	T	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	6.0×10^{-2}		Duchowicz et al. (2020)	Q	
	1.0×10^{-1}		Hilal et al. (2008)	Q	
	9.9×10^{-2}		Modarresi et al. (2007)	Q	67
	2.2×10^{-2}		Fang Lee (2007)	Q	721
	4.7×10^{-2}		Fang Lee (2007)	Q	722
		4800	Kühne et al. (2005)	Q	
	5.2×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	3.5×10^{-2}		Dunnivant et al. (1992)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		4800	Kühne et al. (2005)	?	
2,4,5-trichlorobiphenyl	3.1×10^{-2}	6500	Schwardt et al. (2021)	L	1
$C_{12}H_7Cl_3$	3.1×10^{-2}	6300	Li et al. (2003)	L	366
(PCB-29)	3.3×10^{-2}	6700	Li et al. (2003)	L	367
[15862-07-4]	2.6×10^{-2}	4200	Bamford et al. (2000)	M	
VGVIKVCCUATMNG-UHFFFAOYSA-N	4.9×10^{-2}		Brunner et al. (1990)	M	
	7.7×10^{-3}	5500	Paasivirta and Sinkkonen (2009)	V	
	4.1×10^{-3}		Mackay et al. (2006b)	V	
	4.1×10^{-2}		Mackay et al. (1992a)	V	
	4.2×10^{-2}		Shiu and Mackay (1986)	V	
	3.9×10^{-2}		Burkhard et al. (1985)	V	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.3×10^{-2}		Duchowicz et al. (2020)	Q	
	4.5×10^{-2}		Bhangare et al. (2019)	Q	
	7.9×10^{-2}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	67
	4.0×10^{-2}		Fang Lee (2007)	Q	721
	4.2×10^{-2}		Fang Lee (2007)	Q	722
		5100	Kühne et al. (2005)	Q	
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	3.7×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		4500	Kühne et al. (2005)	?	
2,4,6-trichlorobiphenyl	1.5×10^{-2}		Dunnivant et al. (1988)	M	
$C_{12}H_7Cl_3$	1.5×10^{-2}		Dunnivant and Elzerman (1988)	M	723
(PCB-30)	1.0×10^{-2}		Duchowicz et al. (2020)	V	186
[35693-92-6]	8.5×10^{-3}	5600	Paasivirta and Sinkkonen (2009)	V	
MTLMVEWEYZFYTH-UHFFFAOYSA-N	2.0×10^{-2}		Mackay et al. (2006b)	V	
	2.0×10^{-2}		Mackay et al. (1992a)	V	
	2.0×10^{-2}		Shiu and Mackay (1986)	V	
	1.6×10^{-2}		Burkhard et al. (1985)	V	
	3.5×10^{-2}		Duchowicz et al. (2020)	Q	
	2.9×10^{-2}		Hilal et al. (2008)	Q	
	2.4×10^{-2}		Fang Lee (2007)	Q	721
	2.5×10^{-2}		Fang Lee (2007)	Q	722
	1.7×10^{-2}		Dunnivant et al. (1992)	Q	
2,4',5-trichlorobiphenyl	2.7×10^{-2}	6100	Li et al. (2003)	L	366
$C_{12}H_7Cl_3$	2.9×10^{-2}	6600	Li et al. (2003)	L	367
(PCB-31)	3.4×10^{-2}	4900	Bamford et al. (2002)	M	
[16606-02-3]	5.2×10^{-2}		Brunner et al. (1990)	M	
VAHKBZSAUKPEOV-UHFFFAOYSA-N	3.7×10^{-2}		Murphy et al. (1987)	M	12
	4.9×10^{-2}		Murphy et al. (1983a)	M	24
	1.1×10^{-2}		Atlas et al. (1982)	M	679
	1.3×10^{-2}	5700	Paasivirta and Sinkkonen (2009)	V	
	1.8×10^{-2}		Shiu and Mackay (1986)	V	
	3.9×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	5.5×10^{-2}		Duchowicz et al. (2020)	Q	
	1.0×10^{-1}		Hilal et al. (2008)	Q	
	9.1×10^{-2}		Modarresi et al. (2007)	Q	67
	3.0×10^{-2}		Fang Lee (2007)	Q	721
	4.1×10^{-2}		Fang Lee (2007)	Q	722
	3.6×10^{-2}		Dunnivant et al. (1992)	Q	
	3.5×10^{-2}		Sabljić and Güsten (1989)	Q	
	5.2×10^{-2}		Duchowicz et al. (2020)	?	185, 21

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4',6-trichlorobiphenyl	1.2×10^{-2}	5700	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_7Cl_3$	2.7×10^{-2}		Burkhard et al. (1985)	V	
(PCB-32)	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
[38444-77-8]	6.0×10^{-2}		Duchowicz et al. (2020)	Q	299
IHIDFKLAWYPTKB-UHFFFAOYSA-N	7.5×10^{-2}		Hilal et al. (2008)	Q	
	6.9×10^{-2}		Modarresi et al. (2007)	Q	67
	1.8×10^{-2}		Fang Lee (2007)	Q	721
	4.1×10^{-2}		Fang Lee (2007)	Q	722
	2.5×10^{-2}		Dunnivant et al. (1992)	Q	
	2.4×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,3',4'-trichlorobiphenyl	3.6×10^{-2}	5100	Bamford et al. (2002)	M	
$C_{12}H_7Cl_3$	4.4×10^{-2}		Murphy et al. (1987)	M	12
(PCB-33)	6.6×10^{-2}		Murphy et al. (1983a)	M	24
[38444-86-9]	2.5×10^{-2}		Westcott et al. (1981)	M	
RIMXLXBUOQMDHV-UHFFFAOYSA-N	1.3×10^{-2}	5600	Paasivirta and Sinkkonen (2009)	V	
			Mackay et al. (2006b)	V	683
	2.3×10^{-2}		Mackay et al. (1992a)	V	
	2.3×10^{-2}		Shiu and Mackay (1986)	V	
	5.9×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	299
	1.1×10^{-1}		Hilal et al. (2008)	Q	
	7.0×10^{-2}		Modarresi et al. (2007)	Q	67
	7.7×10^{-2}		Fang Lee (2007)	Q	721
	5.0×10^{-2}		Fang Lee (2007)	Q	722
	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
	4.5×10^{-2}		Sabljić and Güsten (1989)	Q	
	6.2×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,3',5'-trichlorobiphenyl	1.3×10^{-2}	5800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_7Cl_3$	3.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-34)	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
[37680-68-5]	6.0×10^{-2}		Duchowicz et al. (2020)	Q	184
GXVMAQACUOSFJF-UHFFFAOYSA-N	7.3×10^{-2}		Hilal et al. (2008)	Q	
	7.1×10^{-2}		Modarresi et al. (2007)	Q	67
	1.1×10^{-1}		Fang Lee (2007)	Q	721
	3.9×10^{-2}		Fang Lee (2007)	Q	722
	2.3×10^{-2}		Dunnivant et al. (1992)	Q	
	2.0×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3',4-trichlorobiphenyl	1.8×10^{-2}	5600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_7Cl_3$	1.2×10^{-1}		Burkhard et al. (1985)	V	
(PCB-35)	9.5×10^{-2}		Fang Lee (2007)	Q	721
[37680-69-6]	5.9×10^{-2}		Fang Lee (2007)	Q	722
JHBVPKZLIBDTJR-UHFFFAOYSA-N	5.5×10^{-2}		Dunnivant et al. (1992)	Q	
	4.4×10^{-2}		Sabljić and Güsten (1989)	Q	
3,3',5-trichlorobiphenyl	5.8×10^{-2}		Brunner et al. (1990)	M	
$C_{12}H_7Cl_3$	1.3×10^{-2}	5600	Paasivirta and Sinkkonen (2009)	V	
(PCB-36)	7.2×10^{-2}		Burkhard et al. (1985)	V	
[38444-87-0]	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
RIBGNAJQTOXRDK-UHFFFAOYSA-N	6.0×10^{-2}		Duchowicz et al. (2020)	Q	299
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	8.8×10^{-2}		Modarresi et al. (2007)	Q	67
	1.3×10^{-1}		Fang Lee (2007)	Q	721
	4.7×10^{-2}		Fang Lee (2007)	Q	722
	5.8×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.9×10^{-2}		Dunnivant et al. (1992)	Q	
	1.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	5.8×10^{-2}		Duchowicz et al. (2020)	?	185, 21
3,4,4'-trichlorobiphenyl	9.9×10^{-2}		Brunner et al. (1990)	M	
$C_{12}H_7Cl_3$	6.5×10^{-2}		Murphy et al. (1987)	M	12
(PCB-37)	1.2×10^{-2}		Atlas et al. (1982)	M	679
[38444-90-5]	1.3×10^{-2}	5400	Paasivirta and Sinkkonen (2009)	V	
YZANRISAORXTHU-UHFFFAOYSA-N	1.2×10^{-2}		Shiu and Mackay (1986)	V	
	1.4×10^{-1}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	67
	4.8×10^{-2}		Fang Lee (2007)	Q	721
	6.1×10^{-2}		Fang Lee (2007)	Q	722
	6.5×10^{-2}		Dunnivant et al. (1992)	Q	
	6.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	9.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
3,4,5-trichlorobiphenyl	1.2×10^{-2}	5400	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_7Cl_3$	1.3×10^{-1}		Burkhard et al. (1985)	V	
(PCB-38)	8.8×10^{-2}		Fang Lee (2007)	Q	721
[53555-66-1]	5.2×10^{-2}		Fang Lee (2007)	Q	722
BSFZSQRJGZHMMV-UHFFFAOYSA-N	4.2×10^{-2}		Dunnivant et al. (1992)	Q	
	4.8×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4',5-trichlorobiphenyl	1.2×10^{-2}	5600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_7Cl_3$	8.0×10^{-2}		Burkhard et al. (1985)	V	
(PCB-39)	6.6×10^{-2}		Fang Lee (2007)	Q	721
[38444-88-1]	4.4×10^{-2}		Fang Lee (2007)	Q	722
SYSBNFJJSJLZMM-UHFFFAOYSA-N	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	2.3×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,3'-tetrachlorobiphenyl	3.6×10^{-2}	3600	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	9.9×10^{-2}		Brunner et al. (1990)	M	
(PCB-40)	4.9×10^{-2}		Dunnivant et al. (1988)	M	
[38444-93-8]	4.9×10^{-2}		Dunnivant and Elzerman (1988)	M	723
VTLYHLREPCPDKX-UHFFFAOYSA-N	6.1×10^{-2}		Murphy et al. (1987)	M	12
	8.2×10^{-2}		Oliver (1985)	M	
	1.8×10^{-3}	5300	Paasivirta and Sinkkonen (2009)	V	
	4.6×10^{-2}		Mackay et al. (2006b)	V	
	4.6×10^{-2}		Mackay et al. (1992a)	V	
	4.5×10^{-2}		Shiu and Mackay (1986)	V	
	4.9×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.9×10^{-1}		Duchowicz et al. (2020)	Q	299
	1.1×10^{-1}		Hilal et al. (2008)	Q	
	6.8×10^{-2}		Modarresi et al. (2007)	Q	67
	1.2×10^{-1}		Fang Lee (2007)	Q	721
	9.7×10^{-2}		Fang Lee (2007)	Q	722
	2.3×10^{-1}		Yaffe et al. (2003)	Q	248, 272
	6.5×10^{-2}		English and Carroll (2001)	Q	230, 231
	5.4×10^{-2}		Dunnivant et al. (1992)	Q	
	9.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,2',3,4-tetrachlorobiphenyl	4.9×10^{-2}		Murphy et al. (1987)	M	12
$C_{12}H_6Cl_4$	1.6×10^{-2}	6200	Paasivirta and Sinkkonen (2009)	V	
(PCB-41)	4.2×10^{-2}		Burkhard et al. (1985)	V	
[52663-59-9]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
SEWHDNLIHDBVDZ-UHFFFAOYSA-N	1.4×10^{-1}		Duchowicz et al. (2020)	Q	184
	6.9×10^{-2}		Hilal et al. (2008)	Q	
	8.7×10^{-2}		Modarresi et al. (2007)	Q	67
	7.9×10^{-2}		Fang Lee (2007)	Q	721
	7.1×10^{-2}		Fang Lee (2007)	Q	722
	4.0×10^{-2}		Dunnivant et al. (1992)	Q	
	4.8×10^{-2}		Sabljić and Güsten (1989)	Q	
	7.0×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,2',3,4'-tetrachlorobiphenyl	2.8×10^{-2}	3100	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	5.0×10^{-2}		Murphy et al. (1987)	M	12
(PCB-42)	8.6×10^{-3}	5900	Paasivirta and Sinkkonen (2009)	V	
[36559-22-5]	3.4×10^{-2}		Burkhard et al. (1985)	V	
ALFHIHDQSYXSGP-UHFFFAOYSA-N	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	299
	7.2×10^{-2}		Hilal et al. (2008)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.1×10^{-2}		Modarresi et al. (2007)	Q	67
	6.0×10^{-2}		Fang Lee (2007)	Q	721
	6.7×10^{-2}		Fang Lee (2007)	Q	722
	3.9×10^{-2}		Dunnivant et al. (1992)	Q	
	3.1×10^{-2}		Sabljić and Güsten (1989)	Q	
	7.0×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,2',3,5-tetrachlorobiphenyl	1.3×10^{-2}	6300	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	2.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-43)	1.1×10^{-1}		Fang Lee (2007)	Q	721
[70362-46-8]	6.1×10^{-2}		Fang Lee (2007)	Q	722
NRBNBYFPJCCKTO-UHFFFAOYSA-N	2.9×10^{-2}		Dunnivant et al. (1992)	Q	
	2.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,5'-tetrachlorobiphenyl	5.4×10^{-3}		Bhangare et al. (2019)	M	725
$C_{12}H_6Cl_4$	3.4×10^{-2}		Bhangare et al. (2019)	M	726
(PCB-44)	3.6×10^{-2}	3100	Bamford et al. (2000)	M	
[41464-39-5]	5.2×10^{-2}		Murphy et al. (1987)	M	12
ALDJIKXAHSDLLB-UHFFFAOYSA-N	4.1×10^{-2}		Murphy et al. (1983a)	M	24
	1.3×10^{-2}		Atlas et al. (1982)	M	679
	1.1×10^{-2}	6000	Paasivirta and Sinkkonen (2009)	V	
	2.0×10^{-2}		Shiu and Mackay (1986)	V	
	3.0×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	184
	9.7×10^{-2}		Hilal et al. (2008)	Q	
	7.7×10^{-2}		Modarresi et al. (2007)	Q	67
	1.2×10^{-1}		Fang Lee (2007)	Q	721
	6.7×10^{-2}		Fang Lee (2007)	Q	722
		4600	Kühne et al. (2005)	Q	
	4.3×10^{-2}		Dunnivant et al. (1992)	Q	
	3.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	7.0×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		3400	Kühne et al. (2005)	?	
2,2',3,6-tetrachlorobiphenyl	2.5×10^{-2}	2900	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	3.8×10^{-3}	6000	Paasivirta and Sinkkonen (2009)	V	
(PCB-45)	9.9×10^{-3}		Burkhard et al. (1985)	V	
[70362-45-7]	6.7×10^{-2}		Fang Lee (2007)	Q	721
VHGHHZZTMJLTJX-UHFFFAOYSA-N	5.1×10^{-2}		Fang Lee (2007)	Q	722
	2.8×10^{-2}		Dunnivant et al. (1992)	Q	
	3.1×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,6'-tetrachlorobiphenyl	3.0×10^{-2}	3400	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	3.8×10^{-2}		Murphy et al. (1987)	M	12
(PCB-46)	9.1×10^{-4}	5300	Paasivirta and Sinkkonen (2009)	V	
[41464-47-5]	1.4×10^{-2}		Burkhard et al. (1985)	V	
CUGLICQCTXWQNF-UHFFFAOYSA-N	6.7×10^{-2}		Fang Lee (2007)	Q	721
	5.7×10^{-2}		Fang Lee (2007)	Q	722
	2.9×10^{-2}		Dunnivant et al. (1992)	Q	
	2.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',4,4'-tetrachlorobiphenyl	2.1×10^{-1}		Lau et al. (2006)	M	719
$C_{12}H_6Cl_4$	9.1×10^{-3}		Lau et al. (2006)	M	720
(PCB-47)	1.8×10^{-1}	-6000	Charles and Destaillats (2005)	M	
[2437-79-8]	5.2×10^{-2}		Brunner et al. (1990)	M	
QORAVNMWUNPXAO-UHFFFAOYSA-N	2.0×10^{-2}	6200	Paasivirta and Sinkkonen (2009)	V	
	5.7×10^{-2}		Mackay et al. (2006b)	V	
	5.8×10^{-2}		Mackay et al. (1992a)	V	
	2.0×10^{-3}		Hwang et al. (1992)	V	
	5.9×10^{-2}		Shiu and Mackay (1986)	V	
	2.3×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	6.6×10^{-2}		Duchowicz et al. (2020)	Q	299
	5.0×10^{-2}		Hilal et al. (2008)	Q	
	8.2×10^{-2}		Modarresi et al. (2007)	Q	67
	3.5×10^{-2}		Fang Lee (2007)	Q	721
	4.8×10^{-2}		Fang Lee (2007)	Q	722
	2.7×10^{-2}		Dunnivant et al. (1992)	Q	
	2.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	5.2×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,2',4,5-tetrachlorobiphenyl	2.7×10^{-2}	3000	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	3.9×10^{-2}		Murphy et al. (1987)	M	12
(PCB-48)	6.1×10^{-3}	6100	Paasivirta and Sinkkonen (2009)	V	
[70362-47-9]	2.5×10^{-2}		Burkhard et al. (1985)	V	
XBTHILIDLBPRPM-UHFFFAOYSA-N	6.3×10^{-2}		Fang Lee (2007)	Q	721
	5.3×10^{-2}		Fang Lee (2007)	Q	722
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	3.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',4,5'-tetrachlorobiphenyl	2.7×10^{-2}	3000	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	3.6×10^{-2}		Murphy et al. (1987)	M	12
(PCB-49)	4.9×10^{-2}		Murphy et al. (1983a)	M	24
[41464-40-8]	8.3×10^{-3}	5900	Paasivirta and Sinkkonen (2009)	V	
ZWPVHELAQPIZHO-UHFFFAOYSA-N	5.0×10^{-2}		Shiu and Mackay (1986)	V	
	2.1×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	6.1×10^{-2}		Duchowicz et al. (2020)	Q	299
	6.1×10^{-2}		Hilal et al. (2008)	Q	
	7.6×10^{-2}		Modarresi et al. (2007)	Q	67
	7.0×10^{-2}		Fang Lee (2007)	Q	721

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.5×10^{-2}		Fang Lee (2007)	Q	722
	2.8×10^{-2}		Dunnivant et al. (1992)	Q	
	2.6×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.7×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,2',4,6-tetrachlorobiphenyl	1.6×10^{-2}	2900	Bamford et al. (2000)	M	
$C_{12}H_6Cl_4$	1.3×10^{-2}		Atlas et al. (1982)	M	679
(PCB-50)	9.9×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
[62796-65-0]	1.3×10^{-2}		Shiu and Mackay (1986)	V	
VLLVVZDKBSYMCG-UHFFFAOYSA-N	7.3×10^{-3}		Burkhard et al. (1985)	V	
	3.1×10^{-2}		Bhangare et al. (2019)	Q	
	3.9×10^{-2}		Fang Lee (2007)	Q	721
	2.8×10^{-2}		Fang Lee (2007)	Q	722
		3600	Kühne et al. (2005)	Q	
	1.6×10^{-2}		Dunnivant et al. (1992)	Q	
	1.7×10^{-2}		Sabljić and Güsten (1989)	Q	
		3100	Kühne et al. (2005)	?	
2,2',4,6'-tetrachlorobiphenyl	2.5×10^{-2}	6300	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	9.9×10^{-3}		Burkhard et al. (1985)	V	
(PCB-51)	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
[68194-04-7]	6.6×10^{-2}		Duchowicz et al. (2020)	Q	184
WVHNUGRFECMVLQ-UHFFFAOYSA-N	7.3×10^{-2}		Hilal et al. (2008)	Q	
	5.9×10^{-2}		Modarresi et al. (2007)	Q	67
	3.8×10^{-2}		Fang Lee (2007)	Q	721
	4.0×10^{-2}		Fang Lee (2007)	Q	722
	1.9×10^{-2}		Dunnivant et al. (1992)	Q	
	2.0×10^{-2}		Sabljić and Güsten (1989)	Q	
	7.0×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,2',5,5'-tetrachlorobiphenyl	3.5×10^{-2}	6600	Li et al. (2003)	L	366
$C_{12}H_6Cl_4$	4.0×10^{-2}	6800	Li et al. (2003)	L	367
(PCB-52)	4.9×10^{-3}		Bhangare et al. (2019)	M	725
[35693-99-3]	2.9×10^{-2}		Bhangare et al. (2019)	M	726
HCWZEPKLWVAEOV-UHFFFAOYSA-N	3.2×10^{-2}	3700	Bamford et al. (2000)	M	
	4.2×10^{-2}	6200	ten Hulscher et al. (1992)	M	
	4.9×10^{-2}		Brunner et al. (1990)	M	
	2.9×10^{-2}		Dunnivant et al. (1988)	M	
	2.9×10^{-2}		Dunnivant and Elzerman (1988)	M	723
	4.1×10^{-2}		Murphy et al. (1987)	M	12
	8.2×10^{-2}		Oliver (1985)	M	
	4.5×10^{-2}		Murphy et al. (1983a)	M	24
	1.1×10^{-2}		Atlas et al. (1982)	M	679
			Westcott et al. (1981)	M	727
	3.7×10^{-3}	5700	Paasivirta and Sinkkonen (2009)	V	
	2.1×10^{-2}		Mackay et al. (2006b)	V	
	2.1×10^{-2}		Mackay et al. (1992a)	V	
	1.2×10^{-1}		McLachlan et al. (1990)	V	373
	2.1×10^{-2}		Shiu and Mackay (1986)	V	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.9×10^{-2}		Burkhard et al. (1985)	V	
	1.2×10^{-2}	7700	Paasivirta et al. (1999)	T	
	3.8×10^{-2}		Murphy et al. (1983b)	X	724, 24
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	5.6×10^{-2}		Duchowicz et al. (2020)	Q	184
	7.9×10^{-2}		Hilal et al. (2008)	Q	
	6.5×10^{-2}		Modarresi et al. (2007)	Q	67
	9.7×10^{-2}		Fang Lee (2007)	Q	721
	4.6×10^{-2}		Fang Lee (2007)	Q	722
		4200	Kühne et al. (2005)	Q	
	3.1×10^{-2}		Dunnivant et al. (1992)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		4900	Kühne et al. (2005)	?	
2,2',5,6'-tetrachlorobiphenyl $C_{12}H_6Cl_4$ (PCB-53) [41464-41-9] SFTUSTXGTCCSHX-UHFFFAOYSA-N	2.4×10^{-2}		Dunnivant et al. (1988)	M	
	2.4×10^{-2}		Dunnivant and Elzerman (1988)	M	723
	3.5×10^{-2}		Murphy et al. (1987)	M	12
	3.3×10^{-2}		Murphy et al. (1983a)	M	24
	5.4×10^{-2}		Duchowicz et al. (2020)	V	186
	1.6×10^{-3}	5500	Paasivirta and Sinkkonen (2009)	V	
	3.3×10^{-2}		Shiu and Mackay (1986)	V	
	8.9×10^{-3}		Burkhard et al. (1985)	V	
	6.1×10^{-2}		Duchowicz et al. (2020)	Q	
	8.8×10^{-2}		Hilal et al. (2008)	Q	
	5.9×10^{-2}		Modarresi et al. (2007)	Q	67
	5.3×10^{-2}		Fang Lee (2007)	Q	721
	4.1×10^{-2}		Fang Lee (2007)	Q	722
	2.3×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',6,6'-tetrachlorobiphenyl $C_{12}H_6Cl_4$ (PCB-54) [15968-05-5] PXAGFNRKXSYIHU-UHFFFAOYSA-N	4.9×10^{-2}		Brunner et al. (1990)	M	
	1.8×10^{-2}		Dunnivant et al. (1988)	M	
	1.8×10^{-2}		Dunnivant and Elzerman (1988)	M	723
	1.0×10^{-4}	4800	Paasivirta and Sinkkonen (2009)	V	
	5.3×10^{-3}		Burkhard et al. (1985)	V	
	6.7×10^{-2}		Dunnivant et al. (1988)	C	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	6.6×10^{-2}		Duchowicz et al. (2020)	Q	184
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	6.5×10^{-2}		Modarresi et al. (2007)	Q	67
	3.3×10^{-2}		Fang Lee (2007)	Q	721
	2.7×10^{-2}		Fang Lee (2007)	Q	722
	5.2×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.7×10^{-2}		Dunnivant et al. (1992)	Q	
	4.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',4-tetrachlorobiphenyl	9.6×10^{-3}	5900	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	8.7×10^{-2}		Burkhard et al. (1985)	V	
(PCB-55)	9.9×10^{-2}		Fang Lee (2007)	Q	721
[74338-24-2]	9.3×10^{-2}		Fang Lee (2007)	Q	722
ZKGSEEWIVLAUNH-UHFFFAOYSA-N	5.4×10^{-2}		Dunnivant et al. (1992)	Q	
	4.3×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',4'-tetrachlorobiphenyl	3.8×10^{-2}	3800	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	6.1×10^{-2}		Murphy et al. (1987)	M	12
(PCB-56)	4.9×10^{-3}	5400	Paasivirta and Sinkkonen (2009)	V	
[41464-43-1]	1.1×10^{-1}		Burkhard et al. (1985)	V	
UNCGJRRROFURDV-UHFFFAOYSA-N	7.5×10^{-2}		Fang Lee (2007)	Q	721
	9.7×10^{-2}		Fang Lee (2007)	Q	722
	6.5×10^{-2}		Dunnivant et al. (1992)	Q	
	7.5×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',5-tetrachlorobiphenyl	8.9×10^{-3}	6100	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	5.1×10^{-2}		Burkhard et al. (1985)	V	
(PCB-57)	1.4×10^{-1}		Fang Lee (2007)	Q	721
[70424-67-8]	7.8×10^{-2}		Fang Lee (2007)	Q	722
DHDBTLFALXRTLB-UHFFFAOYSA-N	3.6×10^{-2}		Dunnivant et al. (1992)	Q	
	2.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',5'-tetrachlorobiphenyl	2.3×10^{-3}	5400	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	6.2×10^{-2}		Burkhard et al. (1985)	V	
(PCB-58)	1.5×10^{-1}		Fang Lee (2007)	Q	721
[41464-49-7]	8.1×10^{-2}		Fang Lee (2007)	Q	722
IOPBNBSKOPJKEG-UHFFFAOYSA-N	3.9×10^{-2}		Dunnivant et al. (1992)	Q	
	2.4×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',6-tetrachlorobiphenyl	4.4×10^{-2}	6600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	2.9×10^{-2}		Burkhard et al. (1985)	V	
(PCB-59)	8.3×10^{-2}		Fang Lee (2007)	Q	721
[74472-33-6]	8.3×10^{-2}		Fang Lee (2007)	Q	722
WZNAMGYIQPAXDH-UHFFFAOYSA-N	3.2×10^{-2}		Dunnivant et al. (1992)	Q	
	2.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,4,4'-tetrachlorobiphenyl	6.1×10^{-2}		Murphy et al. (1987)	M	12
$C_{12}H_6Cl_4$	1.2×10^{-2}		Atlas et al. (1982)	M	679
(PCB-60)	2.9×10^{-3}	5500	Paasivirta and Sinkkonen (2009)	V	
[33025-41-1]	9.7×10^{-2}		Burkhard et al. (1985)	V	
XLDBTRJKXLKYTC-UHFFFAOYSA-N	4.9×10^{-2}		Fang Lee (2007)	Q	721
	9.2×10^{-2}		Fang Lee (2007)	Q	722
	6.5×10^{-2}		Dunnivant et al. (1992)	Q	
	6.5×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4,5-tetrachlorobiphenyl	4.9×10^{-2}	6600	Li et al. (2003)	L	366
$C_{12}H_6Cl_4$	5.0×10^{-2}	7200	Li et al. (2003)	L	367
(PCB-61)	9.6×10^{-3}		Duchowicz et al. (2020)	V	186
[33284-53-6]	4.9×10^{-3}	5600	Paasivirta and Sinkkonen (2009)	V	
HLQDGCWIOSOMDP-UHFFFAOYSA-N	8.7×10^{-2}		Burkhard et al. (1985)	V	
	9.6×10^{-2}		Duchowicz et al. (2020)	Q	
	9.0×10^{-2}		Fang Lee (2007)	Q	721
	8.4×10^{-2}		Fang Lee (2007)	Q	722
	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
	5.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,4,6-tetrachlorobiphenyl	4.7×10^{-2}		Brunner et al. (1990)	M	
$C_{12}H_6Cl_4$	7.1×10^{-3}	6000	Paasivirta and Sinkkonen (2009)	V	
(PCB-62)	3.3×10^{-2}		Burkhard et al. (1985)	V	
[54230-22-7]	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
HOBRTVXSIVSXIA-UHFFFAOYSA-N	5.7×10^{-2}		Duchowicz et al. (2020)	Q	299
	4.0×10^{-2}		Hilal et al. (2008)	Q	
	1.8×10^{-1}		Modarresi et al. (2007)	Q	67
	5.5×10^{-2}		Fang Lee (2007)	Q	721
	6.4×10^{-2}		Fang Lee (2007)	Q	722
	2.7×10^{-2}		Dunnivant et al. (1992)	Q	
	2.7×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.7×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,3,4',5-tetrachlorobiphenyl	2.5×10^{-2}	3000	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	3.4×10^{-2}		Murphy et al. (1987)	M	12
(PCB-63)	9.4×10^{-3}	6100	Paasivirta and Sinkkonen (2009)	V	
[74472-34-7]	5.6×10^{-2}		Burkhard et al. (1985)	V	
CITMYAMXIZQCJD-UHFFFAOYSA-N	6.8×10^{-2}		Fang Lee (2007)	Q	721
	7.1×10^{-2}		Fang Lee (2007)	Q	722
	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
	3.4×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,4',6-tetrachlorobiphenyl	2.5×10^{-2}	2900	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	5.8×10^{-2}		Murphy et al. (1987)	M	12
(PCB-64)	7.9×10^{-3}	6000	Paasivirta and Sinkkonen (2009)	V	
[52663-58-8]	3.2×10^{-2}		Burkhard et al. (1985)	V	
FXRXQYZZALWWGA-UHFFFAOYSA-N	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	7.7×10^{-2}		Duchowicz et al. (2020)	Q	299
	1.1×10^{-1}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	67
	4.2×10^{-2}		Fang Lee (2007)	Q	721
	7.7×10^{-2}		Fang Lee (2007)	Q	722
	3.6×10^{-2}		Dunnivant et al. (1992)	Q	
	3.5×10^{-2}		Sabljić and Güsten (1989)	Q	
	7.0×10^{-2}		Duchowicz et al. (2020)	?	185, 21

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,5,6-tetrachlorobiphenyl	4.9×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	3.7×10^{-2}		Burkhard et al. (1985)	V	
(PCB-65)	5.3×10^{-2}		Hilal et al. (2008)	Q	
[33284-54-7]	1.4×10^{-1}		Modarresi et al. (2007)	Q	67
BLAYIQLVUNIICD-UHFFFAOYSA-N	7.6×10^{-2}		Fang Lee (2007)	Q	721
	9.9×10^{-2}		Fang Lee (2007)	Q	722
	2.9×10^{-2}		Dunnivant et al. (1992)	Q	
	3.2×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3',4,4'-tetrachlorobiphenyl	2.7×10^{-2}	3500	Bamford et al. (2000)	M	
$C_{12}H_6Cl_4$	4.9×10^{-2}		Murphy et al. (1987)	M	12
(PCB-66)	3.0×10^{-3}	5300	Paasivirta and Sinkkonen (2009)	V	
[32598-10-0]	1.2×10^{-2}		Shiu and Mackay (1986)	V	
RKLLTEAEZIJBAU-UHFFFAOYSA-N	7.3×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	299
	2.9×10^{-2}		Bhangare et al. (2019)	Q	
	2.1×10^{-1}		Hilal et al. (2008)	Q	
	8.5×10^{-2}		Modarresi et al. (2007)	Q	67
	4.3×10^{-2}		Fang Lee (2007)	Q	721
	6.8×10^{-2}		Fang Lee (2007)	Q	722
		5200	Kühne et al. (2005)	Q	
	4.9×10^{-2}		Dunnivant et al. (1992)	Q	
	3.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	8.2×10^{-2}		Duchowicz et al. (2020)	?	185, 21
		3800	Kühne et al. (2005)	?	
2,3',4,5-tetrachlorobiphenyl	9.9×10^{-2}		Brunner et al. (1990)	M	
$C_{12}H_6Cl_4$	1.6×10^{-2}	6200	Paasivirta and Sinkkonen (2009)	V	
(PCB-67)	5.2×10^{-2}		Burkhard et al. (1985)	V	
[73575-53-8]	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
LQEGJNOKOZHBBZ-UHFFFAOYSA-N	7.7×10^{-2}		Duchowicz et al. (2020)	Q	299
	1.9×10^{-1}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	67
	7.9×10^{-2}		Fang Lee (2007)	Q	721
	6.8×10^{-2}		Fang Lee (2007)	Q	722
	4.2×10^{-2}		Dunnivant et al. (1992)	Q	
	3.4×10^{-2}		Sabljić and Güsten (1989)	Q	
	9.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,3',4,5'-tetrachlorobiphenyl	7.2×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	4.3×10^{-2}		Burkhard et al. (1985)	V	
(PCB-68)	8.7×10^{-2}		Fang Lee (2007)	Q	721
[73575-52-7]	5.2×10^{-2}		Fang Lee (2007)	Q	722
KTTXLLZIBIDUCR-UHFFFAOYSA-N	2.6×10^{-2}		Dunnivant et al. (1992)	Q	
	1.8×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3',4,6-tetrachlorobiphenyl	1.9×10^{-2}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	2.1×10^{-2}		Burkhard et al. (1985)	V	
(PCB-69)	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
[60233-24-1]	5.0×10^{-2}		Duchowicz et al. (2020)	Q	
CKUBKYSLNCKBOI-UHFFFAOYSA-N	7.9×10^{-2}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	67
	4.8×10^{-2}		Fang Lee (2007)	Q	721
	4.5×10^{-2}		Fang Lee (2007)	Q	722
	2.0×10^{-2}		Dunnivant et al. (1992)	Q	
	1.6×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.7×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,3',4',5-tetrachlorobiphenyl	3.3×10^{-2}	3500	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	9.9×10^{-2}		Brunner et al. (1990)	M	
(PCB-70)	5.2×10^{-2}		Murphy et al. (1987)	M	12
[32598-11-1]	1.1×10^{-1}		Brownawell (1986)	M	294
KENZYIHFBRWMOD-UHFFFAOYSA-N	4.9×10^{-2}		Murphy et al. (1983a)	M	24
	4.0×10^{-3}	5400	Paasivirta and Sinkkonen (2009)	V	
	5.0×10^{-2}		Shiu and Mackay (1986)	V	
	6.5×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.0×10^{-1}		Duchowicz et al. (2020)	Q	299
	2.0×10^{-1}		Hilal et al. (2008)	Q	
	7.2×10^{-2}		Modarresi et al. (2007)	Q	67
	6.0×10^{-2}		Fang Lee (2007)	Q	721
	6.4×10^{-2}		Fang Lee (2007)	Q	722
	4.9×10^{-2}		Dunnivant et al. (1992)	Q	
	5.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	9.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,3',4',6-tetrachlorobiphenyl	1.8×10^{-2}	6000	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	4.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-71)	3.6×10^{-2}		Fang Lee (2007)	Q	721
[41464-46-4]	7.0×10^{-2}		Fang Lee (2007)	Q	722
WYVBETQIUHPLFO-UHFFFAOYSA-N	3.1×10^{-2}		Dunnivant et al. (1992)	Q	
	3.1×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3',5,5'-tetrachlorobiphenyl	4.0×10^{-3}	5700	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	3.9×10^{-2}		Burkhard et al. (1985)	V	
(PCB-72)	1.2×10^{-1}		Fang Lee (2007)	Q	721
[41464-42-0]	5.3×10^{-2}		Fang Lee (2007)	Q	722
WBTMFEPLVQOWFI-UHFFFAOYSA-N	2.7×10^{-2}		Dunnivant et al. (1992)	Q	
	2.1×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3',5',6-tetrachlorobiphenyl	6.4×10^{-3}	5900	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	2.6×10^{-2}		Burkhard et al. (1985)	V	
(PCB-73)	7.4×10^{-2}		Fang Lee (2007)	Q	721
[74338-23-1]	6.0×10^{-2}		Fang Lee (2007)	Q	722
HDULUCZRGGWTMZ-UHFFFAOYSA-N	1.9×10^{-2}		Dunnivant et al. (1992)	Q	
	1.6×10^{-2}		Sabljić and Güsten (1989)	Q	
2,4,4',5-tetrachlorobiphenyl	2.6×10^{-2}	3000	Bamford et al. (2002)	M	
$C_{12}H_6Cl_4$	9.9×10^{-2}		Brunner et al. (1990)	M	
(PCB-74)	4.7×10^{-2}		Murphy et al. (1987)	M	12
[32690-93-0]	4.8×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
TULCXSBAPHCWCF-UHFFFAOYSA-N	5.8×10^{-2}		Burkhard et al. (1985)	V	
	4.5×10^{-2}		Keshavarz et al. (2022)	Q	
	7.7×10^{-2}		Duchowicz et al. (2020)	Q	184
	2.0×10^{-1}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	67
	3.9×10^{-2}		Fang Lee (2007)	Q	721
	6.5×10^{-2}		Fang Lee (2007)	Q	722
	4.6×10^{-2}		Dunnivant et al. (1992)	Q	
	4.7×10^{-2}		Sabljić and Güsten (1989)	Q	
	9.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,4,4',6-tetrachlorobiphenyl	2.1×10^{-2}	6400	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	2.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-75)	2.4×10^{-2}		Fang Lee (2007)	Q	721
[32598-12-2]	4.4×10^{-2}		Fang Lee (2007)	Q	722
RZFZBHKDGHISSH-UHFFFAOYSA-N	2.1×10^{-2}		Dunnivant et al. (1992)	Q	
	1.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3',4',5'-tetrachlorobiphenyl	7.7×10^{-2}		Murphy et al. (1987)	M	12
$C_{12}H_6Cl_4$	2.3×10^{-3}	5500	Paasivirta and Sinkkonen (2009)	V	
(PCB-76)	8.2×10^{-2}		Burkhard et al. (1985)	V	
[70362-48-0]	1.4×10^{-1}		Fang Lee (2007)	Q	721
QILUYCYPNYWMIL-UHFFFAOYSA-N	7.0×10^{-2}		Fang Lee (2007)	Q	722
	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
	4.4×10^{-2}		Sabljić and Güsten (1989)	Q	
3,3',4,4'-tetrachlorobiphenyl	1.2×10^{-2}		Bhangare et al. (2019)	M	725
$C_{12}H_6Cl_4$	7.1×10^{-2}		Bhangare et al. (2019)	M	726
(PCB-77)	3.1×10^{-2}		Lau et al. (2006)	M	719
[32598-13-3]	1.8×10^{-2}		Lau et al. (2006)	M	720
UQMGJOKDKOLIDP-UHFFFAOYSA-N	9.1×10^{-2}		Fang et al. (2006)	M	
	2.9×10^{-2}	13000	Charles and Destaillats (2005)	M	33
	6.2×10^{-2}	4800	Bamford et al. (2000)	M	
	1.0×10^{-1}		Dunnivant et al. (1988)	M	
	1.0×10^{-1}		Dunnivant and Elzerman (1988)	M	723
	6.0×10^{-4}	4600	Paasivirta and Sinkkonen (2009)	V	
	5.8×10^{-2}		Mackay et al. (2006b)	V	
	5.8×10^{-1}		Mackay et al. (1992a)	V	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.9×10^{-1}		Shiu and Mackay (1986)	V	
	2.3×10^{-1}		Burkhard et al. (1985)	V	
	8.3×10^{-3}	7400	Paasivirta et al. (1999)	T	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.9×10^{-1}		Duchowicz et al. (2020)	Q	
	3.6×10^{-1}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	67
	9.4×10^{-2}		Fang Lee (2007)	Q	721
	8.0×10^{-2}		Fang Lee (2007)	Q	722
		6100	Kühne et al. (2005)	Q	
	9.6×10^{-2}		Dunnivant et al. (1992)	Q	
	7.9×10^{-2}		Meylan and Howard (1991)	Q	
	1.0		Duchowicz et al. (2020)	?	185, 21
		5600	Kühne et al. (2005)	?	
3,3',4,5-tetrachlorobiphenyl	5.1×10^{-3}	5600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	1.7×10^{-1}		Burkhard et al. (1985)	V	
(PCB-78)	1.7×10^{-1}		Fang Lee (2007)	Q	721
[70362-49-1]	7.5×10^{-2}		Fang Lee (2007)	Q	722
SXFLURRQRFKBNN-UHFFFAOYSA-N	6.0×10^{-2}		Dunnivant et al. (1992)	Q	
	4.4×10^{-2}		Sabljić and Güsten (1989)	Q	
3,3',4,5'-tetrachlorobiphenyl	3.8×10^{-3}	5400	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	1.4×10^{-1}		Burkhard et al. (1985)	V	
(PCB-79)	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
[41464-48-6]	1.1×10^{-1}		Duchowicz et al. (2020)	Q	299
QLCTXEMDCZGPCG-UHFFFAOYSA-N	2.5×10^{-1}		Hilal et al. (2008)	Q	
	8.2×10^{-2}		Modarresi et al. (2007)	Q	67
	1.9×10^{-1}		Fang Lee (2007)	Q	721
	6.3×10^{-2}		Fang Lee (2007)	Q	722
	5.0×10^{-2}		Dunnivant et al. (1992)	Q	
	2.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	?	185, 21
3,3',5,5'-tetrachlorobiphenyl	9.4×10^{-4}	5100	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_6Cl_4$	8.0×10^{-2}		Burkhard et al. (1985)	V	
(PCB-80)	2.6×10^{-1}		Fang Lee (2007)	Q	721
[33284-52-5]	5.2×10^{-2}		Fang Lee (2007)	Q	722
UTMWFJSRHLYRPY-UHFFFAOYSA-N	2.6×10^{-2}		Dunnivant et al. (1992)	Q	
	1.6×10^{-2}		Sabljić and Güsten (1989)	Q	
3,4,4',5-tetrachlorobiphenyl	8.8×10^{-2}		Fang et al. (2006)	M	
$C_{12}H_6Cl_4$	4.1×10^{-2}	4000	Bamford et al. (2002)	M	
(PCB-81)	2.0×10^{-3}	5300	Paasivirta and Sinkkonen (2009)	V	
[70362-50-4]	1.9×10^{-1}		Burkhard et al. (1985)	V	
BHWVLZJTVIYLIV-UHFFFAOYSA-N	8.6×10^{-2}		Fang Lee (2007)	Q	721
	7.2×10^{-2}		Fang Lee (2007)	Q	722
	6.9×10^{-2}		Dunnivant et al. (1992)	Q	
	6.7×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4-pentachlorobiphenyl	2.7×10^{-2}	5100	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	8.4×10^{-2}		Murphy et al. (1987)	M	12
(PCB-82)	4.9×10^{-2}		Murphy et al. (1983a)	M	24
[52663-62-4]	3.2×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
AUGNBQPSMWGAJE-UHFFFAOYSA-N	5.0×10^{-2}		Shiu and Mackay (1986)	V	
	8.0×10^{-2}		Burkhard et al. (1985)	V	
	1.6×10^{-1}		Fang Lee (2007)	Q	721
	1.5×10^{-1}		Fang Lee (2007)	Q	722
	6.7×10^{-2}		Dunnivant et al. (1992)	Q	
	8.1×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,3',5-pentachlorobiphenyl	2.3×10^{-2}	3600	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	6.0×10^{-2}		Murphy et al. (1987)	M	12
(PCB-83)	7.7×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
[60145-20-2]	4.7×10^{-2}		Burkhard et al. (1985)	V	
SUBRHHYLRGOTHL-UHFFFAOYSA-N	2.2×10^{-1}		Fang Lee (2007)	Q	721
	1.4×10^{-1}		Fang Lee (2007)	Q	722
	4.7×10^{-2}		Dunnivant et al. (1992)	Q	
	3.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,3',6-pentachlorobiphenyl	5.7×10^{-2}		Murphy et al. (1987)	M	12
$C_{12}H_5Cl_5$	2.3×10^{-3}	6000	Paasivirta and Sinkkonen (2009)	V	
(PCB-84)	1.9×10^{-2}		Burkhard et al. (1985)	V	
[52663-60-2]	1.3×10^{-1}		Fang Lee (2007)	Q	721
QVWUJLANSDKRAH-UHFFFAOYSA-N	1.2×10^{-1}		Fang Lee (2007)	Q	722
	3.9×10^{-2}		Dunnivant et al. (1992)	Q	
	4.3×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4,4'-pentachlorobiphenyl	2.3×10^{-2}	3100	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	1.5×10^{-1}		Brunner et al. (1990)	M	
(PCB-85)	6.0×10^{-2}		Murphy et al. (1987)	M	12
[65510-45-4]	2.8×10^{-2}	6600	Paasivirta and Sinkkonen (2009)	V	
LACXVZHAJMVESG-UHFFFAOYSA-N	5.6×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.6×10^{-1}		Duchowicz et al. (2020)	Q	
	9.2×10^{-2}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	67
	7.8×10^{-2}		Fang Lee (2007)	Q	721
	1.1×10^{-1}		Fang Lee (2007)	Q	722
	5.1×10^{-2}		Dunnivant et al. (1992)	Q	
	4.0×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.5×10^{-1}		Duchowicz et al. (2020)	?	185, 21

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,5-pentachlorobiphenyl	3.2×10^{-3}		Duchowicz et al. (2020)	V	186
$C_{12}H_5Cl_5$	8.9×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
(PCB-86)	6.6×10^{-3}		Mackay et al. (2006b)	V	
[55312-69-1]	6.6×10^{-3}		Mackay et al. (1992a)	V	
AIURIRUDHVDRFQ-UHFFFAOYSA-N	6.6×10^{-3}		Shiu and Mackay (1986)	V	
	1.2×10^{-2}		Burkhard et al. (1985)	V	
	1.4×10^{-1}		Duchowicz et al. (2020)	Q	
	7.5×10^{-2}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Fang Lee (2007)	Q	721
	1.2×10^{-1}		Fang Lee (2007)	Q	722
	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
	5.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4,5'-pentachlorobiphenyl	2.7×10^{-2}	3900	Bamford et al. (2000)	M	
$C_{12}H_5Cl_5$	7.8×10^{-2}		Murphy et al. (1987)	M	12
(PCB-87)	1.4×10^{-1}		Brownawell (1986)	M	294
[38380-02-8]	3.0×10^{-2}		Murphy et al. (1983a)	M	24
OPKYDBFRKPQCBS-UHFFFAOYSA-N	4.1×10^{-3}	6000	Paasivirta and Sinkkonen (2009)	V	
	4.0×10^{-2}		Mackay et al. (2006b)	V	
	4.0×10^{-2}		Mackay et al. (1992a)	V	
	4.0×10^{-2}		Shiu and Mackay (1986)	V	
	5.0×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.5×10^{-1}		Duchowicz et al. (2020)	Q	299
	2.3×10^{-2}		Bhangare et al. (2019)	Q	
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Fang Lee (2007)	Q	721
	1.0×10^{-1}		Fang Lee (2007)	Q	722
		5000	Kühne et al. (2005)	Q	
	5.4×10^{-2}		Dunnivant et al. (1992)	Q	
	5.5×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.3×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		4200	Kühne et al. (2005)	?	
2,2',3,4,6-pentachlorobiphenyl	9.6×10^{-3}	6800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	7.3×10^{-3}		Burkhard et al. (1985)	V	
(PCB-88)	1.2×10^{-1}		Fang Lee (2007)	Q	721
[55215-17-3]	7.8×10^{-2}		Fang Lee (2007)	Q	722
QGDKRLQRLFUJPP-UHFFFAOYSA-N	2.6×10^{-2}		Dunnivant et al. (1992)	Q	
	2.9×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4,6'-pentachlorobiphenyl	2.2×10^{-2}	2500	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	4.3×10^{-3}	6100	Paasivirta and Sinkkonen (2009)	V	
(PCB-89)	2.4×10^{-2}		Burkhard et al. (1985)	V	
[73575-57-2]	8.7×10^{-2}		Fang Lee (2007)	Q	721
GLOOIONSKMZYQZ-UHFFFAOYSA-N	9.8×10^{-2}		Fang Lee (2007)	Q	722
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	3.4×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4',5-pentachlorobiphenyl	2.1×10^{-2}	6600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	3.3×10^{-2}		Burkhard et al. (1985)	V	
(PCB-90)	1.1×10^{-1}		Fang Lee (2007)	Q	721
[68194-07-0]	8.8×10^{-2}		Fang Lee (2007)	Q	722
SUOAMBOBSWRMNQ-UHFFFAOYSA-N	3.4×10^{-2}		Dunnivant et al. (1992)	Q	
	2.6×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4',6-pentachlorobiphenyl	1.9×10^{-2}	1200	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	3.6×10^{-2}		Murphy et al. (1987)	M	12
(PCB-91)	1.1×10^{-2}	6500	Paasivirta and Sinkkonen (2009)	V	
[68194-05-8]	1.4×10^{-2}		Burkhard et al. (1985)	V	
CXKIGWXPPVZSQK-UHFFFAOYSA-N	6.6×10^{-2}		Fang Lee (2007)	Q	721
	8.3×10^{-2}		Fang Lee (2007)	Q	722
	2.9×10^{-2}		Dunnivant et al. (1992)	Q	
	2.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,5,5'-pentachlorobiphenyl	2.2×10^{-2}	2900	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	1.2×10^{-2}	6500	Paasivirta and Sinkkonen (2009)	V	
(PCB-92)	3.0×10^{-2}		Burkhard et al. (1985)	V	
[52663-61-3]	2.2×10^{-1}		Fang Lee (2007)	Q	721
CRCBRZBVCDKPGA-UHFFFAOYSA-N	9.5×10^{-2}		Fang Lee (2007)	Q	722
	3.8×10^{-2}		Dunnivant et al. (1992)	Q	
	3.1×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,5,6-pentachlorobiphenyl	4.1×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	8.3×10^{-3}		Burkhard et al. (1985)	V	
(PCB-93)	1.2×10^{-1}		Fang Lee (2007)	Q	721
[73575-56-1]	1.3×10^{-1}		Fang Lee (2007)	Q	722
BMXRLHMJGHJGLR-UHFFFAOYSA-N	2.9×10^{-2}		Dunnivant et al. (1992)	Q	
	3.5×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,5,6'-pentachlorobiphenyl	4.5×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	1.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-94)	1.2×10^{-1}		Fang Lee (2007)	Q	721
[73575-55-0]	9.1×10^{-2}		Fang Lee (2007)	Q	722
FJUVPPYNSDTRQV-UHFFFAOYSA-N	2.5×10^{-2}		Dunnivant et al. (1992)	Q	
	2.3×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,5',6-pentachlorobiphenyl	2.1×10^{-2}	2500	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	5.0×10^{-2}		Murphy et al. (1987)	M	12
(PCB-95)	3.3×10^{-3}	6200	Paasivirta and Sinkkonen (2009)	V	
[38379-99-6]	1.2×10^{-2}		Burkhard et al. (1985)	V	
GXNNLIMMEXHBKV-UHFFFAOYSA-N	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	7.9×10^{-2}		Duchowicz et al. (2020)	Q	
	1.3×10^{-1}		Fang Lee (2007)	Q	721
	9.0×10^{-2}		Fang Lee (2007)	Q	722
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	3.4×10^{-2}		Sabljić and Güsten (1989)	Q	
	8.2×10^{-2}		Duchowicz et al. (2020)	?	185, 21

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,6,6'-pentachlorobiphenyl	8.7×10^{-4}	5800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	7.2×10^{-3}		Burkhard et al. (1985)	V	
(PCB-96)	7.4×10^{-2}		Fang Lee (2007)	Q	721
[73575-54-9]	6.5×10^{-2}		Fang Lee (2007)	Q	722
QQFGAXUIQVKBKU-UHFFFAOYSA-N	2.4×10^{-2}		Dunnivant et al. (1992)	Q	
	2.6×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4',5'-pentachlorobiphenyl	2.3×10^{-2}	3600	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	1.3×10^{-1}		Brunner et al. (1990)	M	
(PCB-97)	6.6×10^{-2}		Murphy et al. (1987)	M	12
[41464-51-1]	8.6×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
JTUSORDQZVOEAZ-UHFFFAOYSA-N	4.8×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.5×10^{-1}		Duchowicz et al. (2020)	Q	
	1.5×10^{-1}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Modarresi et al. (2007)	Q	67
	1.2×10^{-1}		Fang Lee (2007)	Q	721
	1.1×10^{-1}		Fang Lee (2007)	Q	722
	5.5×10^{-2}		Dunnivant et al. (1992)	Q	
	5.5×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.3×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,4',6'-pentachlorobiphenyl	5.5×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	1.5×10^{-2}		Burkhard et al. (1985)	V	
(PCB-98)	7.6×10^{-2}		Fang Lee (2007)	Q	721
[60233-25-2]	6.5×10^{-2}		Fang Lee (2007)	Q	722
GOFFZTAPOOICFT-UHFFFAOYSA-N	2.5×10^{-2}		Dunnivant et al. (1992)	Q	
	2.0×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',4,4',5-pentachlorobiphenyl	2.2×10^{-2}		Lau et al. (2006)	M	719
$C_{12}H_5Cl_5$	4.2×10^{-3}		Lau et al. (2006)	M	720
(PCB-99)	8.8×10^{-3}	8700	Charles and Destaillats (2005)	M	33
[38380-01-7]	2.1×10^{-2}	1900	Bamford et al. (2002)	M	
LMQJBFRGXHMNOX-UHFFFAOYSA-N	1.3×10^{-1}		Brunner et al. (1990)	M	
	4.6×10^{-2}		Murphy et al. (1987)	M	12
	2.1×10^{-2}	6600	Paasivirta and Sinkkonen (2009)	V	
	3.4×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	8.6×10^{-2}		Duchowicz et al. (2020)	Q	299
	6.2×10^{-2}		Fang Lee (2007)	Q	721
	7.9×10^{-2}		Fang Lee (2007)	Q	722
	4.0×10^{-2}		Dunnivant et al. (1992)	Q	
	3.3×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.3×10^{-1}		Duchowicz et al. (2020)	?	185, 21

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',4,4',6-pentachlorobiphenyl	9.7×10^{-3}	6600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	1.0×10^{-2}		Burkhard et al. (1985)	V	
(PCB-100)	3.8×10^{-2}		Fang Lee (2007)	Q	721
[39485-83-1]	4.6×10^{-2}		Fang Lee (2007)	Q	722
RKUAZJIXKHPFRK-UHFFFAOYSA-N	1.8×10^{-2}		Dunnivant et al. (1992)	Q	
	1.6×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',4,5,5'-pentachlorobiphenyl	3.2×10^{-2}	6800	Li et al. (2003)	L	366
$C_{12}H_5Cl_5$	4.1×10^{-2}	7500	Li et al. (2003)	L	367
(PCB-101)	6.9×10^{-3}		Bhangare et al. (2019)	M	725
[37680-73-2]	2.0×10^{-2}		Bhangare et al. (2019)	M	726
LAHWLEDBADHJGA-UHFFFAOYSA-N	2.4×10^{-2}	3600	Bamford et al. (2000)	M	
	3.9×10^{-2}		Dunnivant et al. (1988)	M	
	3.9×10^{-2}		Dunnivant and Elzerman (1988)	M	723
	5.5×10^{-2}		Murphy et al. (1987)	M	12
	1.4×10^{-1}		Oliver (1985)	M	
			Westcott et al. (1981)	M	728
	8.9×10^{-3}	6400	Paasivirta and Sinkkonen (2009)	V	
	2.8×10^{-2}		Mackay et al. (2006b)	V	
	2.8×10^{-2}		Mackay et al. (1992a)	V	
	2.9×10^{-2}		Shiu and Mackay (1986)	V	
	3.1×10^{-2}		Burkhard et al. (1985)	V	
	2.0×10^{-2}	8100	Paasivirta et al. (1999)	T	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	7.9×10^{-2}		Duchowicz et al. (2020)	Q	184
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	67
	1.3×10^{-1}		Fang Lee (2007)	Q	721
	7.9×10^{-2}		Fang Lee (2007)	Q	722
		4600	Kühne et al. (2005)	Q	
	1.2×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	6.1×10^{-2}		English and Carroll (2001)	Q	230, 231
	4.0×10^{-2}		Dunnivant et al. (1992)	Q	
	1.1×10^{-1}		Meylan and Howard (1991)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		3900	Kühne et al. (2005)	?	
2,2',4,5,6'-pentachlorobiphenyl	1.1×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_5Cl_5$	6.3×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
(PCB-102)	1.5×10^{-2}		Burkhard et al. (1985)	V	
[68194-06-9]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
BWWVXHRLMPBDCK-UHFFFAOYSA-N	8.6×10^{-2}		Duchowicz et al. (2020)	Q	
	8.8×10^{-2}		Hilal et al. (2008)	Q	
	1.3×10^{-1}		Modarresi et al. (2007)	Q	67
	6.9×10^{-2}		Fang Lee (2007)	Q	721
	7.7×10^{-2}		Fang Lee (2007)	Q	722
	2.7×10^{-2}		Dunnivant et al. (1992)	Q	
	2.8×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

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	1.1×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',4,5',6-pentachlorobiphenyl	8.1×10^{-3}	6600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	9.1×10^{-3}		Burkhard et al. (1985)	V	
(PCB-103)	7.7×10^{-2}		Fang Lee (2007)	Q	721
[60145-21-3]	4.6×10^{-2}		Fang Lee (2007)	Q	722
PQHZWWBJPCNNGI-UHFFFAOYSA-N	2.0×10^{-2}		Dunnivant et al. (1992)	Q	
	1.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',4,6,6'-pentachlorobiphenyl	1.5×10^{-2}	1700	Bamford et al. (2000)	M	
$C_{12}H_5Cl_5$	1.1×10^{-2}		Dunnivant et al. (1988)	M	
(PCB-104)	1.1×10^{-2}		Dunnivant and Elzerman (1988)	M	723
[56558-16-8]	2.8×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
MTCPZNVSDFCBBE-UHFFFAOYSA-N	4.3×10^{-2}		Mackay et al. (2006b)	V	
	7.2×10^{-2}		Mackay et al. (1992a)	V	
	5.4×10^{-3}		Burkhard et al. (1985)	V	
	2.0×10^{-2}		Bhangare et al. (2019)	Q	
	4.2×10^{-2}		Fang Lee (2007)	Q	721
	3.4×10^{-2}		Fang Lee (2007)	Q	722
		3100	Kühne et al. (2005)	Q	
	1.3×10^{-2}		Dunnivant et al. (1992)	Q	
		2000	Kühne et al. (2005)	?	
2,3,3',4,4'-pentachlorobiphenyl	3.0×10^{-2}	6800	Li et al. (2003)	L	366
$C_{12}H_5Cl_5$	7.2×10^{-2}	7500	Li et al. (2003)	L	367
(PCB-105)	1.8×10^{-1}		Fang et al. (2006)	M	
[32598-14-4]	3.0×10^{-2}	9100	Bamford et al. (2000)	M	
WIDHRBRBACOVOY-UHFFFAOYSA-N	1.2×10^{-2}		Duchowicz et al. (2020)	V	186
	5.0×10^{-3}	5700	Paasivirta and Sinkkonen (2009)	V	
	1.8×10^{-1}		Burkhard et al. (1985)	V	
	2.9×10^{-2}	8300	Paasivirta et al. (1999)	T	
	2.7×10^{-1}		Duchowicz et al. (2020)	Q	
	2.0×10^{-2}		Bhangare et al. (2019)	Q	
	9.7×10^{-2}		Fang Lee (2007)	Q	721
	1.4×10^{-1}		Fang Lee (2007)	Q	722
	9.9×10^{-2}		Dunnivant et al. (1992)	Q	
	1.6×10^{-1}		Sabljić and Güsten (1989)	Q	
2,3,3',4,5-pentachlorobiphenyl	1.3×10^{-2}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	2.5×10^{-2}		Burkhard et al. (1985)	V	
(PCB-106)	1.8×10^{-1}		Fang Lee (2007)	Q	721
[70424-69-0]	1.4×10^{-1}		Fang Lee (2007)	Q	722
BQENMISTWGTJIJ-UHFFFAOYSA-N	6.0×10^{-2}		Dunnivant et al. (1992)	Q	
	5.1×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',4',5-pentachlorobiphenyl	4.3×10^{-2}	2200	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	1.7×10^{-1}		Murphy et al. (1987)	M	12
(PCB-107)	9.1×10^{-3}	6200	Paasivirta and Sinkkonen (2009)	V	
[70424-68-9]	1.0×10^{-1}		Burkhard et al. (1985)	V	
PVYBHVJTMRRXLG-UHFFFAOYSA-N	2.0×10^{-1}		Fang Lee (2007)	Q	721
	1.2×10^{-1}		Fang Lee (2007)	Q	722
	6.2×10^{-2}		Dunnivant et al. (1992)	Q	
	4.9×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',4,5'-pentachlorobiphenyl	4.1×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	1.0×10^{-1}		Burkhard et al. (1985)	V	
(PCB-108)	1.1×10^{-1}		Fang Lee (2007)	Q	721
[70362-41-3]	1.1×10^{-1}		Fang Lee (2007)	Q	722
MPCDNZSLJWJDNW-UHFFFAOYSA-N	5.6×10^{-2}		Dunnivant et al. (1992)	Q	
	2.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',4,6-pentachlorobiphenyl	1.5×10^{-2}	6600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	2.1×10^{-2}		Burkhard et al. (1985)	V	
(PCB-109)	1.4×10^{-1}		Fang Lee (2007)	Q	721
[74472-35-8]	1.2×10^{-1}		Fang Lee (2007)	Q	722
XGQBSVVYMVILEL-UHFFFAOYSA-N	3.5×10^{-2}		Dunnivant et al. (1992)	Q	
	2.5×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',4',6-pentachlorobiphenyl	2.3×10^{-2}	5200	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	9.3×10^{-2}		Murphy et al. (1987)	M	12
(PCB-110)	2.7×10^{-2}		Murphy et al. (1983a)	M	24
[38380-03-9]	1.8×10^{-2}	6400	Paasivirta and Sinkkonen (2009)	V	
ARXHIJMGSIYYRZ-UHFFFAOYSA-N	5.8×10^{-2}		Burkhard et al. (1985)	V	
	8.3×10^{-2}		Fang Lee (2007)	Q	721
	1.4×10^{-1}		Fang Lee (2007)	Q	722
		5000	Kühne et al. (2005)	Q	
	5.0×10^{-2}		Dunnivant et al. (1992)	Q	
	5.2×10^{-2}		Sabljić and Güsten (1989)	Q	
		4300	Kühne et al. (2005)	?	
2,3,3',5,5'-pentachlorobiphenyl	6.5×10^{-3}	6200	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	6.2×10^{-2}		Burkhard et al. (1985)	V	
(PCB-111)	2.7×10^{-1}		Fang Lee (2007)	Q	721
[39635-32-0]	7.8×10^{-2}		Fang Lee (2007)	Q	722
QMUDLTGWHILKHH-UHFFFAOYSA-N	3.7×10^{-2}		Dunnivant et al. (1992)	Q	
	2.0×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',5,6-pentachlorobiphenyl	7.8×10^{-3}	6600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	2.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-112)	1.5×10^{-1}		Fang Lee (2007)	Q	721
[74472-36-9]	2.0×10^{-1}		Fang Lee (2007)	Q	722
NTKSJAPQYKCFPP-UHFFFAOYSA-N	3.7×10^{-2}		Dunnivant et al. (1992)	Q	
	3.0×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',5',6-pentachlorobiphenyl	1.5×10^{-2}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	3.5×10^{-2}		Burkhard et al. (1985)	V	
(PCB-113)	1.7×10^{-1}		Fang Lee (2007)	Q	721
[68194-10-5]	1.2×10^{-1}		Fang Lee (2007)	Q	722
YDGFMDPEJCJZEV-UHFFFAOYSA-N	3.0×10^{-2}		Dunnivant et al. (1992)	Q	
	2.1×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,4,4',5-pentachlorobiphenyl	5.3×10^{-2}		Fang et al. (2006)	M	
$C_{12}H_5Cl_5$	1.4×10^{-1}		Murphy et al. (1987)	M	12
(PCB-114)	1.2×10^{-2}	6400	Paasivirta and Sinkkonen (2009)	V	
[74472-37-0]	2.8×10^{-2}		Burkhard et al. (1985)	V	
SXZSFWHOSHAKMN-UHFFFAOYSA-N	8.9×10^{-2}		Fang Lee (2007)	Q	721
	1.3×10^{-1}		Fang Lee (2007)	Q	722
	6.9×10^{-2}		Dunnivant et al. (1992)	Q	
	8.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,4,4',6-pentachlorobiphenyl	2.6×10^{-2}	6900	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	2.3×10^{-2}		Burkhard et al. (1985)	V	
(PCB-115)	5.4×10^{-2}		Fang Lee (2007)	Q	721
[74472-38-1]	1.1×10^{-1}		Fang Lee (2007)	Q	722
IOVARPVVZDOPGQ-UHFFFAOYSA-N	4.0×10^{-2}		Dunnivant et al. (1992)	Q	
	3.2×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,4,5,6-pentachlorobiphenyl	4.3×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	5.5×10^{-2}		Burkhard et al. (1985)	V	
(PCB-116)	9.9×10^{-2}		Fang Lee (2007)	Q	721
[18259-05-7]	1.8×10^{-1}		Fang Lee (2007)	Q	722
GGMPTLAAIUQMIE-UHFFFAOYSA-N	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	4.3×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,4',5,6-pentachlorobiphenyl	1.5×10^{-3}	5900	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	2.7×10^{-2}		Burkhard et al. (1985)	V	
(PCB-117)	7.5×10^{-2}		Fang Lee (2007)	Q	721
[68194-11-6]	1.7×10^{-1}		Fang Lee (2007)	Q	722
ZDDZPDTVCZLFFC-UHFFFAOYSA-N	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
	4.0×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3',4,4',5-pentachlorobiphenyl	3.1×10^{-2}	6800	Li et al. (2003)	L	366
$C_{12}H_5Cl_5$	6.9×10^{-2}	7600	Li et al. (2003)	L	367
(PCB-118)	4.6×10^{-3}		Bhangare et al. (2019)	M	725
[31508-00-6]	1.9×10^{-2}		Bhangare et al. (2019)	M	726
IUTPYMGCWINGEY-UHFFFAOYSA-N	1.1×10^{-2}		Lau et al. (2006)	M	719
	5.6×10^{-3}		Lau et al. (2006)	M	720
	5.7×10^{-2}		Fang et al. (2006)	M	
	1.8×10^{-2}	14000	Charles and Destaillats (2005)	M	33
	2.8×10^{-2}	6000	Bamford et al. (2000)	M	
	1.2×10^{-1}		Murphy et al. (1987)	M	12
	2.5×10^{-2}		Murphy et al. (1983a)	M	24
	3.4×10^{-2}		Duchowicz et al. (2020)	V	186
	6.6×10^{-3}	6000	Paasivirta and Sinkkonen (2009)	V	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^{-1}		Burkhard et al. (1985)	V	
	2.6×10^{-2}	8100	Paasivirta et al. (1999)	T	
	1.5×10^{-1}		Duchowicz et al. (2020)	Q	
	7.8×10^{-2}		Fang Lee (2007)	Q	721
	1.0×10^{-1}		Fang Lee (2007)	Q	722
		5600	Kühne et al. (2005)	Q	
	7.9×10^{-2}		Dunnivant et al. (1992)	Q	
	8.5×10^{-2}		Sabljić and Güsten (1989)	Q	
		6300	Kühne et al. (2005)	?	
2,3',4,4',6-pentachlorobiphenyl	1.5×10^{-2}	4600	Bamford et al. (2002)	M	
$C_{12}H_5Cl_5$	1.5×10^{-2}	6500	Paasivirta and Sinkkonen (2009)	V	
(PCB-119)	4.4×10^{-2}		Burkhard et al. (1985)	V	
[56558-17-9]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
OAEQTHQGPZKTQP-UHFFFAOYSA-N	9.4×10^{-2}		Duchowicz et al. (2020)	Q	184
	1.6×10^{-1}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Modarresi et al. (2007)	Q	67
	4.7×10^{-2}		Fang Lee (2007)	Q	721
	7.4×10^{-2}		Fang Lee (2007)	Q	722
	3.2×10^{-2}		Dunnivant et al. (1992)	Q	
	2.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.3×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,3',4,5,5'-pentachlorobiphenyl	1.8×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_5Cl_5$	3.9×10^{-3}	6000	Paasivirta and Sinkkonen (2009)	V	
(PCB-120)	6.4×10^{-2}		Burkhard et al. (1985)	V	
[68194-12-7]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
ZLGYJAIAVPVCNF-UHFFFAOYSA-N	8.6×10^{-2}		Duchowicz et al. (2020)	Q	299
	2.5×10^{-1}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	67
	1.6×10^{-1}		Fang Lee (2007)	Q	721
	8.3×10^{-2}		Fang Lee (2007)	Q	722
	4.0×10^{-2}		Dunnivant et al. (1992)	Q	
	2.4×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.8×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,3',4,5',6-pentachlorobiphenyl	8.5×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	2.6×10^{-2}		Burkhard et al. (1985)	V	
(PCB-121)	9.6×10^{-2}		Fang Lee (2007)	Q	721
[56558-18-0]	6.2×10^{-2}		Fang Lee (2007)	Q	722
XBVSGJGMWSKAKL-UHFFFAOYSA-N	1.8×10^{-2}		Dunnivant et al. (1992)	Q	
	1.3×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',4',5'-pentachlorobiphenyl	1.6×10^{-1}		Murphy et al. (1987)	M	12
$C_{12}H_5Cl_5$	4.3×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
(PCB-122)	1.6×10^{-1}		Burkhard et al. (1985)	V	
[76842-07-4]	2.8×10^{-1}		Fang Lee (2007)	Q	721
GWOWBISZHLPYEK-UHFFFAOYSA-N	1.4×10^{-1}		Fang Lee (2007)	Q	722
	7.9×10^{-2}		Dunnivant et al. (1992)	Q	
	7.2×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3',4,4',5'-pentachlorobiphenyl	4.6×10^{-2}		Fang et al. (2006)	M	
$C_{12}H_5Cl_5$	3.7×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
(PCB-123)	1.1×10^{-1}		Burkhard et al. (1985)	V	
[65510-44-3]	1.4×10^{-1}		Fang Lee (2007)	Q	721
YAHNWSSFXMVPOU-UHFFFAOYSA-N	9.3×10^{-2}		Fang Lee (2007)	Q	722
	5.7×10^{-2}		Dunnivant et al. (1992)	Q	
	3.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3',4',5,5'-pentachlorobiphenyl	1.9×10^{-1}		Murphy et al. (1987)	M	12
$C_{12}H_5Cl_5$	4.5×10^{-3}	5900	Paasivirta and Sinkkonen (2009)	V	
(PCB-124)	1.0×10^{-1}		Burkhard et al. (1985)	V	
[70424-70-3]	2.8×10^{-1}		Fang Lee (2007)	Q	721
PIVBPZFQXKMHBD-UHFFFAOYSA-N	9.4×10^{-2}		Fang Lee (2007)	Q	722
	5.8×10^{-2}		Dunnivant et al. (1992)	Q	
	5.1×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3',4',5',6-pentachlorobiphenyl	2.3×10^{-3}	5800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	6.7×10^{-2}		Burkhard et al. (1985)	V	
(PCB-125)	1.5×10^{-1}		Fang Lee (2007)	Q	721
[74472-39-2]	1.1×10^{-1}		Fang Lee (2007)	Q	722
WAZUWHGJMMZVHH-UHFFFAOYSA-N	3.4×10^{-2}		Dunnivant et al. (1992)	Q	
	3.0×10^{-2}		Sabljić and Güsten (1989)	Q	
3,3',4,4',5-pentachlorobiphenyl	1.0×10^{-1}		Fang et al. (2006)	M	
$C_{12}H_5Cl_5$	4.8×10^{-2}	12000	Bamford et al. (2000)	M	
(PCB-126)	1.6×10^{-3}	5400	Paasivirta and Sinkkonen (2009)	V	
[57465-28-8]	3.6×10^{-1}		Burkhard et al. (1985)	V	
REHONNLQRWTIFF-UHFFFAOYSA-N	6.5×10^{-2}	8800	Paasivirta et al. (1999)	T	
	1.8×10^{-2}		Bhangare et al. (2019)	Q	
	1.7×10^{-1}		Fang Lee (2007)	Q	721
	1.0×10^{-1}		Fang Lee (2007)	Q	722
	1.2×10^{-1}		Dunnivant et al. (1992)	Q	
	1.8×10^{-1}		Sabljić and Güsten (1989)	Q	
3,3',4,5,5'-pentachlorobiphenyl	2.2×10^{-3}	5600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_5Cl_5$	2.2×10^{-1}		Burkhard et al. (1985)	V	
(PCB-127)	3.4×10^{-1}		Fang Lee (2007)	Q	721
[39635-33-1]	8.4×10^{-2}		Fang Lee (2007)	Q	722
MXVAYAXIPRGORY-UHFFFAOYSA-N	6.3×10^{-2}		Dunnivant et al. (1992)	Q	
	2.9×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,4'-hexachlorobiphenyl	2.8×10^{-2}	14000	Bamford et al. (2000)	M	
$C_{12}H_4Cl_6$	7.6×10^{-1}		Brunner et al. (1990)	M	
(PCB-128)	3.3×10^{-1}		Dunnivant et al. (1988)	M	
[38380-07-3]	3.3×10^{-1}		Dunnivant and Elzerman (1988)	M	723
BTAGRXWGMYTPBY-UHFFFAOYSA-N	1.7×10^{-1}		Murphy et al. (1987)	M	12
	2.0×10^{-2}		Murphy et al. (1983a)	M	24
	6.9×10^{-3}	6100	Paasivirta and Sinkkonen (2009)	V	
	8.4×10^{-2}		Mackay et al. (2006b)	V	
	8.4×10^{-2}		Mackay et al. (1992a)	V	
	8.3×10^{-2}		Shiu and Mackay (1986)	V	
	1.5×10^{-1}		Burkhard et al. (1985)	V	
	2.0×10^{-2}		Murphy et al. (1983b)	X	724, 24
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	3.8×10^{-1}		Duchowicz et al. (2020)	Q	299
	1.5×10^{-2}		Bhangare et al. (2019)	Q	
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	67
	1.5×10^{-1}		Fang Lee (2007)	Q	721
	2.4×10^{-1}		Fang Lee (2007)	Q	722
	1.2×10^{-1}		English and Carroll (2001)	Q	230, 231
	9.5×10^{-2}		Dunnivant et al. (1992)	Q	
	7.6×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,3',4,5-hexachlorobiphenyl	3.4×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_4Cl_6$	6.4×10^{-3}	6400	Paasivirta and Sinkkonen (2009)	V	
(PCB-129)	2.5×10^{-2}		Burkhard et al. (1985)	V	
[55215-18-4]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
VQQKIXKPMJTUMP-UHFFFAOYSA-N	2.7×10^{-1}		Duchowicz et al. (2020)	Q	
	1.6×10^{-1}		Hilal et al. (2008)	Q	
	2.2×10^{-1}		Modarresi et al. (2007)	Q	67
	2.9×10^{-1}		Fang Lee (2007)	Q	721
	2.6×10^{-1}		Fang Lee (2007)	Q	722
	7.1×10^{-2}		Dunnivant et al. (1992)	Q	
	1.2×10^{-1}		Sabljić and Güsten (1989)	Q	
	3.4×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,3',4,5'-hexachlorobiphenyl	2.7×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_4Cl_6$	9.2×10^{-2}		Murphy et al. (1987)	M	12
(PCB-130)	5.9×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
[52663-66-8]	8.7×10^{-2}		Burkhard et al. (1985)	V	
YFSLABAYQDPWPF-UHFFFAOYSA-N	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	
	1.9×10^{-1}		Hilal et al. (2008)	Q	
	2.0×10^{-1}		Modarresi et al. (2007)	Q	67
	3.1×10^{-1}		Fang Lee (2007)	Q	721
	2.1×10^{-1}		Fang Lee (2007)	Q	722
	6.5×10^{-2}		Dunnivant et al. (1992)	Q	
	5.1×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,3',4,6-hexachlorobiphenyl	1.5×10^{-1}		Murphy et al. (1987)	M	12
$C_{12}H_4Cl_6$	3.0×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
(PCB-131)	1.6×10^{-2}		Burkhard et al. (1985)	V	
[61798-70-7]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
WDLTVNWWEZJMPF-UHFFFAOYSA-N	1.6×10^{-1}		Duchowicz et al. (2020)	Q	299
	1.6×10^{-1}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	67
	1.7×10^{-1}		Fang Lee (2007)	Q	721
	1.9×10^{-1}		Fang Lee (2007)	Q	722
	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
	3.8×10^{-2}		Sabljić and Güsten (1989)	Q	
	2.5×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,3',4,6'-hexachlorobiphenyl	4.0×10^{-2}	2400	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	2.2×10^{-1}		Brunner et al. (1990)	M	
(PCB-132)	4.1×10^{-3}	6400	Paasivirta and Sinkkonen (2009)	V	
[38380-05-1]	3.6×10^{-2}		Burkhard et al. (1985)	V	
OKBJVIVEFXPEOU-UHFFFAOYSA-N	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	299
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	1.6×10^{-1}		Modarresi et al. (2007)	Q	67
	1.7×10^{-1}		Fang Lee (2007)	Q	721
	2.1×10^{-1}		Fang Lee (2007)	Q	722
	2.3×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	4.9×10^{-2}		Dunnivant et al. (1992)	Q	
	6.1×10^{-2}		Sabljić and Güsten (1989)	Q	
	2.2×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,3',5,5'-hexachlorobiphenyl	4.1×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	5.2×10^{-2}		Burkhard et al. (1985)	V	
(PCB-133)	1.8×10^{-1}		Hilal et al. (2008)	Q	
[35694-04-3]	4.3×10^{-1}		Fang Lee (2007)	Q	721
AJKLKINFZLWHQE-UHFFFAOYSA-N	2.0×10^{-1}		Fang Lee (2007)	Q	722
	4.8×10^{-2}		Dunnivant et al. (1992)	Q	
	3.0×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,3',5,6-hexachlorobiphenyl	1.2×10^{-2}	7300	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	2.0×10^{-1}		Brunner et al. (1990)	M	
(PCB-134)	1.0×10^{-1}		Murphy et al. (1987)	M	12
[52704-70-8]	1.7×10^{-2}		Murphy et al. (1983a)	M	24
RVWLHPJFOKUPNM-UHFFFAOYSA-N	2.8×10^{-3}	6400	Paasivirta and Sinkkonen (2009)	V	
	1.8×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.5×10^{-1}		Duchowicz et al. (2020)	Q	299
	2.0×10^{-1}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	67
	2.4×10^{-1}		Fang Lee (2007)	Q	721

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

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	3.2×10^{-1}		Fang Lee (2007)	Q	722
	4.3×10^{-2}		Dunnivant et al. (1992)	Q	
	4.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	2.0×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,3',5,6'-hexachlorobiphenyl	1.5×10^{-2}	5500	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	1.8×10^{-1}		Brunner et al. (1990)	M	
(PCB-135)	7.0×10^{-2}		Murphy et al. (1987)	M	12
[52744-13-5]	4.8×10^{-3}	6600	Paasivirta and Sinkkonen (2009)	V	
UUTNFLRSJBQQJM-UHFFFAOYSA-N	2.1×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	184
	2.3×10^{-1}		Hilal et al. (2008)	Q	
	1.9×10^{-1}		Modarresi et al. (2007)	Q	67
	2.4×10^{-1}		Fang Lee (2007)	Q	721
	2.1×10^{-1}		Fang Lee (2007)	Q	722
	3.7×10^{-2}		Dunnivant et al. (1992)	Q	
	3.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.8×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,3',6,6'-hexachlorobiphenyl	9.0×10^{-3}	5400	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	1.1×10^{-1}		Brunner et al. (1990)	M	
(PCB-136)	4.4×10^{-2}		Murphy et al. (1987)	M	12
[38411-22-2]	1.6×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
FZFUUSROAHKTTF-UHFFFAOYSA-N	1.1×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	299
	2.7×10^{-1}		Hilal et al. (2008)	Q	
	1.5×10^{-1}		Modarresi et al. (2007)	Q	67
	1.4×10^{-1}		Fang Lee (2007)	Q	721
	1.6×10^{-1}		Fang Lee (2007)	Q	722
	3.1×10^{-2}		Dunnivant et al. (1992)	Q	
	3.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,4,4',5-hexachlorobiphenyl	4.5×10^{-2}	3200	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	1.5×10^{-1}		Murphy et al. (1987)	M	12
(PCB-137)	2.1×10^{-2}		Murphy et al. (1983a)	M	24
[35694-06-5]	1.8×10^{-2}	6800	Paasivirta and Sinkkonen (2009)	V	
CKLLRBPBZLTGDJ-UHFFFAOYSA-N	1.8×10^{-2}		Burkhard et al. (1985)	V	
	1.4×10^{-1}		Fang Lee (2007)	Q	721
	1.7×10^{-1}		Fang Lee (2007)	Q	722
	5.3×10^{-2}		Dunnivant et al. (1992)	Q	
	4.7×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,4',5'-hexachlorobiphenyl	2.5×10^{-2}	7100	Li et al. (2003)	L	366
$C_{12}H_4Cl_6$	3.3×10^{-2}	7700	Li et al. (2003)	L	367
(PCB-138)	2.2×10^{-2}	10000	Bamford et al. (2000)	M	
[35065-28-2]	4.7×10^{-1}		Brunner et al. (1990)	M	
RPUMZMSNLZHIGZ-UHFFFAOYSA-N	1.3×10^{-1}		Murphy et al. (1987)	M	12
	1.4×10^{-1}		Brownawell (1986)	M	294
	2.1×10^{-2}		Murphy et al. (1983a)	M	24
	1.8×10^{-2}	6800	Paasivirta and Sinkkonen (2009)	V	
	1.2×10^{-2}		Shiu and Mackay (1986)	V	
	9.1×10^{-2}		Burkhard et al. (1985)	V	
	4.7×10^{-2}	8700	Paasivirta et al. (1999)	T	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.5×10^{-2}		Bhangare et al. (2019)	Q	
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	2.2×10^{-1}		Modarresi et al. (2007)	Q	67
	1.6×10^{-1}		Fang Lee (2007)	Q	721
	1.8×10^{-1}		Fang Lee (2007)	Q	722
	5.2×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	7.6×10^{-2}		Dunnivant et al. (1992)	Q	
	9.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,4,4',6-hexachlorobiphenyl	1.4×10^{-2}	6900	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	1.1×10^{-2}		Burkhard et al. (1985)	V	
(PCB-139)	8.6×10^{-2}		Fang Lee (2007)	Q	721
[56030-56-9]	1.3×10^{-1}		Fang Lee (2007)	Q	722
SPOPSCCFZQFGDL-UHFFFAOYSA-N	3.0×10^{-2}		Dunnivant et al. (1992)	Q	
	2.6×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4,4',6'-hexachlorobiphenyl	1.7×10^{-2}	7000	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	2.7×10^{-2}		Burkhard et al. (1985)	V	
(PCB-140)	8.5×10^{-2}		Fang Lee (2007)	Q	721
[59291-64-4]	1.1×10^{-1}		Fang Lee (2007)	Q	722
XBBRGUHRZBZMPP-UHFFFAOYSA-N	3.2×10^{-2}		Dunnivant et al. (1992)	Q	
	2.3×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4,5,5'-hexachlorobiphenyl	2.0×10^{-2}	8400	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	4.3×10^{-1}		Brunner et al. (1990)	M	
(PCB-141)	1.0×10^{-1}		Murphy et al. (1987)	M	12
[52712-04-6]	2.5×10^{-2}		Murphy et al. (1983a)	M	24
UCLKLGIYGBLTSM-UHFFFAOYSA-N	1.0×10^{-2}	6700	Paasivirta and Sinkkonen (2009)	V	
	2.5×10^{-2}		Shiu and Mackay (1986)	V	
	1.6×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.5×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.3×10^{-1}		Hilal et al. (2008)	Q	
	2.0×10^{-1}		Modarresi et al. (2007)	Q	67
	2.9×10^{-1}		Fang Lee (2007)	Q	721

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.8×10^{-1}		Fang Lee (2007)	Q	722
	5.7×10^{-2}		Dunnivant et al. (1992)	Q	
	6.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.3×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,4,5,6-hexachlorobiphenyl	4.0×10^{-3}	6900	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	1.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-142)	1.6×10^{-1}		Fang Lee (2007)	Q	721
[41411-61-4]	2.4×10^{-1}		Fang Lee (2007)	Q	722
RUEIBQJFGMERJD-UHFFFAOYSA-N	3.1×10^{-2}		Dunnivant et al. (1992)	Q	
	4.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4,5,6'-hexachlorobiphenyl	6.5×10^{-3}	6600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	7.8×10^{-3}		Burkhard et al. (1985)	V	
(PCB-143)	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
[68194-15-0]	1.6×10^{-1}		Duchowicz et al. (2020)	Q	184
UQPQKLGBEKEZBV-UHFFFAOYSA-N	1.6×10^{-1}		Hilal et al. (2008)	Q	
	1.7×10^{-1}		Modarresi et al. (2007)	Q	67
	1.6×10^{-1}		Fang Lee (2007)	Q	721
	1.9×10^{-1}		Fang Lee (2007)	Q	722
	3.4×10^{-2}		Dunnivant et al. (1992)	Q	
	3.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	2.5×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,4,5',6-hexachlorobiphenyl	7.0×10^{-2}		Murphy et al. (1987)	M	12
$C_{12}H_4Cl_6$	1.6×10^{-2}		Murphy et al. (1983a)	M	24
(PCB-144)	1.2×10^{-2}	7000	Paasivirta and Sinkkonen (2009)	V	
[68194-14-9]	1.7×10^{-2}		Shiu and Mackay (1986)	V	
CXXRQFOKRZJAJA-UHFFFAOYSA-N	1.0×10^{-2}		Burkhard et al. (1985)	V	
	1.8×10^{-1}		Fang Lee (2007)	Q	721
	1.4×10^{-1}		Fang Lee (2007)	Q	722
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
	3.1×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4,6,6'-hexachlorobiphenyl	1.5×10^{-3}	6400	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	5.9×10^{-3}		Burkhard et al. (1985)	V	
(PCB-145)	9.6×10^{-2}		Fang Lee (2007)	Q	721
[74472-40-5]	1.1×10^{-1}		Fang Lee (2007)	Q	722
JZFZCLFEPXCRCA-UHFFFAOYSA-N	2.1×10^{-2}		Dunnivant et al. (1992)	Q	
	2.4×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4',5,5'-hexachlorobiphenyl	1.7×10^{-2}	7100	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	3.9×10^{-1}		Brunner et al. (1990)	M	
(PCB-146)	1.1×10^{-1}		Murphy et al. (1987)	M	12
[51908-16-8]	1.2×10^{-2}	6800	Paasivirta and Sinkkonen (2009)	V	
BQHCQAQLTCQFJZ-UHFFFAOYSA-N	5.4×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	184
	2.0×10^{-1}		Hilal et al. (2008)	Q	
	2.2×10^{-1}		Modarresi et al. (2007)	Q	67

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{-1}		Fang Lee (2007)	Q	721
	1.6×10^{-1}		Fang Lee (2007)	Q	722
	5.3×10^{-2}		Dunnivant et al. (1992)	Q	
	4.0×10^{-2}		Sabljić and Güsten (1989)	Q	
	3.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,4',5,6-hexachlorobiphenyl	1.9×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_4Cl_6$	3.1×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
(PCB-147)	1.3×10^{-2}		Burkhard et al. (1985)	V	
[68194-13-8]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
AQONCPKMJSBHQT-UHFFFAOYSA-N	8.7×10^{-2}		Duchowicz et al. (2020)	Q	299
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	67
	1.2×10^{-1}		Fang Lee (2007)	Q	721
	2.1×10^{-1}		Fang Lee (2007)	Q	722
	3.1×10^{-2}		Dunnivant et al. (1992)	Q	
	3.1×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,4',5,6'-hexachlorobiphenyl	1.2×10^{-2}	7000	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	1.6×10^{-2}		Burkhard et al. (1985)	V	
(PCB-148)	1.2×10^{-1}		Fang Lee (2007)	Q	721
[74472-41-6]	1.0×10^{-1}		Fang Lee (2007)	Q	722
CTVRBEKNQHJPLX-UHFFFAOYSA-N	2.3×10^{-2}		Dunnivant et al. (1992)	Q	
	1.7×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4',5',6-hexachlorobiphenyl	1.5×10^{-2}	5500	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	6.7×10^{-2}		Murphy et al. (1987)	M	12
(PCB-149)	3.3×10^{-2}		Murphy et al. (1983a)	M	24
[38380-04-0]	7.2×10^{-3}		Duchowicz et al. (2020)	V	186
LKHLFUVHHXCNJH-UHFFFAOYSA-N	1.0×10^{-2}	6800	Paasivirta and Sinkkonen (2009)	V	
	3.3×10^{-2}		Shiu and Mackay (1986)	V	
	2.2×10^{-2}		Burkhard et al. (1985)	V	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	
	1.3×10^{-1}		Fang Lee (2007)	Q	721
	1.7×10^{-1}		Fang Lee (2007)	Q	722
	2.1×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	4.2×10^{-2}		Dunnivant et al. (1992)	Q	
	4.5×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',3,4',6,6'-hexachlorobiphenyl	6.5×10^{-3}	6900	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	8.2×10^{-3}		Burkhard et al. (1985)	V	
(PCB-150)	7.2×10^{-2}		Fang Lee (2007)	Q	721
[68194-08-1]	8.0×10^{-2}		Fang Lee (2007)	Q	722
RPPNJBZNXQNKNM-UHFFFAOYSA-N	2.0×10^{-2}		Dunnivant et al. (1992)	Q	
	1.9×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

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2,2',3,5,5',6-hexachlorobiphenyl	1.4×10^{-2}	4500	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	1.7×10^{-1}		Brunner et al. (1990)	M	
(PCB-151)	6.3×10^{-2}		Murphy et al. (1987)	M	12
[52663-63-5]	3.3×10^{-2}		Murphy et al. (1983a)	M	24
UHCLFIWDCYOTOL-UHFFFAOYSA-N	5.2×10^{-3}	6700	Paasivirta and Sinkkonen (2009)	V	
	3.3×10^{-2}		Shiu and Mackay (1986)	V	
	1.2×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	7.9×10^{-2}		Duchowicz et al. (2020)	Q	
	1.6×10^{-1}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	67
	2.4×10^{-1}		Fang Lee (2007)	Q	721
	2.4×10^{-1}		Fang Lee (2007)	Q	722
	3.5×10^{-2}		Dunnivant et al. (1992)	Q	
	3.8×10^{-2}		Sabljić and Güsten (1989)	Q	
	1.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,5,6,6'-hexachlorobiphenyl	1.3×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	6.8×10^{-3}		Burkhard et al. (1985)	V	
(PCB-152)	1.3×10^{-1}		Fang Lee (2007)	Q	721
[68194-09-2]	1.9×10^{-1}		Fang Lee (2007)	Q	722
CLODVDBWNVQLGO-UHFFFAOYSA-N	2.3×10^{-2}		Dunnivant et al. (1992)	Q	
	2.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',4,4',5,5'-hexachlorobiphenyl	4.0×10^{-2}	7100	Li et al. (2003)	L	366
$C_{12}H_4Cl_6$	5.1×10^{-2}	7900	Li et al. (2003)	L	367
(PCB-153)	1.9×10^{-2}	8000	Bamford et al. (2000)	M	
[35065-27-1]	4.3×10^{-1}		Brunner et al. (1990)	M	
MVWHGTYKUMDIHL-UHFFFAOYSA-N	7.5×10^{-2}		Dunnivant et al. (1988)	M	
	7.5×10^{-2}		Dunnivant and Elzerman (1988)	M	723
	1.0×10^{-1}		Murphy et al. (1987)	M	12
	1.6×10^{-1}		Oliver (1985)	M	
	2.8×10^{-2}		Murphy et al. (1983a)	M	24
	1.1×10^{-2}	6700	Paasivirta and Sinkkonen (2009)	V	
	2.3×10^{-2}		Mackay et al. (2006b)	V	
	2.3×10^{-2}		Mackay et al. (1992a)	V	
	2.3×10^{-2}		Shiu and Mackay (1986)	V	
	5.6×10^{-2}		Burkhard et al. (1985)	V	
	1.7×10^{-2}	8400	Paasivirta et al. (1999)	T	
	2.8×10^{-2}		Murphy et al. (1983b)	X	724, 24
	8.0×10^{-2}		Dunnivant et al. (1988)	C	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.1×10^{-1}		Duchowicz et al. (2020)	Q	299
	1.7×10^{-2}		Bhangare et al. (2019)	Q	
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	2.4×10^{-1}		Modarresi et al. (2007)	Q	67
	1.2×10^{-1}		Fang Lee (2007)	Q	721
	1.4×10^{-1}		Fang Lee (2007)	Q	722

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

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	2.9×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	6.0×10^{-2}		Dunnivant et al. (1992)	Q	
	4.3×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',4,4',5,6'-hexachlorobiphenyl	1.3×10^{-2}	5600	Bamford et al. (2000)	M	
$C_{12}H_4Cl_6$	1.7×10^{-2}	7100	Paasivirta and Sinkkonen (2009)	V	
(PCB-154)	1.7×10^{-2}		Burkhard et al. (1985)	V	
[60145-22-4]	1.8×10^{-2}		Bhangare et al. (2019)	Q	
QXZHEJWDLVUFFB-UHFFFAOYSA-N	6.8×10^{-2}		Fang Lee (2007)	Q	721
	8.7×10^{-2}		Fang Lee (2007)	Q	722
	2.6×10^{-2}		Dunnivant et al. (1992)	Q	
	2.0×10^{-2}		Sabljić and Güsten (1989)	Q	
2,2',4,4',6,6'-hexachlorobiphenyl	1.3×10^{-2}	7100	Li et al. (2003)	L	366
$C_{12}H_4Cl_6$	1.1×10^{-2}	7600	Li et al. (2003)	L	367
(PCB-155)	1.3×10^{-2}		Dunnivant et al. (1988)	M	
[33979-03-2]	1.3×10^{-2}		Dunnivant and Elzerman (1988)	M	723
ICOAEPDGFWLUTI-UHFFFAOYSA-N	3.9×10^{-3}		Duchowicz et al. (2020)	V	186
	4.6×10^{-3}	6900	Paasivirta and Sinkkonen (2009)	V	
	1.2×10^{-2}		Mackay et al. (2006b)	V	
	1.2×10^{-2}		Mackay et al. (1992a)	V	
	1.2×10^{-3}		Shiu and Mackay (1986)	V	
	6.4×10^{-3}		Burkhard et al. (1985)	V	
	8.6×10^{-2}		Dunnivant et al. (1988)	C	
	4.8×10^{-2}		Duchowicz et al. (2020)	Q	
	4.2×10^{-2}		Fang Lee (2007)	Q	721
	4.2×10^{-2}		Fang Lee (2007)	Q	722
	1.2×10^{-2}		Dunnivant et al. (1992)	Q	
2,3,3',4,4',5-hexachlorobiphenyl	6.8×10^{-2}		Fang et al. (2006)	M	
$C_{12}H_4Cl_6$	2.9×10^{-2}	13000	Bamford et al. (2002)	M	
(PCB-156)	1.1×10^{-2}		Murphy et al. (1983a)	M	24
[38380-08-4]	6.9×10^{-2}		Duchowicz et al. (2020)	V	186
LCXMEXLGMKFLQO-UHFFFAOYSA-N	5.9×10^{-3}	6200	Paasivirta and Sinkkonen (2009)	V	
	1.1×10^{-2}		Shiu and Mackay (1986)	V	
	5.7×10^{-2}		Burkhard et al. (1985)	V	
	2.7×10^{-1}		Duchowicz et al. (2020)	Q	
	1.8×10^{-1}		Fang Lee (2007)	Q	721
	2.0×10^{-1}		Fang Lee (2007)	Q	722
	1.1×10^{-1}		Dunnivant et al. (1992)	Q	
	4.5×10^{-1}		Sabljić and Güsten (1989)	Q	
2,3,3',4,4',5'-hexachlorobiphenyl	6.0×10^{-2}		Fang et al. (2006)	M	
$C_{12}H_4Cl_6$	3.4×10^{-2}	16000	Bamford et al. (2002)	M	
(PCB-157)	1.7×10^{-2}		Murphy et al. (1983a)	M	24
[69782-90-7]	2.3×10^{-3}	5900	Paasivirta and Sinkkonen (2009)	V	
YTWXDQVNPCIEOX-UHFFFAOYSA-N	1.7×10^{-2}		Shiu and Mackay (1986)	V	
	3.0×10^{-1}		Burkhard et al. (1985)	V	
	1.9×10^{-1}		Fang Lee (2007)	Q	721

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.0×10^{-1}		Fang Lee (2007)	Q	722
		6300	Kühne et al. (2005)	Q	
	1.2×10^{-1}		Dunnivant et al. (1992)	Q	
	1.5×10^{-1}		Sabljić and Güsten (1989)	Q	
		5100	Kühne et al. (2005)	?	
2,3,3',4,4',6-hexachlorobiphenyl	2.1×10^{-2}	9600	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	2.3×10^{-1}		Murphy et al. (1987)	M	12
(PCB-158)	1.5×10^{-2}		Murphy et al. (1983a)	M	24
[74472-42-7]	9.2×10^{-3}	6600	Paasivirta and Sinkkonen (2009)	V	
ZQUPQXINXTWCQR-UHFFFAOYSA-N	1.5×10^{-2}		Shiu and Mackay (1986)	V	
	4.8×10^{-2}		Burkhard et al. (1985)	V	
	1.1×10^{-1}		Fang Lee (2007)	Q	721
	1.9×10^{-1}		Fang Lee (2007)	Q	722
	6.0×10^{-2}		Dunnivant et al. (1992)	Q	
	4.6×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',4,5,5'-hexachlorobiphenyl	4.9×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_4Cl_6$	2.9×10^{-3}	6100	Paasivirta and Sinkkonen (2009)	V	
(PCB-159)	3.4×10^{-2}		Burkhard et al. (1985)	V	
[39635-35-3]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
YZKLGRAIIIGOHB-UHFFFAOYSA-N	1.6×10^{-1}		Duchowicz et al. (2020)	Q	184
	2.6×10^{-1}		Hilal et al. (2008)	Q	
	1.9×10^{-1}		Modarresi et al. (2007)	Q	67
	3.6×10^{-1}		Fang Lee (2007)	Q	721
	1.8×10^{-1}		Fang Lee (2007)	Q	722
	6.3×10^{-2}		Dunnivant et al. (1992)	Q	
	3.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,3,3',4,5,6-hexachlorobiphenyl	4.9×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_4Cl_6$	7.9×10^{-3}	7100	Paasivirta and Sinkkonen (2009)	V	
(PCB-160)	4.0×10^{-2}		Burkhard et al. (1985)	V	
[41411-62-5]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
JHJMZCXLJXRCHK-UHFFFAOYSA-N	1.1×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.2×10^{-1}		Hilal et al. (2008)	Q	
	3.8×10^{-1}		Modarresi et al. (2007)	Q	67
	2.0×10^{-1}		Fang Lee (2007)	Q	721
	3.3×10^{-1}		Fang Lee (2007)	Q	722
	4.6×10^{-2}		Dunnivant et al. (1992)	Q	
	3.9×10^{-2}		Sabljić and Güsten (1989)	Q	
	4.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,3,3',4,5',6-hexachlorobiphenyl	9.2×10^{-3}	6800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	2.9×10^{-2}		Burkhard et al. (1985)	V	
(PCB-161)	2.2×10^{-1}		Fang Lee (2007)	Q	721
[74472-43-8]	1.7×10^{-1}		Fang Lee (2007)	Q	722
UNPTZXSJGZTGJJ-UHFFFAOYSA-N	3.5×10^{-2}		Dunnivant et al. (1992)	Q	
	2.0×10^{-2}		Sabljić and Güsten (1989)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',4',5,5'-hexachlorobiphenyl	3.7×10^{-3}	6200	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	1.8×10^{-1}		Burkhard et al. (1985)	V	
(PCB-162)	2.7×10^{-1}		Fang Lee (2007)	Q	721
[39635-34-2]	1.8×10^{-1}		Fang Lee (2007)	Q	722
AHZUOPSGLWYCNF-UHFFFAOYSA-N	7.5×10^{-2}		Dunnivant et al. (1992)	Q	
	4.8×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',4',5,6-hexachlorobiphenyl	2.1×10^{-2}	9700	Bamford et al. (2002)	M	
$C_{12}H_4Cl_6$	6.6×10^{-1}		Brunner et al. (1990)	M	
(PCB-163)	4.9×10^{-3}	6400	Paasivirta and Sinkkonen (2009)	V	
[74472-44-9]	5.4×10^{-2}		Burkhard et al. (1985)	V	
ZAGRQXMWMRUYRB-UHFFFAOYSA-N	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.5×10^{-1}		Duchowicz et al. (2020)	Q	299
	2.5×10^{-1}		Hilal et al. (2008)	Q	
	2.6×10^{-1}		Modarresi et al. (2007)	Q	67
	1.5×10^{-1}		Fang Lee (2007)	Q	721
	3.1×10^{-1}		Fang Lee (2007)	Q	722
	6.0×10^{-2}		Dunnivant et al. (1992)	Q	
	6.3×10^{-2}		Sabljić and Güsten (1989)	Q	
	6.6×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,3,3',4',5',6-hexachlorobiphenyl	9.5×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	1.0×10^{-1}		Burkhard et al. (1985)	V	
(PCB-164)	1.6×10^{-1}		Fang Lee (2007)	Q	721
[74472-45-0]	2.3×10^{-1}		Fang Lee (2007)	Q	722
HAZQOLYHFUUJJN-UHFFFAOYSA-N	5.6×10^{-2}		Dunnivant et al. (1992)	Q	
	5.0×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3,3',5,5',6-hexachlorobiphenyl	3.4×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_4Cl_6$	2.5×10^{-3}	6400	Paasivirta and Sinkkonen (2009)	V	
(PCB-165)	3.2×10^{-2}		Burkhard et al. (1985)	V	
[74472-46-1]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
ZEATXTCWXKQPHO-UHFFFAOYSA-N	8.7×10^{-2}		Duchowicz et al. (2020)	Q	
	1.6×10^{-1}		Hilal et al. (2008)	Q	
	2.1×10^{-1}		Modarresi et al. (2007)	Q	67
	3.0×10^{-1}		Fang Lee (2007)	Q	721
	2.9×10^{-1}		Fang Lee (2007)	Q	722
	3.6×10^{-2}		Dunnivant et al. (1992)	Q	
	2.2×10^{-2}		Sabljić and Güsten (1989)	Q	
	3.4×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,3,4,4',5,6-hexachlorobiphenyl	3.5×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	4.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-166)	1.2×10^{-1}		Hilal et al. (2008)	Q	
[41411-63-6]	3.1×10^{-1}		Modarresi et al. (2007)	Q	67
BTOCFTAWZMMTNB-UHFFFAOYSA-N	9.8×10^{-2}		Fang Lee (2007)	Q	721
	2.9×10^{-1}		Fang Lee (2007)	Q	722
		4100	Kühne et al. (2005)	Q	
	5.4×10^{-2}		Dunnivant et al. (1992)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

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	5.7×10^{-2}		Sabljić and Güsten (1989)	Q	
		5800	Kühne et al. (2005)	?	
2,3',4,4',5,5'-hexachlorobiphenyl	7.8×10^{-2}		Fang et al. (2006)	M	
$C_{12}H_4Cl_6$	2.7×10^{-2}	13000	Bamford et al. (2002)	M	
(PCB-167)	7.3×10^{-3}	6400	Paasivirta and Sinkkonen (2009)	V	
[52663-72-6]	1.9×10^{-1}		Burkhard et al. (1985)	V	
AZXHAWRMEPZSSV-UHFFFAOYSA-N	1.6×10^{-1}		Fang Lee (2007)	Q	721
	1.4×10^{-1}		Fang Lee (2007)	Q	722
	9.0×10^{-2}		Dunnivant et al. (1992)	Q	
	8.0×10^{-2}		Sabljić and Güsten (1989)	Q	
2,3',4,4',5',6-hexachlorobiphenyl	1.1×10^{-2}	6700	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_4Cl_6$	7.7×10^{-2}		Burkhard et al. (1985)	V	
(PCB-168)	9.4×10^{-2}		Fang Lee (2007)	Q	721
[59291-65-5]	1.2×10^{-1}		Fang Lee (2007)	Q	722
PITHIPNORFGJPI-UHFFFAOYSA-N	3.6×10^{-2}		Dunnivant et al. (1992)	Q	
	2.1×10^{-2}		Sabljić and Güsten (1989)	Q	
3,3',4,4',5,5'-hexachlorobiphenyl	8.1×10^{-2}		Fang et al. (2006)	M	
$C_{12}H_4Cl_6$	4.7×10^{-2}	19000	Bamford et al. (2002)	M	
(PCB-169)	4.0×10^{-4}	5100	Paasivirta and Sinkkonen (2009)	V	
[32774-16-6]	6.4×10^{-1}		Burkhard et al. (1985)	V	
ZHLICBPIXDOFFG-UHFFFAOYSA-N	2.3×10^{-2}	9000	Paasivirta et al. (1999)	T	
	3.4×10^{-1}		Fang Lee (2007)	Q	721
	1.3×10^{-1}		Fang Lee (2007)	Q	722
	1.5×10^{-1}		Dunnivant et al. (1992)	Q	
	1.7×10^{-1}		Sabljić and Güsten (1989)	Q	
2,2',3,3',4,4',5-heptachlorobiphenyl	4.8×10^{-2}	20000	Bamford et al. (2000)	M	
$C_{12}H_3Cl_7$	1.1		Brunner et al. (1990)	M	
(PCB-170)	6.6×10^{-1}		Murphy et al. (1987)	M	12
[35065-30-6]	7.8×10^{-3}	6600	Paasivirta and Sinkkonen (2009)	V	
RMPWIIKNWPVWNG-UHFFFAOYSA-N	5.2×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	3.9×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.5×10^{-2}		Bhangare et al. (2019)	Q	
	2.1×10^{-1}		Hilal et al. (2008)	Q	
	3.2×10^{-1}		Modarresi et al. (2007)	Q	67
	2.8×10^{-1}		Fang Lee (2007)	Q	721
	4.0×10^{-1}		Fang Lee (2007)	Q	722
	1.1×10^{-1}		Dunnivant et al. (1992)	Q	
	1.1		Duchowicz et al. (2020)	?	185, 21

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,4',6-heptachlorobiphenyl	2.9×10^{-2}		Duchowicz et al. (2020)	V	186
$C_{12}H_3Cl_7$	1.3×10^{-2}	7100	Paasivirta and Sinkkonen (2009)	V	
(PCB-171)	1.9×10^{-1}		Mackay et al. (2006b)	V	
[52663-71-5]	1.9×10^{-1}		Mackay et al. (1992a)	V	
TZMHVHLTPWKZCI-UHFFFAOYSA-N	1.9×10^{-1}		Shiu and Mackay (1986)	V	
	3.4×10^{-2}		Burkhard et al. (1985)	V	
	2.3×10^{-1}		Duchowicz et al. (2020)	Q	
	2.1×10^{-1}		Hilal et al. (2008)	Q	
	2.8×10^{-1}		Modarresi et al. (2007)	Q	67
	1.7×10^{-1}		Fang Lee (2007)	Q	721
	3.1×10^{-1}		Fang Lee (2007)	Q	722
	5.7×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,3',4,5,5'-heptachlorobiphenyl	7.6×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_3Cl_7$	8.3×10^{-3}	6800	Paasivirta and Sinkkonen (2009)	V	
(PCB-172)	3.1×10^{-2}		Burkhard et al. (1985)	V	
[52663-74-8]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
HOPMUCXYRNOABF-UHFFFAOYSA-N	2.1×10^{-1}		Duchowicz et al. (2020)	Q	184
	3.2×10^{-1}		Modarresi et al. (2007)	Q	67
	5.6×10^{-1}		Fang Lee (2007)	Q	721
	3.8×10^{-1}		Fang Lee (2007)	Q	722
	8.3×10^{-2}		Dunnivant et al. (1992)	Q	
	7.6		Duchowicz et al. (2020)	?	185, 21
2,2',3,3',4,5,6-heptachlorobiphenyl	7.0×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_3Cl_7$	1.3×10^{-3}	6500	Paasivirta and Sinkkonen (2009)	V	
(PCB-173)	3.3×10^{-2}		Burkhard et al. (1985)	V	
[68194-16-1]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
PAYFWJAKKLILIT-UHFFFAOYSA-N	2.1×10^{-1}		Duchowicz et al. (2020)	Q	
	1.8×10^{-1}		Hilal et al. (2008)	Q	
	3.5×10^{-1}		Modarresi et al. (2007)	Q	67
	3.1×10^{-1}		Fang Lee (2007)	Q	721
	5.9×10^{-1}		Fang Lee (2007)	Q	722
	5.4×10^{-2}		Dunnivant et al. (1992)	Q	
	7.0×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,3',4,5,6'-heptachlorobiphenyl	2.2×10^{-2}	14000	Bamford et al. (2002)	M	
$C_{12}H_3Cl_7$	7.0×10^{-1}		Brunner et al. (1990)	M	
(PCB-174)	2.0×10^{-1}		Murphy et al. (1987)	M	12
[38411-25-5]	5.4×10^{-3}	6700	Paasivirta and Sinkkonen (2009)	V	
ZDLMBNHYTPHDLF-UHFFFAOYSA-N	1.3×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	299
	2.6×10^{-1}		Hilal et al. (2008)	Q	
	3.3×10^{-1}		Modarresi et al. (2007)	Q	67
	3.1×10^{-1}		Fang Lee (2007)	Q	721

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.3×10^{-1}		Fang Lee (2007)	Q	722
	5.8×10^{-2}		Dunnivant et al. (1992)	Q	
	7.0×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,3',4,5',6- heptachlorobiphenyl	1.0×10^{-2}	7200	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_3Cl_7$	2.0×10^{-2}		Burkhard et al. (1985)	V	
(PCB-175)	3.4×10^{-1}		Fang Lee (2007)	Q	721
[40186-70-7]	3.0×10^{-1}		Fang Lee (2007)	Q	722
KJBDZJFSYQUNJT-UHFFFAOYSA-N	4.4×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,3',4,6,6'- heptachlorobiphenyl	1.1×10^{-1}		Murphy et al. (1987)	M	12
$C_{12}H_3Cl_7$	8.5×10^{-3}	7200	Paasivirta and Sinkkonen (2009)	V	
(PCB-176)	1.0×10^{-2}		Burkhard et al. (1985)	V	
[52663-65-7]	1.9×10^{-1}		Fang Lee (2007)	Q	721
HGMYRFJAJNYBRX-UHFFFAOYSA-N	2.6×10^{-1}		Fang Lee (2007)	Q	722
	3.3×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,3',4,5',6'- heptachlorobiphenyl	2.1×10^{-2}	13000	Bamford et al. (2002)	M	
$C_{12}H_3Cl_7$	3.0×10^{-1}		Murphy et al. (1987)	M	12
(PCB-177)	4.5×10^{-3}		Murphy et al. (1983a)	M	24
[52663-70-4]	3.4×10^{-3}	6600	Paasivirta and Sinkkonen (2009)	V	
CXOYNJAHPUASHN-UHFFFAOYSA-N	3.8×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Fang Lee (2007)	Q	721
	5.3×10^{-1}		Fang Lee (2007)	Q	722
	6.0×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,3',5,5',6- heptachlorobiphenyl	1.5×10^{-2}	11000	Bamford et al. (2002)	M	
$C_{12}H_3Cl_7$	4.3×10^{-1}		Brunner et al. (1990)	M	
(PCB-178)	1.5×10^{-1}		Murphy et al. (1987)	M	12
[52663-67-9]	1.0×10^{-2}	7200	Paasivirta and Sinkkonen (2009)	V	
WCIBKXHMIXUQHK-UHFFFAOYSA-N	2.3×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.2×10^{-1}		Duchowicz et al. (2020)	Q	184
	2.7×10^{-1}		Hilal et al. (2008)	Q	
	3.0×10^{-1}		Modarresi et al. (2007)	Q	67
	4.8×10^{-1}		Fang Lee (2007)	Q	721
	5.6×10^{-1}		Fang Lee (2007)	Q	722
	4.6×10^{-2}		Dunnivant et al. (1992)	Q	
	4.3×10^{-1}		Duchowicz et al. (2020)	?	185, 21

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',5,6,6'- heptachlorobiphenyl	4.1×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_3Cl_7$	4.2×10^{-3}	7000	Paasivirta and Sinkkonen (2009)	V	
(PCB-179)	1.1×10^{-2}		Burkhard et al. (1985)	V	
[52663-64-6]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
XYHVYEUZLSYHDP-UHFFFAOYSA-N	1.2×10^{-1}		Duchowicz et al. (2020)	Q	299
	3.1×10^{-1}		Hilal et al. (2008)	Q	
	3.1×10^{-1}		Modarresi et al. (2007)	Q	67
	2.6×10^{-1}		Fang Lee (2007)	Q	721
	4.8×10^{-1}		Fang Lee (2007)	Q	722
	3.6×10^{-2}		Dunnivant et al. (1992)	Q	
	4.1×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,4,4',5,5'- heptachlorobiphenyl	1.7×10^{-1}	7300	Li et al. (2003)	L	366
$C_{12}H_3Cl_7$	1.2×10^{-1}	7900	Li et al. (2003)	L	367
(PCB-180)	2.7×10^{-2}	17000	Bamford et al. (2000)	M	
[35065-29-3]	9.9×10^{-1}		Brunner et al. (1990)	M	
WBHQEUPUMONIKF-UHFFFAOYSA-N	3.1×10^{-1}		Murphy et al. (1987)	M	12
	1.5×10^{-2}	6900	Paasivirta and Sinkkonen (2009)	V	
	3.3×10^{-2}		Burkhard et al. (1985)	V	
	2.5×10^{-2}	9000	Paasivirta et al. (1999)	T	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	2.1×10^{-1}		Duchowicz et al. (2020)	Q	299
	1.4×10^{-2}		Bhangare et al. (2019)	Q	
	2.1×10^{-1}		Hilal et al. (2008)	Q	
	3.5×10^{-1}		Modarresi et al. (2007)	Q	67
	2.8×10^{-1}		Fang Lee (2007)	Q	721
	3.0×10^{-1}		Fang Lee (2007)	Q	722
	9.2×10^{-2}		Dunnivant et al. (1992)	Q	
	9.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,4,4',5,6-heptachlorobiphenyl	1.2×10^{-2}	7200	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_3Cl_7$	2.4×10^{-2}		Burkhard et al. (1985)	V	
(PCB-181)	1.6×10^{-1}		Fang Lee (2007)	Q	721
[74472-47-2]	3.8×10^{-1}		Fang Lee (2007)	Q	722
DJEUXBQAKBLKPO-UHFFFAOYSA-N	4.3×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,4,4',5,6'- heptachlorobiphenyl	1.7×10^{-2}	12000	Bamford et al. (2002)	M	
$C_{12}H_3Cl_7$	1.7×10^{-2}	7200	Paasivirta and Sinkkonen (2009)	V	
(PCB-182)	1.0×10^{-2}		Burkhard et al. (1985)	V	
[60145-23-5]	1.5×10^{-1}		Fang Lee (2007)	Q	721
RXRLRYZUMSYVLS-UHFFFAOYSA-N	2.1×10^{-1}		Fang Lee (2007)	Q	722
	3.8×10^{-2}		Dunnivant et al. (1992)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,4',5',6- heptachlorobiphenyl	1.7×10^{-2}	12000	Bamford et al. (2002)	M	
$C_{12}H_3Cl_7$	1.5×10^{-1}		Murphy et al. (1987)	M	12
(PCB-183)	1.6×10^{-2}		Murphy et al. (1983a)	M	24
[52663-69-1]	2.4×10^{-2}	7400	Paasivirta and Sinkkonen (2009)	V	
KQBFUDNJKCZEDQ-UHFFFAOYSA-N	2.1×10^{-2}		Burkhard et al. (1985)	V	
	1.7×10^{-1}		Fang Lee (2007)	Q	721
	2.5×10^{-1}		Fang Lee (2007)	Q	722
	4.9×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,4,4',6,6'- heptachlorobiphenyl	8.1×10^{-3}	7200	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_3Cl_7$	7.9×10^{-3}		Burkhard et al. (1985)	V	
(PCB-184)	9.4×10^{-2}		Fang Lee (2007)	Q	721
[74472-48-3]	1.3×10^{-1}		Fang Lee (2007)	Q	722
OBIUJJSQKPGKME-UHFFFAOYSA-N	2.2×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,4,5,5',6-heptachlorobiphenyl	6.2×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_3Cl_7$	4.9×10^{-3}	7000	Paasivirta and Sinkkonen (2009)	V	
(PCB-185)	2.2×10^{-2}		Burkhard et al. (1985)	V	
[52712-05-7]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
PYZHTHZEHQHHEN-UHFFFAOYSA-N	1.1×10^{-1}		Duchowicz et al. (2020)	Q	299
	1.5×10^{-1}		Hilal et al. (2008)	Q	
	3.4×10^{-1}		Modarresi et al. (2007)	Q	67
	3.1×10^{-1}		Fang Lee (2007)	Q	721
	4.3×10^{-1}		Fang Lee (2007)	Q	722
	4.6×10^{-2}		Dunnivant et al. (1992)	Q	
	6.2×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,4,5,6,6'-heptachlorobiphenyl	9.6×10^{-4}	6500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_3Cl_7$	1.3×10^{-2}		Burkhard et al. (1985)	V	
(PCB-186)	1.7×10^{-1}		Fang Lee (2007)	Q	721
[74472-49-4]	3.7×10^{-1}		Fang Lee (2007)	Q	722
FGDPOTMRBQHPJK-UHFFFAOYSA-N	2.7×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,4',5,5',6- heptachlorobiphenyl	1.6×10^{-2}	12000	Bamford et al. (2000)	M	
$C_{12}H_3Cl_7$	1.2×10^{-1}		Murphy et al. (1987)	M	12
(PCB-187)	1.3×10^{-2}	7200	Paasivirta and Sinkkonen (2009)	V	
[52663-68-0]	2.4×10^{-2}		Burkhard et al. (1985)	V	
UDMZPLROONOSEF-UHFFFAOYSA-N	2.4×10^{-1}		Fang Lee (2007)	Q	721
	4.3×10^{-1}		Fang Lee (2007)	Q	722
	4.9×10^{-2}		Dunnivant et al. (1992)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4',5,6,6'-heptachlorobiphenyl	8.8×10^{-3}	7500	Bamford et al. (2000)	M	
$C_{12}H_3Cl_7$	4.8×10^{-3}	7100	Paasivirta and Sinkkonen (2009)	V	
(PCB-188)	8.8×10^{-3}		Burkhard et al. (1985)	V	
[74487-85-7]	1.6×10^{-2}		Bhangare et al. (2019)	Q	
MMTJWDQKGUNSDK-UHFFFAOYSA-N	1.3×10^{-1}		Fang Lee (2007)	Q	721
	2.3×10^{-1}		Fang Lee (2007)	Q	722
	2.2×10^{-2}		Dunnivant et al. (1992)	Q	
2,3,3',4,4',5,5'-heptachlorobiphenyl	8.4×10^{-2}		Fang et al. (2006)	M	
$C_{12}H_3Cl_7$	4.1×10^{-3}	6300	Paasivirta and Sinkkonen (2009)	V	
(PCB-189)	1.1×10^{-1}		Burkhard et al. (1985)	V	
[39635-31-9]	3.4×10^{-1}		Fang Lee (2007)	Q	721
XUAWBXBYHDRROL-UHFFFAOYSA-N	3.0×10^{-1}		Fang Lee (2007)	Q	722
	1.5×10^{-1}		Dunnivant et al. (1992)	Q	
2,3,3',4,4',5,6-heptachlorobiphenyl	1.5×10^{-2}	7000	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_3Cl_7$	9.9×10^{-2}		Burkhard et al. (1985)	V	
(PCB-190)	1.9×10^{-1}		Fang Lee (2007)	Q	721
[41411-64-7]	5.3×10^{-1}		Fang Lee (2007)	Q	722
TYEDCFVCFDKSBK-UHFFFAOYSA-N	8.8×10^{-2}		Dunnivant et al. (1992)	Q	
2,3,3',4,4',5',6-heptachlorobiphenyl	2.1×10^{-2}	7200	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_3Cl_7$	5.8×10^{-2}		Burkhard et al. (1985)	V	
(PCB-191)	2.1×10^{-1}		Fang Lee (2007)	Q	721
[74472-50-7]	3.2×10^{-1}		Fang Lee (2007)	Q	722
TVFXBXWAXIMLAQ-UHFFFAOYSA-N	7.4×10^{-2}		Dunnivant et al. (1992)	Q	
2,3,3',4,5,5',6-heptachlorobiphenyl	4.9×10^{-3}	6900	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_3Cl_7$	6.1×10^{-2}		Burkhard et al. (1985)	V	
(PCB-192)	3.8×10^{-1}		Fang Lee (2007)	Q	721
[74472-51-8]	5.0×10^{-1}		Fang Lee (2007)	Q	722
ZUTDUGMNROUBOX-UHFFFAOYSA-N	5.2×10^{-2}		Dunnivant et al. (1992)	Q	
2,3,3',4',5,5',6-heptachlorobiphenyl	3.2×10^{-2}	17000	Bamford et al. (2002)	M	
$C_{12}H_3Cl_7$	7.5×10^{-3}	6800	Paasivirta and Sinkkonen (2009)	V	
(PCB-193)	1.0×10^{-1}		Burkhard et al. (1985)	V	
[69782-91-8]	2.9×10^{-1}		Fang Lee (2007)	Q	721
SSTJUBQGYXNFFP-UHFFFAOYSA-N	5.6×10^{-1}		Fang Lee (2007)	Q	722
	7.3×10^{-2}		Dunnivant et al. (1992)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,4',5,5'- octachlorobiphenyl	1.5×10^{-1}	7500	Li et al. (2003)	L	366
$C_{12}H_2Cl_8$	2.3×10^{-1}	8200	Li et al. (2003)	L	367
(PCB-194)	1.0×10^{-1}	20000	Bamford et al. (2002)	M	
[35694-08-7]	9.9×10^{-1}		Brunner et al. (1990)	M	
DTMRKGRREZAYAP-UHFFFAOYSA-N	8.0×10^{-3}	6900	Paasivirta and Sinkkonen (2009)	V	
	2.1×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	4.0×10^{-1}		Duchowicz et al. (2020)	Q	184
	2.3×10^{-1}		Hilal et al. (2008)	Q	
	4.8×10^{-1}		Modarresi et al. (2007)	Q	67
	5.6×10^{-1}		Fang Lee (2007)	Q	721
	7.1×10^{-1}		Fang Lee (2007)	Q	722
		6500	Kühne et al. (2005)	Q	
	1.5×10^{-1}		Dunnivant et al. (1992)	Q	
	9.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		6600	Kühne et al. (2005)	?	
2,2',3,3',4,4',5,6- octachlorobiphenyl	7.1×10^{-2}	20000	Bamford et al. (2000)	M	
$C_{12}H_2Cl_8$	9.0×10^{-1}		Brunner et al. (1990)	M	
(PCB-195)	7.1×10^{-3}	7100	Paasivirta and Sinkkonen (2009)	V	
[52663-78-2]	7.8×10^{-2}		Burkhard et al. (1985)	V	
JAHJITLFJSDRCG-UHFFFAOYSA-N	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	3.1×10^{-1}		Duchowicz et al. (2020)	Q	299
	2.4×10^{-1}		Hilal et al. (2008)	Q	
	4.5×10^{-1}		Modarresi et al. (2007)	Q	67
	3.1×10^{-1}		Fang Lee (2007)	Q	721
	1.0		Fang Lee (2007)	Q	722
	8.3×10^{-2}		Dunnivant et al. (1992)	Q	
	9.0×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,3',4,4',5,6'- octachlorobiphenyl	9.9×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_2Cl_8$	1.8×10^{-2}	7400	Paasivirta and Sinkkonen (2009)	V	
(PCB-196)	1.4×10^{-2}		Burkhard et al. (1985)	V	
[42740-50-1]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
BQFCCUSDZLKBJG-UHFFFAOYSA-N	2.4×10^{-1}		Duchowicz et al. (2020)	Q	
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	5.0×10^{-1}		Modarresi et al. (2007)	Q	67
	3.4×10^{-1}		Fang Lee (2007)	Q	721
	6.2×10^{-1}		Fang Lee (2007)	Q	722
	7.6×10^{-2}		Dunnivant et al. (1992)	Q	
	9.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,4',6,6'- octachlorobiphenyl	1.3×10^{-2}	7600	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_2Cl_8$	1.1×10^{-2}		Burkhard et al. (1985)	V	
(PCB-197)	1.9×10^{-1}		Fang Lee (2007)	Q	721
[33091-17-7]	4.2×10^{-1}		Fang Lee (2007)	Q	722
YPDBBDKYNWRFMF-UHFFFAOYSA-N	3.9×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,3',4,5,5',6- octachlorobiphenyl	7.0×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_2Cl_8$	3.5×10^{-3}	7000	Paasivirta and Sinkkonen (2009)	V	
(PCB-198)	4.8×10^{-2}		Burkhard et al. (1985)	V	
[68194-17-2]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
PJHBSPRZHUOIAS-UHFFFAOYSA-N	1.7×10^{-1}		Duchowicz et al. (2020)	Q	299
	2.5×10^{-1}		Hilal et al. (2008)	Q	
	4.5×10^{-1}		Modarresi et al. (2007)	Q	67
	6.2×10^{-1}		Fang Lee (2007)	Q	721
	1.0		Fang Lee (2007)	Q	722
	6.4×10^{-2}		Dunnivant et al. (1992)	Q	
	7.0×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,3',4,5,5',6'- octachlorobiphenyl	9.9×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_2Cl_8$	3.4×10^{-3}	7000	Paasivirta and Sinkkonen (2009)	V	
(PCB-199)	2.3×10^{-2}		Burkhard et al. (1985)	V	
[52663-75-9]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
HJBYDWKNARZTMJ-UHFFFAOYSA-N	2.2×10^{-1}		Duchowicz et al. (2020)	Q	299
	2.7×10^{-1}		Hilal et al. (2008)	Q	
	4.7×10^{-1}		Modarresi et al. (2007)	Q	67
	6.2×10^{-1}		Fang Lee (2007)	Q	721
	9.1×10^{-1}		Fang Lee (2007)	Q	722
	4.3×10^{-2}		Dunnivant et al. (1992)	Q	
	9.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,3',4,5,6,6'- octachlorobiphenyl	7.6×10^{-3}	7200	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_2Cl_8$	1.5×10^{-2}		Burkhard et al. (1985)	V	
(PCB-200)	3.4×10^{-1}		Fang Lee (2007)	Q	721
[52663-73-7]	7.7×10^{-1}		Fang Lee (2007)	Q	722
HHXNVASVVVNNDG-UHFFFAOYSA-N	4.1×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,3',4,5',6,6'- octachlorobiphenyl	1.0×10^{-2}	17000	Bamford et al. (2000)	M	
$C_{12}H_2Cl_8$	5.8×10^{-1}		Brunner et al. (1990)	M	
(PCB-201)	1.2×10^{-2}	7500	Paasivirta and Sinkkonen (2009)	V	
[40186-71-8]	1.5×10^{-2}		Burkhard et al. (1985)	V	
LJQOBQLZTUSEJA-UHFFFAOYSA-N	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.3×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.3×10^{-2}		Bhangare et al. (2019)	Q	
	2.9×10^{-1}		Hilal et al. (2008)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	5.1×10^{-1}		Modarresi et al. (2007)	Q	67
	3.7×10^{-1}		Fang Lee (2007)	Q	721
	1.1		Fang Lee (2007)	Q	722
	7.6×10^{-2}		Dunnivant et al. (1992)	Q	
	5.8×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,2',3,3',5,5',6,6'- octachlorobiphenyl	5.5×10^{-1}		Brunner et al. (1990)	M	
$C_{12}H_2Cl_8$	5.0×10^{-3}	7300	Paasivirta and Sinkkonen (2009)	V	
(PCB-202)	2.6×10^{-2}		Mackay et al. (2006b)	V	
[2136-99-4]	2.6×10^{-2}		Mackay et al. (1992a)	V	
JPOPEORRMSDUIP-UHFFFAOYSA-N	2.7×10^{-2}		Shiu and Mackay (1986)	V	
	1.3×10^{-2}		Burkhard et al. (1985)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.2×10^{-1}		Duchowicz et al. (2020)	Q	
	3.7×10^{-1}		Hilal et al. (2008)	Q	
	5.5×10^{-1}		Modarresi et al. (2007)	Q	67
	5.3×10^{-1}		Fang Lee (2007)	Q	721
	1.4		Fang Lee (2007)	Q	722
		4700	Kühne et al. (2005)	Q	
	4.4×10^{-2}		Dunnivant et al. (1992)	Q	
	5.5×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		5000	Kühne et al. (2005)	?	
2,2',3,4,4',5,5',6- octachlorobiphenyl	3.2×10^{-2}	7800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_2Cl_8$	5.0×10^{-2}		Burkhard et al. (1985)	V	
(PCB-203)	1.3×10^{-2}		Bhangare et al. (2019)	Q	
[52663-76-0]	3.1×10^{-1}		Fang Lee (2007)	Q	721
DCPDZFRGNJDWPP-UHFFFAOYSA-N	7.7×10^{-1}		Fang Lee (2007)	Q	722
	7.0×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,4,4',5,6,6'- octachlorobiphenyl	1.1×10^{-2}	7800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_2Cl_8$	1.9×10^{-2}		Burkhard et al. (1985)	V	
(PCB-204)	1.3×10^{-2}		Bhangare et al. (2019)	Q	
[74472-52-9]	1.7×10^{-1}		Fang Lee (2007)	Q	721
JDZUWXRNKHXZFE-UHFFFAOYSA-N	4.5×10^{-1}		Fang Lee (2007)	Q	722
	2.9×10^{-2}		Dunnivant et al. (1992)	Q	
2,3,3',4,4',5,5',6- octachlorobiphenyl	4.4×10^{-3}	6800	Paasivirta and Sinkkonen (2009)	V	
$C_{12}H_2Cl_8$	2.1×10^{-1}		Burkhard et al. (1985)	V	
(PCB-205)	1.2×10^{-2}		Bhangare et al. (2019)	Q	
[74472-53-0]	3.8×10^{-1}		Fang Lee (2007)	Q	721
VXXBCDUYUQKWCK-UHFFFAOYSA-N	9.1×10^{-1}		Fang Lee (2007)	Q	722
	1.1×10^{-1}		Dunnivant et al. (1992)	Q	

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Table A6.3: Polychlorinated biphenyls (PCBs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,4',5,5',6- nonachlorobiphenyl	2.1×10^{-3}	7300	Paasivirta and Sinkkonen (2009)	V	
$C_{12}HCl_9$	1.2		Mackay et al. (2006b)	V	
(PCB-206)	1.2×10^{-2}		Mackay et al. (1992a)	V	
[40186-72-9]	3.6×10^{-2}		Burkhard et al. (1985)	V	
JFIMDKGRGPNPRQ-UHFFFAOYSA-N	1.1×10^{-2}		Bhangare et al. (2019)	Q	
	6.2×10^{-1}		Fang Lee (2007)	Q	721
	2.0		Fang Lee (2007)	Q	722
	1.1×10^{-1}		Dunnivant et al. (1992)	Q	
2,2',3,3',4,4',5,6,6'- nonachlorobiphenyl	1.8×10^{-3}	7500	Paasivirta and Sinkkonen (2009)	V	
$C_{12}HCl_9$	2.8×10^{-2}		Burkhard et al. (1985)	V	
(PCB-207)	1.1×10^{-2}		Bhangare et al. (2019)	Q	
[52663-79-3]	3.3×10^{-1}		Fang Lee (2007)	Q	721
YGDPIDTZOQGPAX-UHFFFAOYSA-N	1.4		Fang Lee (2007)	Q	722
	5.8×10^{-2}		Dunnivant et al. (1992)	Q	
2,2',3,3',4,5,5',6,6'- nonachlorobiphenyl	3.0×10^{-3}	7700	Paasivirta and Sinkkonen (2009)	V	
$C_{12}HCl_9$	3.1×10^{-2}		Burkhard et al. (1985)	V	
(PCB-208)	1.2×10^{-2}		Bhangare et al. (2019)	Q	
[52663-77-1]	6.7×10^{-1}		Fang Lee (2007)	Q	721
XIFFTDRFWYFAPO-UHFFFAOYSA-N	2.5		Fang Lee (2007)	Q	722
	5.9×10^{-2}		Dunnivant et al. (1992)	Q	
decachlorobiphenyl	1.0×10^{-3}		Duchowicz et al. (2020)	V	186
$C_{12}Cl_{10}$	6.7×10^{-4}	7200	Paasivirta and Sinkkonen (2009)	V	
(PCB-209)			Mackay et al. (2006b)	V	683
[2051-24-3]	4.8×10^{-2}		Mackay et al. (1992a)	V	
ONXPZLFXDMAPRO-UHFFFAOYSA-N	4.8×10^{-2}		Shiu and Mackay (1986)	V	
	8.0×10^{-2}		Burkhard et al. (1985)	V	
	2.6×10^{-1}		Duchowicz et al. (2020)	Q	
	1.0×10^{-2}		Bhangare et al. (2019)	Q	
	3.1×10^{-1}		Hilal et al. (2008)	Q	
	6.7×10^{-1}		Fang Lee (2007)	Q	721
	5.0		Fang Lee (2007)	Q	722
		6100	Kühne et al. (2005)	Q	
	8.8×10^{-2}		Dunnivant et al. (1992)	Q	
		7300	Kühne et al. (2005)	?	

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A6.4 Oxygenated chlorocarbons (C, H, O, Cl)

Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
phosgene	5.9×10^{-4}	3800	De Bruyn et al. (1995a)	M	
CCl_2O	6.8×10^{-4}	4200	Manogue and Pigford (1960)	M	
[75-44-5]	7.0×10^{-4}		Yaws (2003)	X	237
YGYAWVDWMABLBF-UHFFFAOYSA-N	5.3×10^{-4}		Hayer et al. (2022)	Q	20
	8.8×10^{-3}		Keshavarz et al. (2022)	Q	
	6.1×10^{-2}		Duchowicz et al. (2020)	Q	
	3.7×10^{-1}		Wang et al. (2017)	Q	80, 238
	1.4×10^{-2}		Wang et al. (2017)	Q	80, 239
	1.1×10^{-4}		Wang et al. (2017)	Q	80, 240
	6.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
	5.9×10^{-4}		Duchowicz et al. (2020)	?	185, 21
	7.1×10^{-4}		Yaws (1999)	?	21
MCM:CCL3OOH	2.1×10^{1}		Wang et al. (2017)	Q	80, 238
CHO_2Cl_3	4.9		Wang et al. (2017)	Q	80, 239
DUBMHDTUZCIGCY-UHFFFAOYSA-N	3.8		Wang et al. (2017)	Q	80, 240
MCM:CH2CLOOH	1.8×10^{1}		Wang et al. (2017)	Q	80, 238
CH_3O_2Cl	6.2×10^{1}		Wang et al. (2017)	Q	80, 239
DUNYOPWYTOSXOC-UHFFFAOYSA-N	1.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CHCL2OOH	4.7×10^{1}		Wang et al. (2017)	Q	80, 238
$CH_2O_2Cl_2$	1.3×10^{2}		Wang et al. (2017)	Q	80, 239
TUIYYMKEIGYDJB-UHFFFAOYSA-N	5.6		Wang et al. (2017)	Q	80, 240
MCM:CCL3OH	4.7		Wang et al. (2017)	Q	80, 238
$CHOCl_3$	8.1×10^{-1}		Wang et al. (2017)	Q	80, 239
GYLIOGDFGLKMOL-UHFFFAOYSA-N	4.0×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CH2CLOH	1.9		Wang et al. (2017)	Q	80, 238
CH_3OCl	1.9×10^{1}		Wang et al. (2017)	Q	80, 239
BCUPGIHTCQJCSI-UHFFFAOYSA-N	1.1×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CHCL2OH	6.6		Wang et al. (2017)	Q	80, 238
CH_2OCl_2	1.2×10^{1}		Wang et al. (2017)	Q	80, 239
GJYVZUKSNFSLCL-UHFFFAOYSA-N	2.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CHOCL	2.2×10^{-1}		Wang et al. (2017)	Q	80, 238
CHOCl	2.0×10^{-2}		Wang et al. (2017)	Q	80, 239
GFAUNYMRSKVDJL-UHFFFAOYSA-N	3.0×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:CLCO2H	3.2×10^{1}		Wang et al. (2017)	Q	80, 238
CHO_2Cl	8.5		Wang et al. (2017)	Q	80, 239
AOGYCOYQMAVAFD-UHFFFAOYSA-N	9.1×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dichloroacetaldehyde	4.7×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_2H_2Cl_2O$	7.4×10^{-1}		Wang et al. (2017)	Q	80, 239
[79-02-7]	1.1×10^{-2}		Wang et al. (2017)	Q	80, 240
NWQWQKUXRJYXFH-UHFFFAOYSA-N	1.2		HSDB (2015)	Q	99
chloroacetyl chloride	2.9×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_2H_2Cl_2O$	1.3×10^{-1}		Wang et al. (2017)	Q	80, 239
[79-04-9]	4.3×10^{-2}		Wang et al. (2017)	Q	80, 240
VGCXGMAHQTYDJK-UHFFFAOYSA-N	4.3×10^{-2}		HSDB (2015)	Q	99
chloral hydrate	2.4×10^{3}		HSDB (2015)	V	
$C_2H_3Cl_3O_2$					
[302-17-0]					
RNFNDJAIBTYOQL-UHFFFAOYSA-N					
chloroacetaldehyde	1.9×10^{-1}		Wang et al. (2017)	Q	80, 238
C_2H_3ClO	2.3		Wang et al. (2017)	Q	80, 239
[107-20-0]	3.5		Wang et al. (2017)	Q	80, 240
QSKPIOLLBIHNAC-UHFFFAOYSA-N	4.1×10^{-1}		HSDB (2015)	Q	99
2-chloroethanol	1.3×10^{1}		Duchowicz et al. (2020)	V	186
C_2H_5ClO	3.3		Duchowicz et al. (2020)	Q	
[107-07-3]	1.1		Wang et al. (2017)	Q	80, 238
SZIFAVKTNFCBPC-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	80, 239
	4.7		Wang et al. (2017)	Q	80, 240
	9.5×10^{1}		HSDB (2015)	Q	99
	2.8×10^{1}		Modarresi et al. (2007)	Q	67
	1.4×10^{1}		Yaffe et al. (2003)	Q	248, 249
	1.7×10^{1}		Katritzky et al. (1998)	Q	
2,2-dichloroethanol	3.7×10^{-1}		Burkholder et al. (2019)	L	
$C_2H_4Cl_2O$	3.7×10^{-1}		Burkholder et al. (2015)	L	
[598-38-9]	3.7×10^{-1}		O'Farrell and Waghorne (2010)	M	
IDJOCJAIQSKSOP-UHFFFAOYSA-N	3.2		Wang et al. (2017)	Q	80, 238
	2.6×10^{1}		Wang et al. (2017)	Q	80, 239
	6.9		Wang et al. (2017)	Q	80, 240
2-chloroethanol-d4	5.0	8700	Hiatt (2013)	M	
ClC_2D_4OH					
[117067-62-6]					
SZIFAVKTNFCBPC-LNLMKGTHSA-N					
MCM:CCL2CL2OOH	3.9×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_2O_2Cl_4$	7.1×10^{1}		Wang et al. (2017)	Q	80, 239
SWNDCAXLXSSRFN-UHFFFAOYSA-N	1.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CCL3CH2OOH	1.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_2H_3O_2Cl_3$	1.8×10^{1}		Wang et al. (2017)	Q	80, 239
RJIYMCLTECJZCN-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	80, 240

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CCL3CO3H	2.6×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2HO_3Cl_3$	5.9		Wang et al. (2017)	Q	80, 239
DRTNVNKYVPOWCY-UHFFFAOYSA-N	1.4		Wang et al. (2017)	Q	80, 240
MCM:CH2CL3OOH	1.2×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_3O_2Cl_3$	3.8×10^{1}		Wang et al. (2017)	Q	80, 239
CHVIFDTZRLKJET-UHFFFAOYSA-N	1.3×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CH2CLCOOH	1.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_2H_5O_2Cl$	6.3×10^{1}		Wang et al. (2017)	Q	80, 239
PIXGNJBYAUTOCI-UHFFFAOYSA-N	5.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CH3CCL2OOH	1.2×10^{1}		Wang et al. (2017)	Q	80, 238
$C_2H_4O_2Cl_2$	1.0×10^{1}		Wang et al. (2017)	Q	80, 239
YUVMNUKOYYKKNS-UHFFFAOYSA-N	8.9		Wang et al. (2017)	Q	80, 240
MCM:CH3CHCLOOH	1.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_2H_5O_2Cl$	2.0×10^{1}		Wang et al. (2017)	Q	80, 239
MCYQTMMYWIXRIL-UHFFFAOYSA-N	5.6		Wang et al. (2017)	Q	80, 240
MCM:CHCL2CO3H	5.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_2O_3Cl_2$	4.3×10^{1}		Wang et al. (2017)	Q	80, 239
VWNSYHZUZUFFDM-UHFFFAOYSA-N	8.9		Wang et al. (2017)	Q	80, 240
MCM:CHCL2COOH	3.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_2H_4O_2Cl_2$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
GJBKLBBJOKITMY-UHFFFAOYSA-N	2.7×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CHCL3OOH	4.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_3O_2Cl_3$	1.2×10^{2}		Wang et al. (2017)	Q	80, 239
AMASFZACKVPSTN-UHFFFAOYSA-N	4.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CLETO3H	2.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_3O_3Cl$	5.5×10^{1}		Wang et al. (2017)	Q	80, 239
JSQPGNJFQUOEPA-UHFFFAOYSA-N	1.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DICLETO2H	1.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_4O_2Cl_2$	7.3×10^{1}		Wang et al. (2017)	Q	80, 239
UPXDMONURWDHKL-UHFFFAOYSA-N	4.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:C2CL2OH2	1.4×10^{5}		Wang et al. (2017)	Q	80, 238
$C_2H_4O_2Cl_2$	1.3×10^{4}		Wang et al. (2017)	Q	80, 239
HHQQTVXFKGIICR-UHFFFAOYSA-N	1.2×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:C2CL2OHOOH	2.8×10^{6}		Wang et al. (2017)	Q	80, 238
$C_2H_4O_3Cl_2$	1.7×10^{4}		Wang et al. (2017)	Q	80, 239
NCBKAYIJWMIXBU-UHFFFAOYSA-N	1.4×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:C2CL32OH	1.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_2H_3O_2Cl_3$	5.1×10^{3}		Wang et al. (2017)	Q	80, 239
MYDJEUINZIFHKK-UHFFFAOYSA-N	2.8×10^{7}		Wang et al. (2017)	Q	80, 240

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:C2CL3HOOOH	3.1×10^{6}		Wang et al. (2017)	Q	80, 238
$C_2H_3O_3Cl_3$	1.0×10^{4}		Wang et al. (2017)	Q	80, 239
KHLAQOPQQHOMKQ-UHFFFAOYSA-N	4.3×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:C2CL3OHOOH	2.6×10^{6}		Wang et al. (2017)	Q	80, 238
$C_2H_3O_3Cl_3$	1.1×10^{4}		Wang et al. (2017)	Q	80, 239
CEKNFZNLLTXCLL-UHFFFAOYSA-N	1.1×10^{4}		Wang et al. (2017)	Q	80, 240
trichloroethanol	1.7		Wang et al. (2017)	Q	80, 238
$C_2H_3OCl_3$	3.9		Wang et al. (2017)	Q	80, 239
[115-20-8]	3.2		Wang et al. (2017)	Q	80, 240
KPWDGTGXUYRARH-UHFFFAOYSA-N					
MCM:CCLOHCOOH	1.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_2H_5O_3Cl$	9.6×10^{3}		Wang et al. (2017)	Q	80, 239
MIFGQALJBIDZDW-UHFFFAOYSA-N	1.0×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:CH2CL3OH	2.9×10^{1}		Wang et al. (2017)	Q	80, 238
$C_2H_3OCl_3$	1.3×10^{1}		Wang et al. (2017)	Q	80, 239
HYCHPIPDVAXCCJ-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CH2OHCCLOH	4.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_2H_5O_2Cl$	4.2×10^{3}		Wang et al. (2017)	Q	80, 239
VVKFXODVPQSIHU-UHFFFAOYSA-N	9.3×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CH3CCL2OH	1.6		Wang et al. (2017)	Q	80, 238
$C_2H_4OCl_2$	2.4		Wang et al. (2017)	Q	80, 239
DNBABSPIEDTPHK-UHFFFAOYSA-N	8.1		Wang et al. (2017)	Q	80, 240
MCM:CH3CHCLOH	1.8		Wang et al. (2017)	Q	80, 238
C_2H_5OCl	8.1		Wang et al. (2017)	Q	80, 239
KJESGYZFVCIMDE-UHFFFAOYSA-N	4.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CHCL2CL2OH	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_2OCl_4$	2.2×10^{1}		Wang et al. (2017)	Q	80, 239
LQINPQOSBLVJBS-UHFFFAOYSA-N	3.7×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CHCL3OH	9.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_2H_3OCl_3$	5.6×10^{1}		Wang et al. (2017)	Q	80, 239
NIBKDWIGIKUFKL-UHFFFAOYSA-N	3.4×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CL2OHCH2OH	4.5×10^{3}		Wang et al. (2017)	Q	80, 238
$C_2H_4O_2Cl_2$	1.6×10^{3}		Wang et al. (2017)	Q	80, 239
ZOZPDNLNQWCVSW-UHFFFAOYSA-N	1.6×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:CL2OHCO3H	9.3×10^{4}		Wang et al. (2017)	Q	80, 238
$C_2H_2O_4Cl_2$	4.7		Wang et al. (2017)	Q	80, 239
MACSTFWYVGNISK-UHFFFAOYSA-N	5.9		Wang et al. (2017)	Q	80, 240
MCM:CL2OHOOH	1.7×10^{5}		Wang et al. (2017)	Q	80, 238
$C_2H_4O_3Cl_2$	4.0×10^{3}		Wang et al. (2017)	Q	80, 239
WOJAYLCSWSBEJV-UHFFFAOYSA-N	4.1×10^{5}		Wang et al. (2017)	Q	80, 240

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CLOHCO3H	1.0×10^{5}		Wang et al. (2017)	Q	80, 238
$C_2H_3O_4Cl$	2.5×10^{2}		Wang et al. (2017)	Q	80, 239
IODLIDNNOHQSDW-UHFFFAOYSA-N	1.3×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:COHCCLOOH	1.2×10^{5}		Wang et al. (2017)	Q	80, 238
$C_2H_5O_3Cl$	5.0×10^{3}		Wang et al. (2017)	Q	80, 239
WXPZQCJQULOKCY-UHFFFAOYSA-N	4.4×10^{3}		Wang et al. (2017)	Q	80, 240
MCM:DICLETOH	2.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_2H_4OCl_2$	3.8×10^{1}		Wang et al. (2017)	Q	80, 239
QXBDFCZHAAOUBY-UHFFFAOYSA-N	3.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:TCE2OH	2.9×10^{5}		Wang et al. (2017)	Q	80, 238
$C_2H_2O_2Cl_4$	2.0×10^{3}		Wang et al. (2017)	Q	80, 239
BVBMRJKFECUARX-UHFFFAOYSA-N	4.2×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:TCEOHOOH	3.4×10^{6}		Wang et al. (2017)	Q	80, 238
$C_2H_2O_3Cl_4$	4.3×10^{3}		Wang et al. (2017)	Q	80, 239
YKIXQGIQZGTABG-UHFFFAOYSA-N	1.4×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:CCLOHCHO	8.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_2H_3O_2Cl$	8.9×10^{1}		Wang et al. (2017)	Q	80, 239
RYRGLFUQPWFXSD-UHFFFAOYSA-N	4.4		Wang et al. (2017)	Q	80, 240
MCM:CL2OHCHO	7.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_2H_2O_2Cl_2$	1.0		Wang et al. (2017)	Q	80, 239
LCOUNIIIIIIWZOM-UHFFFAOYSA-N	6.0×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:CH3COCL	1.5×10^{-1}		Wang et al. (2017)	Q	80, 238
C_2H_3OCl	2.6×10^{-2}		Wang et al. (2017)	Q	80, 239
WETWJCDKMRHUPV-UHFFFAOYSA-N	8.7×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:CHCL2COCL	6.8×10^{-1}		Wang et al. (2017)	Q	80, 238
C_2HOCl_3	6.6×10^{-2}		Wang et al. (2017)	Q	80, 239
FBCCMZVIWNDFMO-UHFFFAOYSA-N	3.6×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:CLCOCH2OOH	1.1×10^{4}		Wang et al. (2017)	Q	80, 238
$C_2H_3O_3Cl$	2.1×10^{2}		Wang et al. (2017)	Q	80, 239
ARKKUYXZQNWAAF-UHFFFAOYSA-N	8.0		Wang et al. (2017)	Q	80, 240
MCM:CLCOCL2OOH	1.6×10^{4}		Wang et al. (2017)	Q	80, 238
$C_2HO_3Cl_3$	3.1×10^{1}		Wang et al. (2017)	Q	80, 239
FXUYMCPKRPYDCU-UHFFFAOYSA-N	2.1		Wang et al. (2017)	Q	80, 240
MCM:CLCOCLOOH	2.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_2H_2O_3Cl_2$	3.9×10^{2}		Wang et al. (2017)	Q	80, 239
WROSSTYSMNZXTC-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CLGLYOX	2.2×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2O_2Cl_2$	1.3×10^{-1}		Wang et al. (2017)	Q	80, 239
CTSLXHKWHWQRSH-UHFFFAOYSA-N	3.6×10^{-4}		Wang et al. (2017)	Q	80, 240

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CCL2OHCOCL	1.3×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2HO_2Cl_3$	1.2		Wang et al. (2017)	Q	80, 239
WBBOIYQGQVKNEO-UHFFFAOYSA-N	1.7×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:CCLOHCOCL	1.4×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_2O_2Cl_2$	5.6×10^{1}		Wang et al. (2017)	Q	80, 239
NABBVDLPPITPRF-UHFFFAOYSA-N	3.5		Wang et al. (2017)	Q	80, 240
MCM:CH2OHCOCL	2.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_2H_3O_2Cl$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
LCIMJULVQOQTEZ-UHFFFAOYSA-N	4.2×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CL1GLYOX	1.4×10^{2}		Wang et al. (2017)	Q	80, 238
C_2HO_2Cl	1.5		Wang et al. (2017)	Q	80, 239
ZNBGBHISQKMEPA-UHFFFAOYSA-N	4.2×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:CLOHCO2H	8.5×10^{4}		Wang et al. (2017)	Q	80, 238
$C_2H_3O_3Cl$	3.6×10^{4}		Wang et al. (2017)	Q	80, 239
SORBEIKZIPTJRS-UHFFFAOYSA-N	1.4×10^{5}		Wang et al. (2017)	Q	80, 240
1,1,1-trichloro-2-propanone $C_3H_3Cl_3O$ [918-00-3] SMZHKGXSEAGRTI-UHFFFAOYSA-N	4.5		HSDB (2015)	Q	99
1,1-dichloro-2-propanone	3.3×10^{-1}		Burkholder et al. (2019)	L	
$C_3H_4Cl_2O$	3.3×10^{-1}		Burkholder et al. (2015)	L	
(1,1-dichloroacetone)	3.3×10^{-1}		O'Farrell and Waghorne (2010)	M	
[513-88-2]	1.6		HSDB (2015)	Q	99
CSVFWMMPUJDVKH-UHFFFAOYSA-N					
carbonochloridic acid, 2-chloroethyl ester $C_3H_4Cl_2O_2$ (chloroethyl chloroformate) [627-11-2] SVDDJQGVOFZBNX-UHFFFAOYSA-N	9.0×10^{-3}		HSDB (2015)	Q	99
carbonochloridic acid, ethyl ester $C_3H_5ClO_2$ (ethyl chloroformate) [541-41-3] RIFGWPKJUGCATF-UHFFFAOYSA-N	3.2×10^{-3}		HSDB (2015)	Q	99
2-chloropropanoic acid $C_3H_5ClO_2$ [598-78-7] GAWAYYRQGQZKCR-UHFFFAOYSA-N	3.8×10^{1}		HSDB (2015)	Q	99

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-dichloro-1-propanol	7.8		Wang et al. (2017)	Q	80, 238
$C_3H_6Cl_2O$	6.9×10^{1}		Wang et al. (2017)	Q	80, 239
[616-23-9]	1.3×10^{1}		Wang et al. (2017)	Q	80, 240
ZXCYIJGIGSDJQQ-UHFFFAOYSA-N	3.3×10^{3}		HSDB (2015)	Q	99
1,3-dichloro-2-propanol	5.8		Meylan and Howard (1991)	V	
$C_3H_6Cl_2O$	1.6×10^{1}		HSDB (2015)	Q	99
[96-23-1]	2.0×10^{1}		Raventos-Duran et al. (2010)	Q	271, 243
DEWLEGDTCGBNGU-UHFFFAOYSA-N	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{1}		Raventos-Duran et al. (2010)	Q	245
	2.6×10^{1}		Hilal et al. (2008)	Q	
	3.0×10^{1}		Modarresi et al. (2007)	Q	67
	1.7×10^{1}		Meylan and Howard (1991)	Q	
3-chloro-1,2-propanediol	1.6×10^{2}		HSDB (2015)	Q	99
$C_3H_7ClO_2$					
[96-24-2]					
SSZWWUDQMAHNAQ-UHFFFAOYSA-N					
1-chloro-2-propanol	5.8		HSDB (2015)	Q	99
C_3H_7ClO					
[127-00-4]					
YYTSGNJTASLUOY-UHFFFAOYSA-N					
2-chloro-1-propanol	5.8		HSDB (2015)	Q	99
C_3H_7ClO					
[78-89-7]					
VZIQXGLTRZLBEX-UHFFFAOYSA-N					
3-chloro-1-propanol	1.3×10^{1}		Ebert et al. (2023)	?	316
C_3H_7ClO					
[627-30-5]					
LAMUXTNQCICZQX-UHFFFAOYSA-N					
trichloroethanal	3.4×10^{3}	3500	Burkholder et al. (2019)	L	460
CCl_3CHO	3.4×10^{3}	3500	Burkholder et al. (2015)	L	460
(trichloroacetaldehyde; chloral)	3.4×10^{3}	3500	Betterton and Hoffmann (1988)	M	460
[75-87-6]	2.2×10^{3}		Keshavarz et al. (2022)	Q	
HFFLGKNGCAIQMO-UHFFFAOYSA-N	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
	2.1×10^{-1}		Wang et al. (2017)	Q	80, 238
	1.6×10^{-2}		Wang et al. (2017)	Q	80, 239
	3.2×10^{-3}		Wang et al. (2017)	Q	80, 240
	1.2×10^{3}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{2}		Raventos-Duran et al. (2010)	Q	244
	3.1		Raventos-Duran et al. (2010)	Q	245
		1700	Kühne et al. (2005)	Q	
	1.7×10^{3}		Meylan and Howard (1991)	Q	
	3.4×10^{3}		Duchowicz et al. (2020)	?	185, 21
		3500	Kühne et al. (2005)	?	

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chloro-2-propanone	5.8×10^{-1}	5400	Burkholder et al. (2019)	L	
$CH_2ClCOCH_3$	5.8×10^{-1}	5400	Burkholder et al. (2015)	L	
(chloroacetone)	5.8×10^{-1}	5400	Sander et al. (2011)	L	
[78-95-5]	5.8×10^{-1}	5400	Betterton (1991)	M	
BULLHNJGPPOUOX-UHFFFAOYSA-N	1.2×10^{-1}		Keshavarz et al. (2022)	Q	
	8.8×10^{-2}		Duchowicz et al. (2020)	Q	299
	1.3×10^{-1}		Wang et al. (2017)	Q	80, 238
	2.0		Wang et al. (2017)	Q	80, 239
	1.2		Wang et al. (2017)	Q	80, 240
	1.6		Raventos-Duran et al. (2010)	Q	271, 243
	1.2		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-1}		Raventos-Duran et al. (2010)	Q	245
	8.8×10^{-1}		Hilal et al. (2008)	Q	
	6.8×10^{-1}		Modarresi et al. (2007)	Q	67
		4400	Kühne et al. (2005)	Q	
	6.0×10^{-1}		Duchowicz et al. (2020)	?	185, 21
		5500	Kühne et al. (2005)	?	
chloroethanoic acid	1.1×10^{3}	9700	Burkholder et al. (2019)	L	
$CH_2ClCOOH$	1.1×10^{3}	9700	Burkholder et al. (2015)	L	
(chloroacetic acid)	1.1×10^{3}	9700	Sander et al. (2011)	L	
[79-11-8]	1.1×10^{3}	9700	Bowden et al. (1998a)	M	
FOCAUTSVDIKZOP-UHFFFAOYSA-N	1.1×10^{3}		Keshavarz et al. (2022)	Q	
	1.3×10^{2}		Duchowicz et al. (2020)	Q	
	2.0×10^{2}		Wang et al. (2017)	Q	80, 238
	3.6×10^{3}		Wang et al. (2017)	Q	80, 239
	1.1×10^{3}		Wang et al. (2017)	Q	80, 240
	1.2×10^{3}		Raventos-Duran et al. (2010)	Q	271, 243
	1.6×10^{3}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	8.8×10^{2}		Hilal et al. (2008)	Q	
	3.1×10^{2}		Modarresi et al. (2007)	Q	67
		8100	Kühne et al. (2005)	Q	
	1.1×10^{3}		Duchowicz et al. (2020)	?	185, 21
		9400	Kühne et al. (2005)	?	
dichloroethanoic acid	1.2×10^{3}	8000	Burkholder et al. (2019)	L	
$CHCl_2COOH$	1.2×10^{3}	8000	Burkholder et al. (2015)	L	
(dichloroacetic acid)	1.2×10^{3}	8000	Sander et al. (2011)	L	
[79-43-6]	1.2×10^{3}	8000	Bowden et al. (1998a)	M	
JXTHNDFMNIQAHM-UHFFFAOYSA-N	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	3.9×10^{2}		Duchowicz et al. (2020)	Q	299
	6.6×10^{2}		Wang et al. (2017)	Q	80, 238
	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
	3.8×10^{2}		Wang et al. (2017)	Q	80, 240
	2.5×10^{3}		Raventos-Duran et al. (2010)	Q	271, 243
	6.2×10^{2}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	245

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.9×10^{2}		Hilal et al. (2008)	Q	
	8.5×10^{2}		Modarresi et al. (2007)	Q	67
		8400	Kühne et al. (2005)	Q	
	2.6×10^{1}		Katritzky et al. (1998)	Q	
	1.2×10^{3}		Duchowicz et al. (2020)	?	185, 21
		8000	Kühne et al. (2005)	?	
trichloroethanoic acid	7.3×10^{2}	8700	Burkholder et al. (2019)	L	
CCl_3COOH	7.3×10^{2}	8700	Burkholder et al. (2015)	L	
(trichloroacetic acid)	7.3×10^{2}	8700	Sander et al. (2011)	L	
[76-03-9]	7.3×10^{2}	8700	Bowden et al. (1998b)	M	
YNJBWRMUSHSURL-UHFFFAOYSA-N	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	2.3×10^{2}		Duchowicz et al. (2020)	Q	
	9.9×10^{2}		Raventos-Duran et al. (2010)	Q	271, 243
	3.9		Raventos-Duran et al. (2010)	Q	244
	3.9×10^{2}		Raventos-Duran et al. (2010)	Q	245
	4.7		Hilal et al. (2008)	Q	
	7.6×10^{2}		Modarresi et al. (2007)	Q	67
		8800	Kühne et al. (2005)	Q	
	7.3×10^{2}		Duchowicz et al. (2020)	?	185, 21
		8600	Kühne et al. (2005)	?	
2,2-dichloro-propanoic acid	1.7×10^{2}		Duchowicz et al. (2020)	V	186
$C_3H_4Cl_2O_2$	3.5×10^{8}		Mackay et al. (2006d)	V	
[75-99-0]	1.8×10^{2}		Duchowicz et al. (2020)	Q	
NDUPDOJHUQKPAG-UHFFFAOYSA-N					
trichloroacetylchloride	2.0×10^{-2}		Mirabel et al. (1996)	M	
CCl_3COCl	2.0×10^{-2}		De Bruyn et al. (1995a)	M	449
[76-02-8]	2.0×10^{-2}		George et al. (1994a)	M	
PVFOMCVHYWHZJE-UHFFFAOYSA-N	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	7.3×10^{-2}		Duchowicz et al. (2020)	Q	184
	3.4×10^{-1}		HSDB (2015)	Q	99
	1.9×10^{-2}		Duchowicz et al. (2020)	?	185, 21
hexachloroacetone	1.0×10^{2}		Zhang et al. (2010)	Q	287, 288
C_3Cl_6O	9.0×10^{-4}		Zhang et al. (2010)	Q	287, 289
[116-16-5]	6.2×10^{-2}		Zhang et al. (2010)	Q	287, 290
DOJXGHGHTWFZHK-UHFFFAOYSA-N	1.8×10^{-1}		Zhang et al. (2010)	Q	287, 291
(chloromethyl)-oxirane	2.9×10^{-1}		Welke et al. (1998)	M	
C_3H_5ClO	3.2×10^{-1}		Duchowicz et al. (2020)	V	186
(epichlorohydrin)	3.3×10^{-1}		HSDB (2015)	V	
[106-89-8]	3.0×10^{-1}		Mackay et al. (2006c)	V	
BRLQWZUYTZBJKN-UHFFFAOYSA-N	3.0×10^{-1}		Mackay et al. (1993)	V	
	2.8×10^{-1}		Goldstein (1982)	X	446
	2.8×10^{-1}	3700	Goldstein (1982)	X	298
	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
	9.9×10^{-2}		Hilal et al. (2008)	Q	
	1.7×10^{-1}		Modarresi et al. (2007)	Q	67

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl chloroethanoate	4.9×10^{-1}	5600	Brockbank (2013)	L	1
$C_3H_5ClO_2$	4.2×10^{-1}		Duchowicz et al. (2020)	V	186
[96-34-4]	4.1×10^{-2}		HSDB (2015)	V	
QABLOFMHHSOFRJ-UHFFFAOYSA-N	3.3×10^{-1}		Duchowicz et al. (2020)	Q	
	2.3×10^{-1}		Hilal et al. (2008)	Q	
	1.2×10^{-1}		Modarresi et al. (2007)	Q	67
MCM:CL12CO3H	1.6×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_4O_3Cl_2$	1.1×10^{2}		Wang et al. (2017)	Q	80, 239
VMJCNPRTZBGZGF-UHFFFAOYSA-N	2.3		Wang et al. (2017)	Q	80, 240
MCM:CL12PRAOOH	1.0×10^{2}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_2Cl_2$	2.5×10^{2}		Wang et al. (2017)	Q	80, 239
WGVINOMLJVZPKZ-UHFFFAOYSA-N	1.5×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CL12PRBOOH	7.1×10^{1}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_2Cl_2$	1.8×10^{1}		Wang et al. (2017)	Q	80, 239
OMIMXWULHYQJIC-UHFFFAOYSA-N	9.3		Wang et al. (2017)	Q	80, 240
MCM:CL12PRCOOH	1.2×10^{2}		Wang et al. (2017)	Q	80, 238
$C_3H_6O_2Cl_2$	3.8×10^{1}		Wang et al. (2017)	Q	80, 239
ULSSYZYIMOSSQB-UHFFFAOYSA-N	3.8×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CL12PRBOH	1.4×10^{1}		Wang et al. (2017)	Q	80, 238
$C_3H_6OCl_2$	1.5×10^{1}		Wang et al. (2017)	Q	80, 239
QEZDCTNHTRSNMD-UHFFFAOYSA-N	2.6×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CL12PRCOH	2.3×10^{1}		Wang et al. (2017)	Q	80, 238
$C_3H_6OCl_2$	1.8×10^{1}		Wang et al. (2017)	Q	80, 239
FLTSEOGWHPJWRV-UHFFFAOYSA-N	4.9×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:CL12PRCHO	1.3		Wang et al. (2017)	Q	80, 238
$C_3H_4OCl_2$	3.5		Wang et al. (2017)	Q	80, 239
IZRKUJREXIKAQM-UHFFFAOYSA-N	5.5×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:CH3CLCOCL	2.7×10^{-1}		Wang et al. (2017)	Q	80, 238
$C_3H_4OCl_2$	3.8×10^{-2}		Wang et al. (2017)	Q	80, 239
JEQDSBVHLKBEIZ-UHFFFAOYSA-N	1.1×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:CH3COCLOOH	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_3H_5O_3Cl$	3.5×10^{2}		Wang et al. (2017)	Q	80, 239
HLLYIZVQRAGDFF-UHFFFAOYSA-N	1.0×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CLCOCLMOOH	1.4×10^{4}		Wang et al. (2017)	Q	80, 238
$C_3H_4O_3Cl_2$	6.0×10^{1}		Wang et al. (2017)	Q	80, 239
RUPGTCZALLJKQM-UHFFFAOYSA-N	1.3		Wang et al. (2017)	Q	80, 240
MCM:CL12CO2H	1.3×10^{3}		Wang et al. (2017)	Q	80, 238
$C_3H_4O_2Cl_2$	3.5×10^{3}		Wang et al. (2017)	Q	80, 239
GKFWNPPZHDYVLI-UHFFFAOYSA-N	8.1×10^{2}		Wang et al. (2017)	Q	80, 240

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-chloro-2-butanone C_4H_7ClO [4091-39-8] OIMRLHCSLQUXLL-UHFFFAOYSA-N	9.5×10^{-2}		Ebert et al. (2023)	?	316
ethyl chloroethanoate $C_4H_7ClO_2$ [105-39-5] VEUUMBGHMNQHGO-UHFFFAOYSA-N	2.6×10^{-1} 2.4×10^{-1} 1.5×10^{-1} 1.2×10^{-1} 1.1×10^{-1} 1.1×10^{-1} 2.4×10^{-1}	6100	Brockbank (2013) Duchowicz et al. (2020) Duchowicz et al. (2020) HSDB (2015) Hilal et al. (2008) Modarresi et al. (2007) Bartelt-Hunt et al. (2008)	L V Q Q Q Q ?	1 186 99 67 21
carbonochloridic acid, 1-methylethyl ester $C_4H_7ClO_2$ [108-23-6] IVRIRQXJSNCSPQ-UHFFFAOYSA-N	2.4×10^{-3}		HSDB (2015)	Q	99
chloroacetic acid anhydride $C_4H_4Cl_2O_3$ [541-88-8] PNVPNXKRAUBJGW-UHFFFAOYSA-N	2.2		HSDB (2015)	Q	99
chlorobutanol C_4H_9ClO [1320-66-7] OSASVXMJTNOKOY-UHFFFAOYSA-N	4.5		HSDB (2015)	Q	99
methyl 2-chloroacetoacetate $C_5H_7ClO_3$ [4755-81-1] GYQRIAVRKLRQKP-UHFFFAOYSA-N	2.3		Ebert et al. (2023)	?	318
3-chloro-4-(dichloromethyl)-2- (5H)-furanone $C_5H_3Cl_3O_2$ [122551-89-7] WNQKLIFDPFSPIZ-UHFFFAOYSA-N	1.5		HSDB (2015)	Q	99
3-chloro-4-(dichloromethyl)-5- hydroxy-2-(5H)-furanone $C_5H_3Cl_3O_3$ [77439-76-0] WNTRMRXAGJOLCU-UHFFFAOYSA-N	3.9×10^{4}		HSDB (2015)	Q	99
1,2,4-trichloro-2-methyl-3- pentanone $C_6H_9Cl_3O$ [145556-04-3] KAUWEMQJFDRELR-UHFFFAOYSA-N	1.9 1.9 1.1×10^{2} 4.1×10^{-1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bis(2-chloroisopropyl) ether	3.0×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_6H_{12}Cl_2O$	3.3×10^{-4}		Zhang et al. (2010)	Q	287, 289
[39638-32-9]	9.5×10^{-1}		Zhang et al. (2010)	Q	287, 290
BULHJTXRZFEUDQ-UHFFFAOYSA-N	1.6×10^{-3}		Zhang et al. (2010)	Q	287, 291
butyl 2,2,3,4,4-pentachloro-3-butenoate	3.9×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_8H_9Cl_5O_2$	3.9×10^{-2}		Zhang et al. (2010)	Q	287, 289
[75147-20-5]	7.9×10^{-2}		Zhang et al. (2010)	Q	287, 290
JZJILZTVTMMGAR-UHFFFAOYSA-N	1.8×10^{-1}		Zhang et al. (2010)	Q	287, 291
3-(2,2-dichlorovinyl)-2,2- dimethylcyclopropane carbonyl chloride	1.6×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_8H_9Cl_3O$	9.7×10^{-3}		Zhang et al. (2010)	Q	287, 289
[52314-67-7]	1.6×10^{-1}		Zhang et al. (2010)	Q	287, 290
CHLAOFANYRDCPD-UHFFFAOYSA-N	8.8×10^{-1}		Zhang et al. (2010)	Q	287, 291
3-(2,2-dichlorovinyl)-2,2- dimethylcyclopropane carboxylic acid	1.9×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_8H_{10}Cl_2O_2$	9.0×10^{1}		Zhang et al. (2010)	Q	287, 289
[55701-05-8]	6.1×10^{4}		Zhang et al. (2010)	Q	287, 290
LLMLSUSAKZVFOA-UHFFFAOYSA-N	6.1×10^{1}		Zhang et al. (2010)	Q	287, 291
hexanoic acid, 3,3-dimethyl-4,6,6,6-tetrachloro, methyl ester	6.7×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_9H_{14}Cl_4O_2$	2.7×10^{-1}		Zhang et al. (2010)	Q	287, 289
[64667-33-0]	6.1×10^{2}		Zhang et al. (2010)	Q	287, 290
POFHGKISWXYKLB-UHFFFAOYSA-N	1.8×10^{-2}		Zhang et al. (2010)	Q	287, 291
methyl 3-(2,2-dichlorovinyl)-2,2- dimethylcyclopropanecarboxylate	6.1×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_9H_{12}Cl_2O_2$	5.2×10^{-2}		Zhang et al. (2010)	Q	287, 289
[61898-95-1]	1.3×10^{-1}		Zhang et al. (2010)	Q	287, 290
QJOOIMSFFIUFKX-UHFFFAOYSA-N	1.7×10^{-1}		Zhang et al. (2010)	Q	287, 291
oxychlordane	6.0×10^{-2}	4300	Paasivirta et al. (1999)	T	
$C_{10}H_4Cl_8O$	1.1×10^{2}		HSDB (2015)	Q	99
[27304-13-8]					
VWGNQYSIWFHEQU-UHFFFAOYSA-N					
kepone	1.8×10^{2}		Duchowicz et al. (2020)	V	186
$C_{10}Cl_{10}O$	1.8×10^{2}		HSDB (2015)	V	
[143-50-0]	2.0×10^{2}		Mackay et al. (2006d)	V	
LHHGDZSESBACKH-UHFFFAOYSA-N	1.5×10^{2}		Duchowicz et al. (2020)	Q	

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bis-(chloromethyl) ether	2.3×10^{-3}		Duchowicz et al. (2020)	V	186
$C_2H_4Cl_2O$	4.8×10^{-2}		Mackay et al. (2006c)	V	
[542-88-1]	4.8×10^{-2}		Mackay et al. (1993)	V	
HRQGCQVOJVTVLU-UHFFFAOYSA-N	4.7×10^{-3}		Ryan et al. (1988)	C	
	1.9×10^{-2}		Duchowicz et al. (2020)	Q	
	4.3×10^{-2}		Modarresi et al. (2007)	Q	67
1,5-dichloro-3-oxapentane	4.8×10^{-1}	6200	Brockbank (2013)	L	1
$C_4H_8Cl_2O$	5.8×10^{-1}		Duchowicz et al. (2020)	V	186
(bis-(2-chloroethyl)-ether)	3.4×10^{-1}		HSDB (2015)	V	
[111-44-4]	3.5×10^{-1}		Mackay et al. (2006c)	V	
ZNSMNVMLTJELDZ-UHFFFAOYSA-N	3.4×10^{-2}		Lide and Frederikse (1995)	V	
	3.5×10^{-1}		Mackay et al. (1993)	V	
	4.6×10^{-1}		Goldstein (1982)	X	446
	4.7×10^{-1}	4100	Goldstein (1982)	X	298
	3.7×10^{-1}		Harrison et al. (1993)	C	
	8.6		Ryan et al. (1988)	C	
	3.4×10^{-2}		Duchowicz et al. (2020)	Q	
	5.2×10^{-2}		Zhang et al. (2010)	Q	287, 288
	2.8×10^{-1}		Zhang et al. (2010)	Q	287, 289
	4.4×10^{-2}		Zhang et al. (2010)	Q	287, 290
	4.6×10^{-3}		Zhang et al. (2010)	Q	287, 291
	2.9×10^{-1}		Hilal et al. (2008)	Q	
	3.7×10^{-1}		Modarresi et al. (2007)	Q	67
		6000	Kühne et al. (2005)	Q	
		6000	Kühne et al. (2005)	?	
2-chloro-1,1-dimethoxyethane	3.2×10^{-1}		Ebert et al. (2023)	?	318
$C_4H_9ClO_2$					
[97-97-2]					
CRZJPEIBPQWDGJ-UHFFFAOYSA-N					
(2-chloroethoxy)-ethene	1.1×10^{-3}		Duchowicz et al. (2020)	V	186
C_4H_7ClO	1.1×10^{-3}		HSDB (2015)	V	
(2-chloroethylvinylether)	3.9×10^{-2}		Mackay et al. (2006c)	V	
[110-75-8]	3.9×10^{-2}		Mackay et al. (1993)	V	
DNJRKFKAFWSXSE-UHFFFAOYSA-N	1.1×10^{-3}		Goldstein (1982)	X	446
	3.1×10^{-2}	2500	Goldstein (1982)	X	298
	4.0×10^{-2}		Ryan et al. (1988)	C	
	4.9×10^{-2}		Duchowicz et al. (2020)	Q	
	2.3×10^{-3}		Hilal et al. (2008)	Q	
	2.1×10^{-2}		Modarresi et al. (2007)	Q	67

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bis-(2-chloroethoxy)-methane	2.6		Duchowicz et al. (2020)	V	186
$C_5H_{10}Cl_2O_2$	2.5		HSDB (2015)	V	
[111-91-1]	2.2×10^{1}		Mackay et al. (2006c)	V	
NLXGURFLBLRZRO-UHFFFAOYSA-N	2.2		Mackay et al. (1993)	V	
	8.8		Goldstein (1982)	X	446
	2.6×10^{1}	5500	Goldstein (1982)	X	298
	3.7×10^{1}		Ryan et al. (1988)	C	
	2.9×10^{-1}		Duchowicz et al. (2020)	Q	
	3.4		Hilal et al. (2008)	Q	
bis-(2-chloroisopropyl) ether	4.2×10^{-1}		Kawamoto and Urano (1989)	M	
$C_6H_{12}Cl_2O$	1.3×10^{-1}		HSDB (2015)	V	
(DCIP)	9.6×10^{-2}		Mackay et al. (2006c)	V	
[108-60-1]	9.6×10^{-2}		Mackay et al. (1993)	V	
QCFYJCYNJLBDRT-UHFFFAOYSA-N	6.5×10^{-2}		Goldstein (1982)	X	446
	6.4×10^{-2}	2800	Goldstein (1982)	X	298
	8.6×10^{-3}		Ryan et al. (1988)	C	
	7.2×10^{-2}		Hilal et al. (2008)	Q	
	2.9×10^{-1}		Modarresi et al. (2007)	Q	67
1,2-bis(2-chloroethoxy)ethane	1.3×10^{1}		HSDB (2015)	V	
$C_6H_{12}Cl_2O_2$	4.7		Modarresi et al. (2007)	Q	67
[112-26-5]					
AGYUOJIYYGGHKV-UHFFFAOYSA-N					
2-hydroxychlorobenzene	1.5		Sheikheldin et al. (2001)	M	12
C_6H_5ClO	3.6	5700	Tabai et al. (1997)	M	11
(*o*-chlorophenol)	1.5		Mackay et al. (2006c)	V	
[95-57-8]	1.2		Fogg and Sangster (2003)	V	729
ISPYQTSUDJAMAB-UHFFFAOYSA-N	1.8×10^{1}		Lide and Frederikse (1995)	V	
	1.5		Mackay et al. (1995)	V	
	1.5		Shiu et al. (1994)	V	
	8.8×10^{-1}		Abraham et al. (1994a)	R	
	1.2		Goldstein (1982)	X	446
	1.2	4600	Goldstein (1982)	X	298
	1.8×10^{1}		Howard (1989)	X	418
	2.1		Ryan et al. (1988)	C	
	2.2		Keshavarz et al. (2022)	Q	
	8.2		Duchowicz et al. (2020)	Q	299
	4.2		Hilal et al. (2008)	Q	
	4.6		Modarresi et al. (2007)	Q	67
		6200	Kühne et al. (2005)	Q	
	9.2×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	1.8×10^{2}		Nirmalakhandan et al. (1997)	Q	
	8.8×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	8.8×10^{-1}		HSDB (2015)	?	419
		5600	Kühne et al. (2005)	?	
	2.6×10^{-1}		Yaws (1999)	?	21
	1.0		Chiou et al. (1980)	?	79

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-hydroxychlorobenzene	7.2		Chao et al. (2017)	M	
C_6H_5ClO	3.4×10^1	6400	Tabai et al. (1997)	M	11
(m-chlorophenol)	4.9		Mackay et al. (2006c)	V	
[108-43-0]	7.3		Fogg and Sangster (2003)	V	
HORNXRXVQWOLPJ-UHFFFAOYSA-N	1.8×10^1		Lide and Frederikse (1995)	V	
	4.9		Mackay et al. (1995)	V	
	4.9		Shiu et al. (1994)	V	
	2.9×10^1		Abraham et al. (1994a)	R	
	1.8×10^1		Howard (1989)	X	418
	4.3		Keshavarz et al. (2022)	Q	
	9.9×10^1		Duchowicz et al. (2020)	Q	299
	1.6×10^1		Hilal et al. (2008)	Q	
	2.5×10^1		Modarresi et al. (2007)	Q	67
		6200	Kühne et al. (2005)	Q	
	3.0×10^1		Yaffe et al. (2003)	Q	248, 249
	1.3×10^1		English and Carroll (2001)	Q	230, 231
	2.4×10^1		Katritzky et al. (1998)	Q	
	1.8×10^2		Nirmalakhandan et al. (1997)	Q	
	2.9×10^1		Duchowicz et al. (2020)	?	185, 21
	2.9×10^1		HSDB (2015)	?	419
		6100	Kühne et al. (2005)	?	
	4.8		Yaws (1999)	?	21, 12
4-hydroxychlorobenzene	6.7		Chao et al. (2017)	M	
C_6H_5ClO	1.4×10^3	11000	Tabai et al. (1997)	M	11
(p-chlorophenol)	1.6×10^1		HSDB (2015)	V	
[106-48-9]	1.1×10^1		Mackay et al. (2006c)	V	
WXNZTHHGJRFXKQ-UHFFFAOYSA-N	1.2×10^1		Fogg and Sangster (2003)	V	
	1.8×10^1		Lide and Frederikse (1995)	V	
	1.1×10^1		Mackay et al. (1995)	V	
	1.1×10^1		Shiu et al. (1994)	V	
	5.8×10^1		Abraham et al. (1994a)	R	
	1.8×10^1		Howard (1989)	X	418
	4.3		Keshavarz et al. (2022)	Q	
	1.5×10^2		Duchowicz et al. (2020)	Q	184
	2.4×10^1		Li et al. (2014)	Q	241
	1.3×10^1		Hilal et al. (2008)	Q	
	9.8		Modarresi et al. (2007)	Q	67
		6200	Kühne et al. (2005)	Q	
	5.8×10^1		Yaffe et al. (2003)	Q	248, 249
	3.4×10^1		Yao et al. (2002)	Q	229
	2.3×10^1		English and Carroll (2001)	Q	230, 260
	3.0×10^1		Katritzky et al. (1998)	Q	
	1.8×10^2		Nirmalakhandan et al. (1997)	Q	
	1.6×10^1		Duchowicz et al. (2020)	?	185, 21
		6400	Kühne et al. (2005)	?	
	7.8		Yaws (1999)	?	21, 12

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.1×10^1		Chiou et al. (1980)	?	79
2,3-dichlorophenol $C_6H_4Cl_2O$ [576-24-9] UMPSXRYVXUPCOS-UHFFFAOYSA-N	2.9		HSDB (2015)	V	
2,4-dichlorophenol $C_6H_4Cl_2O$ [120-83-2] HFZWRUODUSTPEG-UHFFFAOYSA-N	3.4		Sheikheldin et al. (2001)	M	12
	6.6	6800	Tabai et al. (1997)	M	11
	2.3		Duchowicz et al. (2020)	V	186
	2.8		HSDB (2015)	V	
	2.3		Mackay et al. (2006c)	V	
	2.3		Mackay et al. (1995)	V	
	2.3		Shiu et al. (1994)	V	
	9.0		Leuenberger et al. (1985)	V	416
	1.5		Goldstein (1982)	X	446
	1.5	4900	Goldstein (1982)	X	298
	1.8		Ryan et al. (1988)	C	
	2.2×10^1		Duchowicz et al. (2020)	Q	
	3.2×10^1		Zhang et al. (2010)	Q	287, 288
	8.0		Zhang et al. (2010)	Q	287, 289
	1.1		Zhang et al. (2010)	Q	287, 290
	4.6		Zhang et al. (2010)	Q	287, 291
	8.2		Hilal et al. (2008)	Q	
	4.4		Modarresi et al. (2007)	Q	67
		6300	Kühne et al. (2005)	Q	
		7400	Kühne et al. (2005)	?	
2,5-dichlorophenol $C_6H_4Cl_2O$ [583-78-8] RANCECPPZPIPNO-UHFFFAOYSA-N	1.6		HSDB (2015)	V	
2,6-dichlorophenol $C_6H_4Cl_2O$ [87-65-0] HOLHYSJJBXSLMV-UHFFFAOYSA-N	3.7		Duchowicz et al. (2020)	V	186
	3.7		HSDB (2015)	V	
	1.3		Mackay et al. (2006c)	V	
	3.3		Mackay et al. (1995)	V	
	1.2		Duchowicz et al. (2020)	Q	
	3.8		Yaffe et al. (2003)	Q	248, 249
	2.5×10^1		Katritzky et al. (1998)	Q	
3,4-dichlorophenol $C_6H_4Cl_2O$ [95-77-2] WDNBURPWRNALGP-UHFFFAOYSA-N	2.1×10^1		HSDB (2015)	Q	99

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,5-dichlorophenol	4.0×10^{1}		Duchowicz et al. (2020)	V	186
$C_6H_4Cl_2O$	4.1×10^{1}		HSDB (2015)	V	
[591-35-5]	1.8×10^{2}		Duchowicz et al. (2020)	Q	
VPOMSPZBQMDLTM-UHFFFAOYSA-N	4.6×10^{1}		Hilal et al. (2008)	Q	
	1.4×10^{1}		Modarresi et al. (2007)	Q	67
2,3,4-trichlorophenol	2.5		Mackay et al. (2006c)	V	
$C_6H_3Cl_3O$	2.5		Mackay et al. (1995)	V	
[15950-66-0]					
HSQFVBWFPBKHEB-UHFFFAOYSA-N					
2,3,5-trichlorophenol	2.5		Mackay et al. (2006c)	V	
$C_6H_3Cl_3O$	2.5		Mackay et al. (1995)	V	
[933-78-8]					
WWGQHTJIFOQAOC-UHFFFAOYSA-N					
2,4,5-trichlorophenol	6.1		Duchowicz et al. (2020)	V	186
$C_6H_3Cl_3O$	6.2		HSDB (2015)	V	
[95-95-4]	1.9		Mackay et al. (2006c)	V	
LHJGJYXLEPZJPM-UHFFFAOYSA-N	4.6×10^{-1}		Fogg and Sangster (2003)	V	
	1.9		Mackay et al. (1995)	V	
	7.6		Leuenberger et al. (1985)	V	416
	4.6×10^{1}		Duchowicz et al. (2020)	Q	
	2.0×10^{1}		Hilal et al. (2008)	Q	
	5.7		Modarresi et al. (2007)	Q	67
2,3,6-trichlorophenol	4.3×10^{1}		HSDB (2015)	Q	99
$C_6H_3Cl_3O$					
[933-75-5]					
XGCHAIDDPMFRLJ-UHFFFAOYSA-N					
2,4,6-trichlorophenol	1.9×10^{1}		Chao et al. (2017)	M	
$C_6H_3Cl_3O$	2.0		Yoshida et al. (1987)	M	730, 12
[88-06-2]	3.8		Duchowicz et al. (2020)	V	186
LINPIYWFGCPVIE-UHFFFAOYSA-N	3.8		HSDB (2015)	V	
	1.8		Mackay et al. (2006c)	V	
	1.6×10^{2}		Lide and Frederikse (1995)	V	
	1.8		Mackay et al. (1995)	V	
	7.6		Leuenberger et al. (1985)	V	416
	1.4	5000	Goldstein (1982)	X	298
	1.6×10^{1}		Howard (1989)	X	418
	2.4		Ryan et al. (1988)	C	
	2.5		Duchowicz et al. (2020)	Q	
	4.3×10^{1}		Zhang et al. (2010)	Q	287, 288
	2.8×10^{-2}		Zhang et al. (2010)	Q	287, 289
	8.8×10^{-1}		Zhang et al. (2010)	Q	287, 290
	9.7×10^{-1}		Zhang et al. (2010)	Q	287, 291
	2.2		Hilal et al. (2008)	Q	
	3.3		Modarresi et al. (2007)	Q	67
		6400	Kühne et al. (2005)	Q	

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.8		Yaffe et al. (2003)	Q	248, 249
	1.8×10^{1}		Katritzky et al. (1998)	Q	
		6500	Kühne et al. (2005)	?	
3,4,5-trichlorophenol $C_6H_3Cl_3O$ [609-19-8] GBNHEBQXJVDXSW-UHFFFAOYSA-N	4.3×10^{1}		HSDB (2015)	Q	99
2,3,4,5-tetrachlorophenol $C_6H_2Cl_4O$ [4901-51-3] RULKYXXCCZZKDZ-UHFFFAOYSA-N	7.2		Mackay et al. (2006c)	V	
	7.2		Mackay et al. (1995)	V	
	2.8×10^{1}		HSDB (2015)	Q	99
2,3,4,6-tetrachlorophenol $C_6H_2Cl_4O$ [58-90-2] VGVRPFIJEJYOFN-UHFFFAOYSA-N	1.1		Duchowicz et al. (2020)	V	186
	7.6		HSDB (2015)	V	
	2.8		Mackay et al. (2006c)	V	
	2.8		Mackay et al. (1995)	V	
	6.6		Duchowicz et al. (2020)	Q	
	5.8×10^{1}		Zhang et al. (2010)	Q	287, 288
	4.1×10^{-2}		Zhang et al. (2010)	Q	287, 289
	3.9		Zhang et al. (2010)	Q	287, 290
	3.1		Zhang et al. (2010)	Q	287, 291
2,3,5,6-tetrachlorophenol $C_6H_2Cl_4O$ [935-95-5] KEWNKZNZRIAIAK-UHFFFAOYSA-N	4.3		Mackay et al. (2006c)	V	
	4.3		Mackay et al. (1995)	V	
	2.8×10^{1}		HSDB (2015)	Q	99
hydroxypentachlorobenzene C_6HCl_5O (pentachlorophenol) [87-86-5] IZUPBVBPLAPZRR-UHFFFAOYSA-N	4.1×10^{2}		Hellmann (1987)	M	87
	1.3×10^{1}		Mackay et al. (2006c)	V	
			Mackay et al. (2006d)	V	558
	1.1×10^{-2}		Fogg and Sangster (2003)	V	
	1.3×10^{1}		Mackay et al. (1995)	V	
	2.3×10^{1}		Riederer (1990)	V	
	2.3×10^{1}		Suntio et al. (1988)	V	12
	2.2×10^{-1}		Barcelo and Hennion (1997)	X	567
	1.1×10^{-1}	1300	Goldstein (1982)	X	298
	4.7		McCarty (1980)	X	368
	3.4		Ryan et al. (1988)	C	
	7.9×10^{1}		Zhang et al. (2010)	Q	287, 288
	6.0×10^{-2}		Zhang et al. (2010)	Q	287, 289
	6.5		Zhang et al. (2010)	Q	287, 290
	4.0		Zhang et al. (2010)	Q	287, 291
	2.5×10^{-1}		Goodarzi et al. (2010)	Q	568, 569
	1.3×10^{1}		Modarresi et al. (2007)	Q	67
		7800	Kühne et al. (2005)	Q	
	7.9×10^{1}		Meylan and Howard (1991)	Q	
	1.8		Fogg and Sangster (2003)	E	
		7400	Kühne et al. (2005)	?	

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4,5-trichloro-1,2-benzenediol $C_6H_3Cl_3O_2$ (3,4,5-trichlorocatechol) [56961-20-7] FUTDYIMYZIMPBJ-UHFFFAOYSA-N	2.4×10^2		Lei et al. (1999)	V	
4,5-dichloro-1,2-benzenediol $C_6H_4Cl_2O_2$ (4,5-dichlorocatechol) [3428-24-8] ACCHWUWBKYGKNM-UHFFFAOYSA-N	1.3×10^3		Lei et al. (1999)	V	
3,4,5,6-tetrachloro-1,2-benzenediol $C_6H_2Cl_4O_2$ (tetrachlorocatechol) [1198-55-6] RRBMVWQICIXSEO-UHFFFAOYSA-N	2.9×10^1		Lei et al. (1999)	V	
2,3,5,6-tetrachloro-*p*-benzoquinone $C_6Cl_4O_2$ (chloranil) [118-75-2] UGNWTBMOAKPKBL-UHFFFAOYSA-N	1.5×10^3		HSDB (2015)	V	
2-chloro-5-methylphenol C_7H_7ClO [615-74-7] SMFHPCZZAAMJJO-UHFFFAOYSA-N	2.1×10^1		HSDB (2015)	Q	99
4-chloro-2-methylphenol C_7H_7ClO [1570-64-5] RHPUJHQBPORFGV-UHFFFAOYSA-N	8.7		Duchowicz et al. (2020)	V	186
	9.0		Woodrow et al. (1990)	V	
	8.5×10^1		Duchowicz et al. (2020)	Q	
	1.6×10^1		Hilal et al. (2008)	Q	
	1.5		Modarresi et al. (2007)	Q	67
4-chloro-3-methylphenol C_7H_7ClO [59-50-7] CFKMVGJGLGKFKI-UHFFFAOYSA-N	4.0		Duchowicz et al. (2020)	V	186
	4.1		HSDB (2015)	V	
	3.9×10^1		Abraham et al. (1994a)	R	
	4.0		Ryan et al. (1988)	C	
	8.5×10^1		Duchowicz et al. (2020)	Q	
	2.2×10^1		Zhang et al. (2010)	Q	287, 288
	1.3×10^1		Zhang et al. (2010)	Q	287, 289
	2.8×10^1		Zhang et al. (2010)	Q	287, 290
	9.2×10^1		Zhang et al. (2010)	Q	287, 291
	1.2×10^1		Hilal et al. (2008)	Q	
	8.8		Modarresi et al. (2007)	Q	67
	3.9×10^1		Yaffe et al. (2003)	Q	248, 249
	1.7×10^1		English and Carroll (2001)	Q	230, 231
	1.3×10^2		Nirmalakhandan et al. (1997)	Q	

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloro-2-methoxybenzene C_7H_7ClO (2-chloroanisole) [766-51-8] QGRPVMLBTFGQDQ-UHFFFAOYSA-N	1.0×10^{-1} 1.1×10^{-1} 1.8×10^{-1}		Pfeifer et al. (2001) Duchowicz et al. (2020) Duchowicz et al. (2020)	M V Q	731 186
1-chloro-3-methoxybenzene C_7H_7ClO (3-chloroanisole) [2845-89-8] YUKILTJWFRTXGB-UHFFFAOYSA-N	4.5×10^{-2}		Pfeifer et al. (2001)	M	731
1-chloro-4-methoxybenzene C_7H_7ClO (4-chloroanisole) [623-12-1] YRGAYAGBVIXNAQ-UHFFFAOYSA-N	5.8×10^{-2}		Pfeifer et al. (2001)	M	731
1,2-dichloro-3-methoxybenzene $C_7H_6Cl_2O$ (2,3-dichloroanisole) [1984-59-4] HFEASCCDHUVYKU-UHFFFAOYSA-N	2.2×10^{-2}		Pfeifer et al. (2001)	M	731
1,5-dichloro-2-methoxybenzene $C_7H_6Cl_2O$ (2,4-dichloroanisole) [553-82-2] CICQUFBZCADHHX-UHFFFAOYSA-N	1.2×10^{-2}		Pfeifer et al. (2001)	M	731
1,4-dichloro-2-methoxybenzene $C_7H_6Cl_2O$ (2,5-dichloroanisole) [1984-58-3] QKMNFFSBZRGHDJ-UHFFFAOYSA-N	2.1×10^{-2} 5.7×10^{-2} 1.4×10^{-2} 1.4×10^{-1} 4.8×10^{-2}		Pfeifer et al. (2001) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	M Q Q Q Q	731 287, 288 287, 289 287, 290 287, 291
1,3-dichloro-2-methoxybenzene $C_7H_6Cl_2O$ (2,6-dichloroanisole) [1984-65-2] KZLMCDNAVVJKPX-UHFFFAOYSA-N	8.8×10^{-3}		Pfeifer et al. (2001)	M	731
1,2-dichloro-4-methoxybenzene $C_7H_6Cl_2O$ (3,4-dichloroanisole) [36404-30-5] VISJRVXHPNMYRH-UHFFFAOYSA-N	9.2×10^{-3}		Pfeifer et al. (2001)	M	731

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3-dichloro-5-methoxybenzene $C_7H_6Cl_2O$ (3,5-dichloroanisole) [33719-74-3] SSNXYMVLSOMJLU-UHFFFAOYSA-N	2.3×10^{-3}		Pfeifer et al. (2001)	M	731
1,2,3-trichloro-4-methoxybenzene $C_7H_5Cl_3O$ (2,3,4-trichloroanisole) [54135-80-7] FRQUNVLMWIYOLV-UHFFFAOYSA-N	1.3×10^{-2}		Pfeifer et al. (2001)	M	731
1,2,5-trichloro-3-methoxybenzene $C_7H_5Cl_3O$ (2,3,5-trichloroanisole) [54135-81-8] MKERQGLKSFEKAE-UHFFFAOYSA-N	7.6×10^{-3}		Pfeifer et al. (2001)	M	731
1,2,4-trichloro-3-methoxybenzene $C_7H_5Cl_3O$ (2,3,6-trichloroanisole) [50375-10-5] OTFNCXLUCRUNCH-UHFFFAOYSA-N	1.1×10^{-2} 9.8×10^{-3} 1.8×10^{-2} 2.0×10^{-2} 7.6×10^{-2}	4500	Diaz et al. (2005) Pfeifer et al. (2001) Hilal et al. (2008) Modarresi et al. (2007) Meylan and Howard (1991)	M M Q Q Q	 731 67
1,2,4-trichloro-5-methoxybenzene $C_7H_5Cl_3O$ (2,4,5-trichloroanisole) [6130-75-2] SXKBHOQOOGRFJF-UHFFFAOYSA-N	1.1×10^{-2}		Pfeifer et al. (2001)	M	731
1,3,5-trichloro-2-methoxybenzene $C_7H_5Cl_3O$ (2,4,6-trichloroanisole) [87-40-1] WCVOGSZTONGSQY-UHFFFAOYSA-N	2.3×10^{-2} 4.4×10^{-3} 4.6×10^{-3}	5500 640	Wu et al. (2022a) Diaz et al. (2005) Pfeifer et al. (2001)	M M M	 731
1,2,3-trichloro-5-methoxybenzene $C_7H_5Cl_3O$ (3,4,5-trichloroanisole) [54135-82-9] GUCFBWGWRCILHN-UHFFFAOYSA-N	4.4×10^{-3}		Pfeifer et al. (2001)	M	731
1,2,3,4-tetrachloro-5-methoxybenzene $C_7H_4Cl_4O$ (2,3,4,5-tetrachloroanisole) [938-86-3] FUUHMSUPRUNWRQ-UHFFFAOYSA-N	6.5×10^{-3}		Pfeifer et al. (2001)	M	731

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,5-tetrachloro-4-methoxybenzene $C_7H_4Cl_4O$ (2,3,4,6-tetrachloroanisole) [938-22-7] ITXDBGLYYSJNPK-UHFFFAOYSA-N	3.1×10^{-3}		Pfeifer et al. (2001)	M	731
1,2,4,5-tetrachloro-3-methoxybenzene $C_7H_4Cl_4O$ (2,3,5,6-tetrachloroanisole) [6936-40-9] WMMFIDNWZNCBCT-UHFFFAOYSA-N	3.2×10^{-3}		Pfeifer et al. (2001)	M	731
pentachloromethoxybenzene $C_7H_3Cl_5O$ (pentachloroanisole) [1825-21-4] BBABSCYTNHOKOG-UHFFFAOYSA-N	2.1×10^{-3} 5.1×10^{-3}		Pfeifer et al. (2001) HSDB (2015)	M Q	731 99
4,5-dichloro-2-methoxyphenol $C_7H_6Cl_2O_2$ (4,5-dichloroguaiacol) [2460-49-3] HAAFFTHBNFBVKY-UHFFFAOYSA-N	5.2 2.3		Mackay et al. (2006c) Lei et al. (1999)	V V	
3,4,5-trichloro-2-methoxyphenol $C_7H_5Cl_3O_2$ (3,4,5-trichloroguaiacol) [57057-83-7] RKEHLKXRUVUBJN-UHFFFAOYSA-N	1.1×10^{1} 8.3 9.7×10^{1}		Duchowicz et al. (2020) Mackay et al. (2006c) Lei et al. (1999) Duchowicz et al. (2020)	V V V Q	186 420
4,5,6-trichloro-2-methoxyphenol $C_7H_5Cl_3O_2$ (4,5,6-trichloroguaiacol) [2668-24-8] NIAJPNQTKGWEOI-UHFFFAOYSA-N	7.4 7.1		Mackay et al. (2006c) Lei et al. (1999)	V V	
2,3,4,5-tetrachloro-6-methoxyphenol $C_7H_4Cl_4O_2$ (tetrachloroguaiacol) [2539-17-5] YZZVKLJKDFFSFL-UHFFFAOYSA-N	1.4 6.2 6.7 8.4		Duchowicz et al. (2020) Mackay et al. (2006c) Lei et al. (1999) Duchowicz et al. (2020)	V V V Q	186
2-chlorobenzoic acid $C_7H_5ClO_2$ [118-91-2] IKCLCGXPQILATA-UHFFFAOYSA-N	1.5×10^{2} 1.3×10^{2} 3.5×10^{2} 1.4×10^{2}		Duchowicz et al. (2020) Yaws (2003) Duchowicz et al. (2020) Gharagheizi et al. (2010)	V X Q Q	186 237 246

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-chlorobenzoic acid	5.7×10^{1}		Abraham et al. (2019)	Q	
$C_7H_5ClO_2$	2.5×10^{2}		HSDB (2015)	Q	545
[535-80-8]					
LULAYUGMBFYYEX-UHFFFAOYSA-N					
4-chlorobenzoic acid	2.5×10^{1}		Abraham et al. (2019)	Q	
$C_7H_5ClO_2$					
[74-11-3]					
XRHGYUZYPHTUJZ-UHFFFAOYSA-N					
3,4-dichlorobenzoic acid	2.1×10^{1}		Abraham et al. (2019)	Q	
$C_7H_4Cl_2O_2$					
[51-44-5]					
VPHHJAOJUJHJKD-UHFFFAOYSA-N					
2,3,6-trichlorobenzoic acid	4.7×10^{2}		Duchowicz et al. (2020)	V	186
$C_7H_3Cl_3O_2$	6.5×10^{2}		Duchowicz et al. (2020)	Q	
[50-31-7]					
XZIDTOHMJBOSOX-UHFFFAOYSA-N					
1,2,3-trichloro-4,5-dimethoxybenzene	2.7×10^{-1}		Lei et al. (1999)	V	
$C_8H_7Cl_3O_2$					
(3,4,5-trichloroveratrole)					
[16766-29-3]					
VKNITLPENCJQOP-UHFFFAOYSA-N					
1,2,3,4-tetrachloro-5,6-dimethoxybenzene	9.1×10^{-2}		Lei et al. (1999)	V	
$C_8H_6Cl_4O_2$	1.7		Zhang et al. (2010)	Q	287, 288
(tetrachloroveratrole)	2.0		Zhang et al. (2010)	Q	287, 289
[944-61-6]	2.6		Zhang et al. (2010)	Q	287, 290
NCYHCGGUQGDEQW-UHFFFAOYSA-N	7.5×10^{-1}		Zhang et al. (2010)	Q	287, 291
3-chloro-2,6-dimethoxyphenol	4.2×10^{1}		Lei et al. (1999)	V	
$C_8H_9ClO_3$					
(3-chlorosyringol)					
[18113-22-9]					
WYEMCZZCZXKDNC-UHFFFAOYSA-N					
3,5-dichloro-2,6-dimethoxyphenol	1.4×10^{1}		Lei et al. (1999)	V	
$C_8H_8Cl_2O_3$					
(3,5-dichlorosyringol)					
[78782-46-4]					
IDKMFABKPPHDBI-UHFFFAOYSA-N					
3,5-dichloro-2-hydroxybenzoic acid	1.3×10^{3}		Zhang et al. (2010)	Q	287, 288
$C_7H_4Cl_2O_3$	4.3×10^{2}		Zhang et al. (2010)	Q	287, 289
[320-72-9]	7.5×10^{4}		Zhang et al. (2010)	Q	287, 290
CNJGWCQEGROXEE-UHFFFAOYSA-N	2.2×10^{2}		Zhang et al. (2010)	Q	287, 291

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,6-dichloro-2-hydroxybenzoic acid	1.3×10^{3}		Zhang et al. (2010)	Q	287, 288
$C_7H_4Cl_2O_3$	3.4×10^{3}		Zhang et al. (2010)	Q	287, 289
[3401-80-7]	1.1×10^{1}		Zhang et al. (2010)	Q	287, 290
FKIKPQHMWFZFEB-UHFFFAOYSA-N	2.2×10^{2}		Zhang et al. (2010)	Q	287, 291
5-chloro-2-methoxybenzoic acid	2.1×10^{3}		Zhang et al. (2010)	Q	287, 288
$C_8H_7ClO_3$	3.8×10^{1}		Zhang et al. (2010)	Q	287, 289
[3438-16-2]	9.5×10^{3}		Zhang et al. (2010)	Q	287, 290
HULDRQRKKXRXBI-UHFFFAOYSA-N	6.0×10^{3}		Zhang et al. (2010)	Q	287, 291
2-chloroacetophenone C_8H_7ClO [532-27-4] IMACFCSSMIZSPP-UHFFFAOYSA-N	2.8		HSDB (2015)	Q	99
2,2,2',4',5'-pentachloroacetophenone	2.0×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_8H_3Cl_5O$	5.7		Zhang et al. (2010)	Q	287, 289
[1203-86-7]	1.0		Zhang et al. (2010)	Q	287, 290
WKJXVVFAALGBOH-UHFFFAOYSA-N	6.0		Zhang et al. (2010)	Q	287, 291
tetrachloroterephthaloyl chloride	1.0×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_8Cl_6O_2$	1.9×10^{1}		Zhang et al. (2010)	Q	287, 289
[719-32-4]	3.4×10^{-2}		Zhang et al. (2010)	Q	287, 290
YJIRZJAZKDWEIJ-UHFFFAOYSA-N	1.3×10^{3}		Zhang et al. (2010)	Q	287, 291
chloroxylenol	1.9×10^{1}		HSDB (2015)	Q	99
C_8H_9ClO	1.9×10^{1}		Zhang et al. (2010)	Q	287, 288
[88-04-0]	1.5×10^{1}		Zhang et al. (2010)	Q	287, 289
OSDLLIBGSJNGJE-UHFFFAOYSA-N	2.0×10^{1}		Zhang et al. (2010)	Q	287, 290
	5.1×10^{1}		Zhang et al. (2010)	Q	287, 291
4,5,6,7-tetrachloro-1,3-isobenzofurandione	5.2		Zhang et al. (2010)	Q	287, 288
$C_8Cl_4O_3$	1.8×10^{4}		Zhang et al. (2010)	Q	287, 289
[117-08-8]	1.9×10^{2}		Zhang et al. (2010)	Q	287, 290
AUHHYELHRWCWEZ-UHFFFAOYSA-N	4.3×10^{1}		Zhang et al. (2010)	Q	287, 291
3,4,5-trichloro-2,6-dimethoxyphenol $C_8H_7Cl_3O_3$ (trichlorosyringol) [2539-26-6] ZZCSBXFJFLSDRR-UHFFFAOYSA-N	4.5×10^{1}		Lei et al. (1999)	V	
4,5,6,7-tetrachlorophthalide	1.8×10^{1}		Kawamoto and Urano (1989)	M	
$C_8H_2Cl_4O_2$	3.1×10^{3}		Duchowicz et al. (2020)	V	186
[27355-22-2]	8.6		Duchowicz et al. (2020)	Q	
NMWKWBPNKPGATC-UHFFFAOYSA-N					

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dicamba	4.5×10^3		Duchowicz et al. (2020)	V	186
$C_8H_6Cl_2O_3$	2.3×10^4		HSDB (2015)	V	
(banvel)	4.5×10^3		Mackay et al. (2006d)	V	
[1918-00-9]	8.3×10^3		Suntio et al. (1988)	V	12
IWEDIXLBFLAXBO-UHFFFAOYSA-N	8.2×10^1		Barcelo and Hennion (1997)	X	567
	2.2×10^4		Armbrust (2000)	C	
	5.9×10^3		Duchowicz et al. (2020)	Q	
	1.2		Goodarzi et al. (2010)	Q	568, 569
	1.0×10^4		Maniere et al. (2011)	?	165
(2,4-dichlorophenoxy)-ethanoic acid	1.4×10^{-1}		Rice et al. (1997b)	M	732, 12
$C_8H_6Cl_2O_3$	1.2		Rice et al. (1997b)	M	732, 12
((2,4-dichlorophenoxy)-acetic acid; 2,4-D)	2.8×10^2		Duchowicz et al. (2020)	V	186
[94-75-7]	5.0×10^4		Mackay et al. (2006c)	V	
OVSKIKFHRZPJSS-UHFFFAOYSA-N	2.3×10^4		Mackay et al. (2006d)	V	
	4.0×10^3		Mackay et al. (2006d)	V	
	2.9×10^2		Mackay et al. (1995)	V	
	1.8		Riederer (1990)	V	
	1.8		Suntio et al. (1988)	V	12
	7.2×10^4		Howard (1991)	X	412
	9.7×10^2		Howard (1991)	X	412
	5.5×10^6		Armbrust (2000)	C	
	8.7×10^2		Duchowicz et al. (2020)	Q	
	2.5×10^5		Maniere et al. (2011)	?	12, 165
2,4,5-trichlorophenoxyethanoic acid	1.7×10^2		Mackay et al. (2006d)	V	
$C_8H_5Cl_3O_3$	1.7×10^2		Riederer (1990)	V	
(2,4,5-T)	1.7×10^2		Suntio et al. (1988)	V	12
[93-76-5]	8.4×10^5		MacBean (2012a)	?	
SMYMJHWAQXWPDB-UHFFFAOYSA-N					
1,4-dichloro-2,5-dimethoxybenzene	9.7×10^{-2}		Duchowicz et al. (2020)	V	186
$C_8H_8Cl_2O_2$	9.9×10^{-2}		HSDB (2015)	V	
[2675-77-6]			Mackay et al. (2006d)	V	558
PFIADAMVCJPXSF-UHFFFAOYSA-N	9.4×10^{-1}		Duchowicz et al. (2020)	Q	
2,3,6-trichlorophenylacetic acid	8.3×10^{-1}		Mackay et al. (2006d)	V	
$C_8H_5Cl_3O_2$	5.5×10^2		HSDB (2015)	Q	99
[85-34-7]					
QZXCCPZJCKEPSA-UHFFFAOYSA-N					

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methoxy-benzoyl chloride $C_8H_7ClO_2$ (p-anisoyl chloride) [100-07-2] MXMOTZIXVICDSD-UHFFFAOYSA-N	1.3		HSDB (2015)	Q	99
(4-chlorophenoxy)acetic acid $C_8H_7ClO_3$ [122-88-3] SODPIMGUZLOIPE-UHFFFAOYSA-N	1.0×10^5		Ebert et al. (2023)	?	316
isobenzan $C_9H_4Cl_8O$ [297-78-9] LRWHHSXTGZSMSN-UHFFFAOYSA-N	1.7×10^2		HSDB (2015)	Q	99
2-chloro-4-hydroxy-3,5-dimethoxybenzaldehyde $C_9H_9ClO_4$ (2-chlorosyringaldehyde) [76341-69-0] GRIHRCLOUQZXPD-UHFFFAOYSA-N	9.1×10^1		Lei et al. (1999)	V	
2,6-dichloro-4-hydroxy-3,5-dimethoxybenzaldehyde $C_9H_8Cl_2O_4$ (2,6-dichlorosyringaldehyde) [76330-06-8] CTFRWEPMHUGVMM-UHFFFAOYSA-N	2.7×10^2		Lei et al. (1999)	V	
methyl 2,4-dichlorophenoxyethanoate	3.6		Duchowicz et al. (2020)	V	186
$C_9H_8Cl_2O_3$	1.0×10^1		Duchowicz et al. (2020)	Q	
[1928-38-7]	1.8		Hilal et al. (2008)	Q	
HWIGZMADSFQMOI-UHFFFAOYSA-N	1.3		Modarresi et al. (2007)	Q	67
(2-methyl-4-chlorophenoxy)acetic acid	$>9.9\times10^1$		Mabury and Crosby (1996)	M	
$C_9H_9ClO_3$	7.4×10^3		Duchowicz et al. (2020)	V	186
(MCPA)	4.0×10^4		Mackay et al. (2006d)	V	
[94-74-6]	9.9×10^3		Woodrow et al. (1990)	V	
WHKUVVPPKQRRBV-UHFFFAOYSA-N	5.7×10^2		Duchowicz et al. (2020)	Q	
	1.8×10^4		Maniere et al. (2011)	?	165
α-(2,4-dichlorophenoxy)propionic acid $C_9H_8Cl_2O_3$ (dichloroprop) [120-36-5] MZHCENGPTKEIGP-UHFFFAOYSA-N	3.7×10^3		Mackay et al. (2006d)	V	

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(*R*)-2-(2,4-dichlorophenoxy)propanoic acid	4.0×10^4		Mackay et al. (2006d)	V	
$C_9H_8Cl_2O_3$	1.8×10^4		Maniere et al. (2011)	?	241, 165
(dichlorprop-p)					
[15165-67-0]					
MZHCENGPTKEIGP-RXMQYKEDSA-N					
2-(2,4,5-trichlorophenoxy)propanoic acid	3.9×10^4		Mackay et al. (2006d)	V	
$C_9H_7Cl_3O_3$					
[93-72-1]					
ZLSWBLPERHFHIS-UHFFFAOYSA-N					
cloxyfonac	1.0×10^5		Duchowicz et al. (2020)	V	186
$C_9H_9O_4Cl$	1.9×10^6		Duchowicz et al. (2020)	Q	
[6386-63-6]					
ZJRUTGDCLVIVRD-UHFFFAOYSA-N					
tridiphane	1.9×10^{-1}		MacBean (2012a)	?	
$C_{10}H_7Cl_5O$					
[58138-08-2]					
IBZHOAONZVJLOB-UHFFFAOYSA-N					
plifenat	1.1×10^4		MacBean (2012a)	?	
$C_{10}H_7O_2Cl_5$					
[21757-82-4]					
FSGNOVKGEXRRHD-UHFFFAOYSA-N					
chlorfenprop-methyl	4.4		Ebert et al. (2023)	?	365
$C_{10}H_{10}Cl_2O_2$					
[14437-17-3]					
YJKIALIXRCSISK-UHFFFAOYSA-N					
ethyl 2,4-dichlorophenoxyethanoate	3.0		Duchowicz et al. (2020)	V	186
$C_{10}H_{10}Cl_2O_3$	4.3		Duchowicz et al. (2020)	Q	
[533-23-3]	1.2		Hilal et al. (2008)	Q	
JSLBZIVMVVHMDJ-UHFFFAOYSA-N	1.1		Modarresi et al. (2007)	Q	67
mecoprop	1.1×10^4		Duchowicz et al. (2020)	V	186
$C_{10}H_{11}ClO_3$			Mackay et al. (2006d)	V	558
[93-65-2]	9.0×10^1		Barcelo and Hennion (1997)	X	567
WNTGYJSOUMFZEP-UHFFFAOYSA-N	9.0×10^3		Armbrust (2000)	C	
	2.6×10^2		Duchowicz et al. (2020)	Q	
	1.4×10^2		Goodarzi et al. (2010)	Q	568

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(*R*)-2-(4-chloro-2-methylphenoxy)propanoic acid	1.0×10^4		Mackay et al. (2006d)	V	
$C_{10}H_{11}ClO_3$	1.8×10^4		Maniere et al. (2011)	?	12, 165
(mecoprop-p)					
[16484-77-8]					
WNTGYJSOUMFZEP-SSDOTTSWSA-N					
dacthal	4.4		Muir et al. (2004)	L	367
$C_{10}H_6Cl_4O_4$	4.5		Duchowicz et al. (2020)	V	186
(DCPA)	4.5		HSDB (2015)	V	
[1861-32-1]	1.4×10^2		Duchowicz et al. (2020)	Q	
NPOJQCVWMSKXDN-UHFFFAOYSA-N					
4-(2,4-dichlorophenoxy)-butanoic acid	4.3×10^3		HSDB (2015)	Q	99
$C_{10}H_{10}Cl_2O_3$	2.2×10^5		Maniere et al. (2011)	?	241, 165
(2,4-DB)					
[94-82-6]					
YIVXMZJTEQBPQO-UHFFFAOYSA-N					
dichlone	9.7×10^3		HSDB (2015)	Q	99
$C_{10}H_4Cl_2O_2$					
[117-80-6]					
SVPKNMBRVBMTLB-UHFFFAOYSA-N					
1-[(2,3,6-trichlorophenyl)methoxy]propan-2-ol	2.0×10^1		Duchowicz et al. (2020)	V	186
$C_{10}H_{11}Cl_3O_2$	1.7×10^1		Duchowicz et al. (2020)	Q	
(tritac)					
[1861-44-5]					
LJWIIRATRWPHBA-UHFFFAOYSA-N					
(2,4-dichlorophenoxy)-acetic acid 1-methylethyl ester	4.6		Duchowicz et al. (2020)	V	186
$C_{11}H_{12}Cl_2O_3$	4.5		HSDB (2015)	V	
[94-11-1]	2.0		Duchowicz et al. (2020)	Q	
WHOKDONDRZNCBC-UHFFFAOYSA-N					
4-(4-chloro-2-methylphenoxy)butanoic acid	3.6×10^3		Duchowicz et al. (2020)	V	186
$C_{11}H_{13}ClO_3$	3.1×10^3		Mackay et al. (2006d)	V	
(MCPB)	1.7×10^3		Duchowicz et al. (2020)	Q	
[94-81-5]	3.3×10^4		Maniere et al. (2011)	?	241, 165
LLWADFLAOKUBDR-UHFFFAOYSA-N					

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
triclosan	4.7×10^{2}		HSDB (2015)	Q	99
$C_{12}H_7Cl_3O_2$	2.0×10^{3}		Zhang et al. (2010)	Q	287, 288
[3380-34-5]	5.7×10^{1}		Zhang et al. (2010)	Q	287, 289
XEFQLINVKFYRCS-UHFFFAOYSA-N	1.4×10^{3}		Zhang et al. (2010)	Q	287, 290
	8.2×10^{2}		Zhang et al. (2010)	Q	287, 291
monobutyl tetrachlorophthalate	2.0×10^{4}		Zhang et al. (2010)	Q	287, 288
$C_{12}H_{10}Cl_4O_4$	7.5×10^{2}		Zhang et al. (2010)	Q	287, 289
[24261-19-6]	5.1×10^{4}		Zhang et al. (2010)	Q	287, 290
WKYMTJULVAGWJM-UHFFFAOYSA-N	5.1×10^{4}		Zhang et al. (2010)	Q	287, 291
(2,4-dichlorophenoxy)-acetic acid butyl ester	2.0×10^{1}		Duchowicz et al. (2020)	V	186
$C_{12}H_{14}Cl_2O_3$	2.0×10^{1}		HSDB (2015)	V	
[94-80-4]	5.7		Duchowicz et al. (2020)	Q	
UQMRAFJOBWOFNS-UHFFFAOYSA-N					
sucralose	2.5×10^{13}		HSDB (2015)	Q	99
$C_{12}H_{19}Cl_3O_8$					
[56038-13-2]					
BAQAVOSOZGMPRM-QBMZZYIRSA-N					
endrin aldehyde	2.4		Duchowicz et al. (2020)	V	186
$C_{12}H_8Cl_6O$	2.3		HSDB (2015)	V	
[7421-93-4]	4.8		Duchowicz et al. (2020)	Q	
HCTWZIFNBBCVGM-UHFFFAOYSA-N					
clorophene	3.7×10^{3}		Duchowicz et al. (2020)	V	186
$C_{13}H_{11}ClO$	3.7×10^{3}		HSDB (2015)	V	
(4-chloro-2-benzylphenol)	6.5×10^{2}		Duchowicz et al. (2020)	Q	
[120-32-1]					
NCKMMSIFQUPKCK-UHFFFAOYSA-N					
(4-chlorophenyl)phenylmethanone	7.0		HSDB (2015)	Q	99
$C_{13}H_9ClO$					
(4-chlorobenzophenone)					
[134-85-0]					
UGVRJVHOJNYEHR-UHFFFAOYSA-N					
1-(4-chlorophenyl)-4,4-dimethyl-3-pentanone	1.1		Zhang et al. (2010)	Q	287, 288
$C_{13}H_{17}ClO$	7.2×10^{-1}		Zhang et al. (2010)	Q	287, 289
[66346-01-8]	4.2		Zhang et al. (2010)	Q	287, 290
ILQGIJDYSLHIOX-UHFFFAOYSA-N	3.9×10^{-1}		Zhang et al. (2010)	Q	287, 291
hexachlorophene	1.8×10^{7}		HSDB (2015)	Q	99
$C_{13}H_6Cl_6O_2$	1.1×10^{7}		Zhang et al. (2010)	Q	287, 288
[70-30-4]	2.5×10^{5}		Zhang et al. (2010)	Q	287, 289
ACGUYXCXAPNIKK-UHFFFAOYSA-N	1.2×10^{4}		Zhang et al. (2010)	Q	287, 290
	6.5×10^{5}		Zhang et al. (2010)	Q	287, 291

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4'-dichlorobenzophenone	9.2		Zhang et al. (2010)	Q	287, 288
$C_{13}H_8Cl_2O$	6.9		Zhang et al. (2010)	Q	287, 289
[85-29-0]	4.3×10^{1}		Zhang et al. (2010)	Q	287, 290
YXMYPHLWXBXNFF-UHFFFAOYSA-N	6.1×10^{1}		Zhang et al. (2010)	Q	287, 291
1-(4-chlorophenyl)-4,4-dimethylpent-1-en-3-one	4.8		Zhang et al. (2010)	Q	287, 288
$C_{13}H_{15}ClO$	2.2		Zhang et al. (2010)	Q	287, 289
[1577-03-3]	8.2		Zhang et al. (2010)	Q	287, 290
LXJZYHPGRKBVGF-UHFFFAOYSA-N	1.5		Zhang et al. (2010)	Q	287, 291
dichlorophen	8.2×10^{6}		HSDB (2015)	V	
$C_{13}H_{10}Cl_2O_2$	8.5×10^{6}		Mackay et al. (2006d)	V	
[97-23-4]					
MDNWOSOZYLHTCG-UHFFFAOYSA-N					
MCPB ethyl ester	2.0×10^{2}		Duchowicz et al. (2020)	V	186
$C_{13}H_{17}ClO_3$	2.9		Duchowicz et al. (2020)	Q	
[10443-70-6]					
XNKARWLGLZGMGX-UHFFFAOYSA-N					
2-chloro-9,10-anthracenedione	4.2×10^{3}		Zhang et al. (2010)	Q	287, 288
$C_{14}H_7ClO_2$	6.7×10^{2}		Zhang et al. (2010)	Q	287, 289
[131-09-9]	1.4×10^{2}		Zhang et al. (2010)	Q	287, 290
FPKCTSIVDAWGFA-UHFFFAOYSA-N	3.3×10^{4}		Zhang et al. (2010)	Q	287, 291
dicofol	4.1×10^{1}		Duchowicz et al. (2020)	V	186
$C_{14}H_9Cl_5O$	4.1×10^{1}		HSDB (2015)	V	
[115-32-2]	9.6×10^{2}		Duchowicz et al. (2020)	Q	
UOAMTSKGCBMZTC-UHFFFAOYSA-N	1.8×10^{4}		Zhang et al. (2010)	Q	287, 288
	3.1×10^{2}		Zhang et al. (2010)	Q	287, 289
	9.2×10^{1}		Zhang et al. (2010)	Q	287, 290
	3.2×10^{3}		Zhang et al. (2010)	Q	287, 291
bis(2,4-dichlorobenzoyl)peroxide	9.2		Zhang et al. (2010)	Q	287, 288
$C_{14}H_6Cl_4O_4$	1.4×10^{2}		Zhang et al. (2010)	Q	287, 289
[133-14-2]	1.6×10^{3}		Zhang et al. (2010)	Q	287, 290
WRXCBRHBHGNNQA-UHFFFAOYSA-N	3.5×10^{3}		Zhang et al. (2010)	Q	287, 291
dipropyl tetrachlorophthalate	4.7×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_{14}H_{14}Cl_4O_4$	3.0×10^{1}		Zhang et al. (2010)	Q	287, 289
[6928-67-2]	1.0×10^{1}		Zhang et al. (2010)	Q	287, 290
QJRSPJSHRYYBJL-UHFFFAOYSA-N	2.8×10^{1}		Zhang et al. (2010)	Q	287, 291
2-(4-chlorobenzoyl)benzoic acid	3.4×10^{5}		Zhang et al. (2010)	Q	287, 288
$C_{14}H_9ClO_3$	3.6×10^{4}		Zhang et al. (2010)	Q	287, 289
[85-56-3]	7.9×10^{7}		Zhang et al. (2010)	Q	287, 290
YWECCEXWKFHHQJ-UHFFFAOYSA-N	2.1×10^{6}		Zhang et al. (2010)	Q	287, 291

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(2,4,5-trichlorophenoxy)acetic acid butoxyethanol ester $C_{14}H_{17}Cl_3O_4$ [2545-59-7] GLDWASBMYWLQGG-UHFFFAOYSA-N	1.2×10^{2}		HSDB (2015)	Q	99
(2,4-dichlorophenoxy)-acetic acid, 2-butoxyethyl ester $C_{14}H_{18}Cl_2O_4$ [1929-73-3] ZMWGIGHRZQTQRE-UHFFFAOYSA-N	6.2×10^{1} 6.2×10^{1} 6.0×10^{1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
1-chloro-9,10-anthracenedione $C_{14}H_7ClO_2$ (1-chloroanthraquinone) [82-44-0] BOCJQSFSGAZAPQ-UHFFFAOYSA-N	4.3×10^{2} 4.2×10^{3}		Abraham et al. (2019) HSDB (2015)	Q Q	 99
chlorflurenol methyl $C_{15}H_{11}ClO_3$ [2536-31-4] LINPVWIEWJTEEJ-UHFFFAOYSA-N	1.3×10^{3}		Ebert et al. (2023)	?	365
4,4'-(1-methylethylidene)bis(2,6-dichlorophenol) $C_{15}H_{12}Cl_4O_2$ (2,2',6,6'-tetrachlorobisphenol A) [79-95-8] KYPYTERUKNKOLP-UHFFFAOYSA-N	3.5×10^{6}		HSDB (2015)	Q	447
diclofop $C_{15}H_{12}Cl_2O_4$ [40843-25-2] OOLBCHYXZDXLDS-UHFFFAOYSA-N	9.2×10^{5}		Ebert et al. (2023)	?	316
methoxychlor $C_{16}H_{15}Cl_3O_2$ [72-43-5] IAKOZHOLGAGEJT-UHFFFAOYSA-N	4.9×10^{1} 1.0 4.0 5.5 2.8 6.4 4.9×10^{1}		Altschuh et al. (1999) Mackay et al. (2006d) Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Duchowicz et al. (2020)	M V Q Q Q Q ?	 67 185, 21
diclofop-methyl $C_{16}H_{14}Cl_2O_4$ [51338-27-3] BACHBFVBHLGWSL-UHFFFAOYSA-N	5.0 5.0 1.3×10^{2} 2.6×10^{2} 9.5×10^{1}		Duchowicz et al. (2020) Mackay et al. (2006d) Duchowicz et al. (2020) HSDB (2015) Maniere et al. (2011)	V V Q Q ?	186 99 12, 165

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chlorobenzilate $C_{16}H_{14}Cl_2O_3$ [510-15-6] RAPBNVDSDCTNRC-UHFFFAOYSA-N	1.4×10^{2} 2.6×10^{2}		HSDB (2015) MacBean (2012a)	V ?	
(2,4-dichlorophenoxy)-acetic acid 2-ethylhexyl ester $C_{16}H_{22}Cl_2O_3$ [1928-43-4] QZSFJRIWRPJUOH-UHFFFAOYSA-N	5.5×10^{-1} 5.5×10^{-1}		MacBean (2012b) Maniere et al. (2011)	X ?	350 241, 165
(2,4-dichlorophenoxy)-acetic acid, isooctyl ester $C_{16}H_{22}Cl_2O_3$ [25168-26-7] BBPLSOGERZQYQC-UHFFFAOYSA-N	1.0×10^{-1} 3.3×10^{-1} 1.7×10^{-1}		Duchowicz et al. (2020) Duchowicz et al. (2020) HSDB (2015)	V Q Q	186 99
mecoprop-2-butoxyethyl ester $C_{16}H_{23}ClO_4$ [23359-62-8] GWFGUAFFJVHZKY-UHFFFAOYSA-N	5.0		Ebert et al. (2023)	?	318
chloropropylate $C_{17}H_{16}Cl_2O_3$ [5836-10-2] AXGUBXVWZBFQGA-UHFFFAOYSA-N	1.2×10^{3} 1.0×10^{2}		HSDB (2015) MacBean (2012a)	V ?	
MCPA-2-ethylhexyl ester $C_{17}H_{25}ClO_3$ [29450-45-1] IDGRPSMONFWWEK-UHFFFAOYSA-N	2.3×10^{-1}		Ebert et al. (2023)	?	318
1-(2-(2-chloroethoxy)ethoxy)-4-(1,1,3,3-tetramethylbutyl)benzene $C_{18}H_{29}ClO_2$ [65925-28-2] FITQCDWGUKECBJ-UHFFFAOYSA-N	5.3×10^{-1} 1.6 3.8×10^{-1} 8.4×10^{-2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
fenofibrate $C_{20}H_{21}ClO_4$ [49562-28-9] YMTINGFKWWXKFG-UHFFFAOYSA-N	2.2×10^{3}		HSDB (2015)	Q	99
indanofan $C_{20}H_{17}O_3Cl$ [133220-30-1] PMAAYIYCDXGUAP-UHFFFAOYSA-N	1.5×10^{4} 5.4×10^{3}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
spirodiclofen	1.7×10^{2}		HSDB (2015)	V	
$C_{21}H_{24}Cl_2O_4$	$>5.0\times10^{2}$		Maniere et al. (2011)	?	12, 165
[148477-71-8]					
DTDSAWVUFPGDMX-UHFFFAOYSA-N					
permethrin	5.3		Duchowicz et al. (2020)	V	186
$C_{21}H_{20}Cl_2O_3$	4.1		HSDB (2015)	V	
[52645-53-1]	9.0		Mackay et al. (2006d)	V	
RLLPVAHGXHCWKJ-UHFFFAOYSA-N	1.2×10^{1}		Duchowicz et al. (2020)	Q	
chlorophacinone	2.7×10^{6}		Duchowicz et al. (2020)	V	186
$C_{23}H_{15}ClO_3$	4.1×10^{4}		Duchowicz et al. (2020)	Q	
[3691-35-8]					
UDHXJZHVNHGCEC-UHFFFAOYSA-N					
chlormadinone acetate	1.8×10^{4}		HSDB (2015)	Q	99
$C_{23}H_{29}ClO_4$					
[302-22-7]					
QMBJSIBWORFWQT-UHFFFAOYSA-N					
3,4,5,6-tetrachlorophthalic acid bis(2-ethylhexyl) ester	2.8		Zhang et al. (2010)	Q	287, 288
$C_{24}H_{34}Cl_4O_4$	2.3×10^{1}		Zhang et al. (2010)	Q	287, 289
[34832-88-7]	1.0×10^{4}		Zhang et al. (2010)	Q	287, 290
BELGUQVGZMFEAQ-UHFFFAOYSA-N	3.5		Zhang et al. (2010)	Q	287, 291
endosulfan alcohol	7.7×10^{3}		Zhang et al. (2010)	Q	287, 288
$C_9H_8Cl_6O_2$	3.0×10^{6}		Zhang et al. (2010)	Q	287, 289
[2157-19-9]	1.3×10^{5}		Zhang et al. (2010)	Q	287, 290
GTSJHTSVFKEASK-UHFFFAOYSA-N	1.8×10^{5}		Zhang et al. (2010)	Q	287, 291
chlorendic anhydride	1.1×10^{2}		Zhang et al. (2010)	Q	287, 288
$C_9H_2Cl_6O_3$	3.1×10^{4}		Zhang et al. (2010)	Q	287, 289
[115-27-5]	1.5×10^{4}		Zhang et al. (2010)	Q	287, 290
FLBJFXNAEMSXGL-UHFFFAOYSA-N	3.9×10^{7}		Zhang et al. (2010)	Q	287, 291
1,4,5,6,7,7-hexachloro-bicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid	3.3×10^{8}		HSDB (2015)	Q	99
$C_9H_4Cl_6O_4$	3.3×10^{8}		Zhang et al. (2010)	Q	287, 288
[115-28-6]	3.1×10^{9}		Zhang et al. (2010)	Q	287, 289
DJKGDNKYTKCJKD-UHFFFAOYSA-N	3.9×10^{9}		Zhang et al. (2010)	Q	287, 290
	7.3×10^{7}		Zhang et al. (2010)	Q	287, 291

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
heptachlorepoxide	4.8×10^{-1}		Shen and Wania (2005)	L	366
$C_{10}H_5Cl_7O$	5.9×10^{-1}		Shen and Wania (2005)	L	367
[1024-57-3]	9.6×10^{-1}		Chao et al. (2017)	M	
ZXFXBSWRVIQKOD-UHFFFAOYSA-N	5.0×10^{-1}	5200	Cetin et al. (2006)	M	
	4.7×10^{-1}		Altschuh et al. (1999)	M	
	3.1×10^{-1}		Warner et al. (1980)	M	
	5.4×10^{-1}		Hilal et al. (2008)	C	
	1.3×10^{1}		Ryan et al. (1988)	C	
	3.1×10^{-1}		Shen (1982)	C	
	6.6×10^{-1}		Keshavarz et al. (2022)	Q	
	7.7×10^{-1}		Duchowicz et al. (2020)	Q	
	7.3		Hilal et al. (2008)	Q	
	5.4		Modarresi et al. (2007)	Q	67
	4.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
dieldrin	1.0		Shen and Wania (2005)	L	366
$C_{12}H_8OCl_6$	9.1×10^{-1}		Shen and Wania (2005)	L	367
[60-57-1]	9.1×10^{-1}		Mackay and Shiu (1981)	L	
DFBKLUNHFCTMDC-NLUYNBKHSA-N	6.5×10^{-1}		Chao et al. (2017)	M	
	9.2×10^{-1}	5800	Cetin et al. (2006)	M	
	9.8×10^{-1}		Altschuh et al. (1999)	M	
	3.4×10^{-1}		Slater and Spedding (1981)	M	12
	1.7×10^{-1}		Warner et al. (1980)	M	
	8.9×10^{-1}		Mackay et al. (2006d)	V	
	8.9×10^{-1}		Suntio et al. (1988)	V	12
	4.9×10^{1}		Mackay and Leinonen (1975)	V	
	8.8×10^{-3}		Barcelo and Hennion (1997)	X	567
	1.7×10^{-1}		Hilal et al. (2008)	C	
	5.0×10^{1}		Suntio et al. (1988)	C	12
	2.2×10^{1}		Suntio et al. (1988)	C	681
	9.8×10^{-1}		Suntio et al. (1988)	C	681
	1.7×10^{-1}		Suntio et al. (1988)	C	
	4.7×10^{-2}		Suntio et al. (1988)	C	
	1.3		Ryan et al. (1988)	C	
	1.7×10^{-1}		Shen (1982)	C	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	7.2×10^{-1}		Duchowicz et al. (2020)	Q	
	7.4×10^{-4}		Goodarzi et al. (2010)	Q	568, 571
	1.1		Hilal et al. (2008)	Q	
	2.7		Modarresi et al. (2007)	Q	67
	9.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	1.2		MacBean (2012a)	?	
	5.7×10^{1}		Brimblecombe (1986)	?	80

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Table A6.4: Oxygenated chlorocarbons (C, H, O, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
endrin	1.6		Shen and Wania (2005)	L	366
$C_{12}H_8Cl_6O$	9.1×10^{-1}		Shen and Wania (2005)	L	367
[72-20-8]	1.5		Chao et al. (2017)	M	
DFBKLUNHFCTMDC-GKRDHZSOSA-N	1.8	4600	Cetin et al. (2006)	M	
	1.6		Altschuh et al. (1999)	M	
	3.0×10^{1}		Mackay et al. (2006d)	V	
	3.0×10^{1}		Suntio et al. (1988)	V	12
	5.6×10^{3}		Suntio et al. (1988)	C	
	2.4×10^{1}		Ryan et al. (1988)	C	
	1.2		Keshavarz et al. (2022)	Q	
	7.2×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.1		Hilal et al. (2008)	Q	
	2.7		Modarresi et al. (2007)	Q	67
	1.6		Duchowicz et al. (2020)	?	185, 21
1,4,5,6,7,7-hexachlorobicyclo[2.2.1]hept-5-ene-2,3-dicarboxylic acid, dibutyl ester	5.8×10^{2}		Zhang et al. (2010)	Q	287, 288
$C_{17}H_{20}Cl_6O_4$	1.4×10^{2}		Zhang et al. (2010)	Q	287, 289
[1770-80-5]	4.6×10^{3}		Zhang et al. (2010)	Q	287, 290
UJAHPBDUQZFDLA-UHFFFAOYSA-N	8.0×10^{2}		Zhang et al. (2010)	Q	287, 291
di-2-ethylhexyl chlorendate	6.0×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_{25}H_{36}Cl_6O_4$	2.1×10^{2}		Zhang et al. (2010)	Q	287, 289
[4827-55-8]	5.2×10^{3}		Zhang et al. (2010)	Q	287, 290
ONIHOIFWLALAQH-UHFFFAOYSA-N	1.6×10^{2}		Zhang et al. (2010)	Q	287, 291

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A6.5 Polychlorinated diphenyl ethers (PCDEs)

Table A6.5: Polychlorinated diphenyl ethers (PCDEs)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-chlorodiphenyl ether $C_{12}H_9ClO$ (PCDE-1) [2689-07-8] IPBRZLMGGXHHMS-UHFFFAOYSA-N	3.1×10^{-2}		Kurz and Ballschmiter (1999)	V	
3-chlorodiphenyl ether $C_{12}H_9ClO$ (PCDE-2) [6452-49-9] BMURONZFJJPAOK-UHFFFAOYSA-N	1.2×10^{-1} 2.7×10^{-2} 3.0×10^{-1}		Kurz and Ballschmiter (1999) Hilal et al. (2008) Modarresi et al. (2007)	V Q Q	 67
4-chlorodiphenyl ether $C_{12}H_9ClO$ (PCDE-3) [7005-72-3] PGPNJCAMHOJTEF-UHFFFAOYSA-N	1.1×10^{-1} 4.5×10^{-2} 9.0×10^{-2} 4.0×10^{-2} 3.1×10^{-2}		Kurz and Ballschmiter (1999) Mackay et al. (1993) Howard and Meylan (1997) Ryan et al. (1988) Hilal et al. (2008)	V V X C Q	 446
2,3-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-5) [68486-28-2] VSKSUBSGORDMQX-UHFFFAOYSA-N	2.4×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,4-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-7) [51892-26-3] KXIPYLZZJZMMPD-UHFFFAOYSA-N	1.9×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,4'-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-8) [6903-65-7] MWKULKMSBBSGTP-UHFFFAOYSA-N	3.2×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,5-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-9) [24910-69-8] VITXVDNQHXYQSK-UHFFFAOYSA-N	7.9×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,6-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-10) [28419-69-4] IRLZOQDGEAEIPX-UHFFFAOYSA-N	5.0×10^{-2}		Kurz and Ballschmiter (1999)	V	

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Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-12) [55538-69-7] QFQLZVAAQOJUFS-UHFFFAOYSA-N	1.1×10^{-1}		Kurz and Ballschmiter (1999)	V	
3,4'-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-13) [6842-62-2] HPRGYUWRGCTBAV-UHFFFAOYSA-N	1.3×10^{-1}		Kurz and Ballschmiter (1999)	V	
3,5-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-14) [24910-68-7] LEKOWSSKXYFERR-UHFFFAOYSA-N	6.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
4,4'-dichlorodiphenyl ether $C_{12}H_8Cl_2O$ (PCDE-15) [2444-89-5] URUJZHZLCCIILC-UHFFFAOYSA-N	2.1×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,2',4-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-17) [68914-97-6] YXMNUPKWUMIZAV-UHFFFAOYSA-N	4.5×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,3,4-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-21) [85918-32-7] ANKBTLMYMVMWBS-UHFFFAOYSA-N	2.8×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,3,4'-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-22) [157683-71-1] KOTNFWJIMRGVBR-UHFFFAOYSA-N	3.2×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,3,5-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-23) [162853-24-9] MDSPKCWGOVVFJD-UHFFFAOYSA-N	2.2×10^{-1}		Kurz and Ballschmiter (1999)	V	

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Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,6-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-24) [162853-25-0] RQSRPDGSUDRYLH-UHFFFAOYSA-N	3.0×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3',4-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-25) [155999-93-2] BJFOCMRBCBZFJT-UHFFFAOYSA-N	1.5×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,4,4'-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-28) [59039-21-3] PIORTDHJOLELKR-UHFFFAOYSA-N	3.0×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,4,5-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-29) [52322-80-2] UWKZWXCTDPYXHU-UHFFFAOYSA-N	8.9×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,4,6-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-30) [63646-52-6] WXLQUFLKMICSSY-UHFFFAOYSA-N	1.4×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,4',5-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-31) [65075-00-5] FZBSTAVCYOMFMD-UHFFFAOYSA-N	1.6×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,4',6-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-32) [157683-72-2] ZMRFCSWFCKICQE-UHFFFAOYSA-N	4.2×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3',4'-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-33) [61328-44-7] VBNJGYOQZAENPO-UHFFFAOYSA-N	3.4×10^{-1}		Kurz and Ballschmiter (1999)	V	

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Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3',4-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-35) [66794-60-3] BUKLLCIUMZELOH-UHFFFAOYSA-N	2.2×10^{-1}		Kurz and Ballschmiter (1999)	V	
3,4,4'-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-37) [63646-51-5] FTZDEZOARSJHGU-UHFFFAOYSA-N	1.6×10^{-1}		Kurz and Ballschmiter (1999)	V	
3,4,5-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-38) [63646-53-7] ZQCCHNBMSHOJAT-UHFFFAOYSA-N	9.1×10^{-3}		Kurz and Ballschmiter (1999)	V	
3,4',5-trichlorodiphenyl ether $C_{12}H_7Cl_3O$ (PCDE-39) [24910-73-4] CCEZFZGXWFJQEF-UHFFFAOYSA-N	1.6×10^{-1}		Kurz and Ballschmiter (1999)	V	
2,2',3,4-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-41) [220002-37-9] VTTDWGUAWMLHPR-UHFFFAOYSA-N	5.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-42) [147102-63-4] UYVBJPIPRAJEKW-UHFFFAOYSA-N	5.8×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',4,4'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-47) [28076-73-5] ZRWRPGGXCSSBAO-UHFFFAOYSA-N	2.9×10^{-2} 2.8×10^{-1}		Kurz and Ballschmiter (1999) HSDB (2015)	V Q	 99
2,2',4,5-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-48) [162853-26-1] DRVAMLZVBNYSQE-UHFFFAOYSA-N	1.6×10^{-2}		Kurz and Ballschmiter (1999)	V	

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Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',4,5'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-49) [155999-92-1] XIXPEFLLHQAIOY-UHFFFAOYSA-N	2.6×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,3',4-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-55) [220002-39-1] IZISEKJPNSBPRX-UHFFFAOYSA-N	2.3×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,3',4'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-56) [162853-27-2] JVFGXWCLGNACOG-UHFFFAOYSA-N	4.4×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,4,4'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-60) [65075-01-6] ZPOBHUZRVVTGKB-UHFFFAOYSA-N	3.6×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,4,5-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-61) [220002-40-4] QAPPZLVGIXQUJW-UHFFFAOYSA-N	6.6×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,3,4,6-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-62) [85918-33-8] WJZPRRFFZWVZJL-UHFFFAOYSA-N	9.1×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,3,4',5-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-63) [220002-41-5] YHQRYZGDQCSHFO-UHFFFAOYSA-N	1.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,4',6-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-64) [220002-42-6] HJCNTJIMUWQMSA-UHFFFAOYSA-N	3.8×10^{-2}		Kurz and Ballschmiter (1999)	V	

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Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,5,6-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-65) [63646-54-8] UFGXCDQXRUFDMA-UHFFFAOYSA-N	9.3×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,3',4,4'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-66) [61328-46-9] CAWSVYYOUZEMHA-UHFFFAOYSA-N	2.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3',4,5-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-67) [152833-52-8] QDQGECFQVPRMEO-UHFFFAOYSA-N	8.9×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,3',4,5'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-68) [147102-64-5] XORVNHCKWFPDLN-UHFFFAOYSA-N	1.0×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3',4',5-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-70) [159553-67-0] MFTPXFIGIJCNJM-UHFFFAOYSA-N	1.8×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3',4',6-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-71) [130892-66-9] IZZULMOBRTYHMH-UHFFFAOYSA-N	4.6×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,4,4',5-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-74) [61328-45-8] KXOJXWNARBQHNX-UHFFFAOYSA-N	1.9×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,4,4',6-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-75) [63553-30-0] YCWRSOTXXJYCKF-UHFFFAOYSA-N	1.7×10^{-2}		Kurz and Ballschmiter (1999)	V	

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Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3',4,4'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-77) [56348-72-2] DHLVZXZRIZBPKG-UHFFFAOYSA-N	4.1×10^{-2}		Kurz and Ballschmiter (1999)	V	
3,3',4,5'-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-79) [552884-22-7] BUPRSRBWDJVKGG-UHFFFAOYSA-N	1.0×10^{-2}		Kurz and Ballschmiter (1999)	V	
3,4,4',5-tetrachlorodiphenyl ether $C_{12}H_6Cl_4O$ (PCDE-81) [62615-07-0] CAUBBRCOHHHCNG-UHFFFAOYSA-N	1.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,3',4-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-82) [160282-10-0] ABRDPORILGADAP-UHFFFAOYSA-N	8.3×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4,4'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-85) [71585-37-0] RSBUDFTVQYJNHK-UHFFFAOYSA-N	5.2×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4,5'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-87) [160282-09-7] SCLCXTQIVCULDR-UHFFFAOYSA-N	2.2×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4,6'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-89) [85918-35-0] JGXAONSRHOSPTJ-UHFFFAOYSA-N	6.5×10^{-2}		Kurz and Ballschmiter (1999)	V	

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Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4',5-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-90) [157683-73-3] QPEBRZQSEUOWPA-UHFFFAOYSA-N	1.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4',6-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-91) [116995-20-1] BRNKJDZWZYZVNM-UHFFFAOYSA-N	3.9×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4',5'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-97) [160282-08-6] ABYZYVAIOYICJQ-UHFFFAOYSA-N	3.3×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',4,4',5-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-99) [60123-64-0] AVURWLKSFZBANQ-UHFFFAOYSA-N	1.8×10^{-2} 3.8×10^{-2}	 6100	Kurz and Ballschmiter (1999) Paasivirta et al. (1999)	V T	
2,2',4,4',6-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-100) [104294-16-8] FONWDRSQXQZNBN-UHFFFAOYSA-N	2.1×10^{-2} 1.3×10^{-2}	 5800	Kurz and Ballschmiter (1999) Paasivirta et al. (1999)	V T	
2,2',4,5,5'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-101) [131138-21-1] MKIAKZAWONVRFF-UHFFFAOYSA-N	1.6×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',4,5,6'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-102) [130892-67-0] BOJBTUWEQMUWHT-UHFFFAOYSA-N	3.7×10^{-2}		Kurz and Ballschmiter (1999)	V	

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Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',4,4'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-105) [85918-31-6] PKEGIXYNAGGYPN-UHFFFAOYSA-N	4.2×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,3',4,5'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-108) [160282-07-5] HCTKORQPUZCIAO-UHFFFAOYSA-N	1.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,3',4,6-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-109) [727738-64-9] SEIXDCGLHKOBEO-UHFFFAOYSA-N	1.4×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,3',4',6-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-110) [159553-69-2] KASGFDPQAMDPAZ-UHFFFAOYSA-N	3.6×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,4,4',5-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-114) [113464-17-8] WSTVMACYLXUQIM-UHFFFAOYSA-N	1.2×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,4,4',6-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-115) [160282-05-3] LUNNFBBTEHRYMW-UHFFFAOYSA-N	1.1×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,4,5,6-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-116) [22274-42-6] JDWOFUWJURZFFF-UHFFFAOYSA-N	6.6×10^{-3}		Kurz and Ballschmiter (1999)	V	

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Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4',5,6-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-117) [63646-55-9] UETIKWAWMZLQQZ-UHFFFAOYSA-N	1.1×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3',4,4',5-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-118) [60123-65-1] NRAVUGAGYOBXIG-UHFFFAOYSA-N	1.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3',4,4',6-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-119) [157683-74-4] POOXVKSDWCXIBU-UHFFFAOYSA-N	1.3×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3',4,5,5'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-120) [160282-04-2] XIFRTJZLSYOLIU-UHFFFAOYSA-N	4.8×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,3',4,4',5'-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-123) [160282-06-4] BUAXMSGDEZZOJD-UHFFFAOYSA-N	1.3×10^{-2}		Kurz and Ballschmiter (1999)	V	
3,3',4,4',5-pentachlorodiphenyl ether $C_{12}H_5Cl_5O$ (PCDE-126) [94339-59-0] WDBLKMRZRGLISL-UHFFFAOYSA-N	1.0×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,3',4,4'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-128) [71585-39-2] GSWMXIIUDJOXNF-UHFFFAOYSA-N	8.3×10^{-2}		Kurz and Ballschmiter (1999)	V	

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Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,5'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-130) [76621-14-2] JTEWACHFMNTRBB-UHFFFAOYSA-N	1.5×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,3',4,6'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-132) [124076-66-0] YDVYLSIVXYLBBX-UHFFFAOYSA-N	6.2×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4,4',5-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-137) [71585-38-1] LDPJEMNNPDFBCQ-UHFFFAOYSA-N	1.8×10^{-2} 1.9×10^{-2}	 6400	Kurz and Ballschmiter (1999) Paasivirta et al. (1999)	V T	
2,2',3,4,4',5'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-138) [71585-36-9] PHSJJYZIFPWCLZ-UHFFFAOYSA-N	2.9×10^{-2} 2.8×10^{-2}	 6500	Kurz and Ballschmiter (1999) Paasivirta et al. (1999)	V T	
2,2',3,4,4',6-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-139) [106220-83-1] BIWCEXHDIQZFHI-UHFFFAOYSA-N	9.8×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,2',3,4,4',6'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-140) [106220-82-0] XDAOZRZWYVKIAK-UHFFFAOYSA-N	3.0×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4',5,5'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-146) [162853-28-3] SFTBUGPDOJDENF-UHFFFAOYSA-N	1.0×10^{-2}		Kurz and Ballschmiter (1999)	V	

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Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4',5,6-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-147) [116995-18-7] DIBYIHMYEPMGKC-UHFFFAOYSA-N	1.0×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4',5',6-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-149) [85918-37-2] RDKSFIZNZGWNLA-UHFFFAOYSA-N	3.1×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',4,4',5,5'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-153) [71859-30-8] PECXRRMHOQBOIE-UHFFFAOYSA-N	1.3×10^{-2} 1.1×10^{-2}	 6300	Kurz and Ballschmiter (1999) Paasivirta et al. (1999)	V T	
2,2',4,4',5,6'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-154) [106220-81-9] XKQUAQGQLZDDBV-UHFFFAOYSA-N	1.4×10^{-2} 4.4×10^{-3}	 5900	Kurz and Ballschmiter (1999) Paasivirta et al. (1999)	V T	
2,3,3',4,4',5-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-156) [109828-22-0] GHTWMHLFFDEYRE-UHFFFAOYSA-N	1.2×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,3',4,4',5'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-157) [94339-60-3] FEIDIWDEJQVIPO-UHFFFAOYSA-N	2.8×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,3,3',4',5,6-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-163) [155999-97-6] YLAYOOJLJKJGCF-UHFFFAOYSA-N	1.6×10^{-2}		Kurz and Ballschmiter (1999)	V	

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Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4,4',5,6-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-166) [63646-56-0] MXDRLBNLTLOWGV-UHFFFAOYSA-N	5.0×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,3',4,4',5,5'-hexachlorodiphenyl ether $C_{12}H_4Cl_6O$ (PCDE-167) [131138-20-0] DYSUSQZPGJXVAL-UHFFFAOYSA-N	8.3×10^{-3}		Kurz and Ballschmiter (1999)	V	
	9.0×10^{-3}	6200	Paasivirta et al. (1999)	T	
2,2',3,3',4,4',5-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-170) [71585-40-5] BLBURLWSCHSPIS-UHFFFAOYSA-N	2.0×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,3',4,5,6'-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-174) [159553-73-8] DQYYZAABYZAOOC-UHFFFAOYSA-N	1.8×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,3',4,5',6'-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-177) [83992-71-6] RXPQVFMDOJTCKE-UHFFFAOYSA-N	1.4×10^{-2}		Kurz and Ballschmiter (1999)	V	
2,2',3,4,4',5,5'-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-180) [83992-69-2] YBYYCWMPXZRBNJ-UHFFFAOYSA-N	5.0×10^{-3}		Kurz and Ballschmiter (1999)	V	
	1.9×10^{-2}	6800	Paasivirta et al. (1999)	T	

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Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,4',5,6-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-181) [157683-75-5] RPNFRXWGMTYOPA-UHFFFAOYSA-N	3.4×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,2',3,4,4',5,6'-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-182) [88467-63-4] XWRZWPPSQDHTFU-UHFFFAOYSA-N	3.3×10^{-3}	6400	Paasivirta et al. (1999)	T	
2,2',3,4,4',6,6'-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-184) [106220-84-2] WTYSJAGEYAAIFW-UHFFFAOYSA-N	2.0×10^{-1}	7800	Paasivirta et al. (1999)	T	
2,2',3,4',5,5',6-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-187) [109828-23-1] BHJCMMGUFRZLKK-UHFFFAOYSA-N	7.4×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,3,3',4,4',5,5'-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-189) [83992-72-7] JUHPMUOWCYBMEY-UHFFFAOYSA-N	6.2×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,3,3',4,4',5,6-heptachlorodiphenyl ether $C_{12}H_3Cl_7O$ (PCDE-190) [83992-70-5] QLSBRXLSQINWHM-UHFFFAOYSA-N	5.8×10^{-3}		Kurz and Ballschmiter (1999)	V	

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Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,4',5,5'- octachlorodiphenyl ether $C_{12}H_2Cl_8O$ (PCDE-194) [57379-40-5] IXZVOZCULZBCDY-UHFFFAOYSA-N	4.3×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,2',3,3',4,4',5,6- octachlorodiphenyl ether $C_{12}H_2Cl_8O$ (PCDE-195) [65075-02-7] YHUPMPHVHYBYJE-UHFFFAOYSA-N	1.8×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,2',3,3',4,4',5,6'- octachlorodiphenyl ether $C_{12}H_2Cl_8O$ (PCDE-196) [85918-38-3] HYNYIQBCBHJTOZ-UHFFFAOYSA-N	8.7×10^{-3}	7100	Paasivirta et al. (1999)	T	
2,2',3,3',4,4',6,6'- octachlorodiphenyl ether $C_{12}H_2Cl_8O$ (PCDE-197) [117948-62-6] GRWRDFGBFYSOKR-UHFFFAOYSA-N	7.7×10^{-3}	7000	Paasivirta et al. (1999)	T	
2,2',3,3',4,5,5',6'- octachlorodiphenyl ether $C_{12}H_2Cl_8O$ (PCDE-199) [83992-76-1] MRHQOXCYYPFGEE-UHFFFAOYSA-N	2.6×10^{-3}		Kurz and Ballschmiter (1999)	V	
2,2',3,4,4',5,5',6- octachlorodiphenyl ether $C_{12}H_2Cl_8O$ (PCDE-203) [83992-75-0] PKOSPVZTRLMBSK-UHFFFAOYSA-N	2.3×10^{-3}		Kurz and Ballschmiter (1999)	V	

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Table A6.5: Polychlorinated diphenyl ethers (PCDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,4',5,5',6- nonachlorodiphenyl ether $C_{12}HCl_9O$ (PCDE-206) [83992-73-8] FPEYJPVHPGDXDD-UHFFFAOYSA-N	5.1×10^{-4}		Kurz and Ballschmiter (1999)	V	
decachlorodiphenyl ether $C_{12}Cl_{10}O$ (PCDE-209) [31710-30-2] CIPFDHFTBYJKQB-UHFFFAOYSA-N	7.1×10^{-5}		Kurz and Ballschmiter (1999)	V	

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A6.6 Polychlorinated dibenzofuranes (PCDFs)

Table A6.6: Polychlorinated dibenzofuranes (PCDFs)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chlorodibenzofuran $C_{12}H_7ClO$ (PCDF-1) [84761-86-4] WRSMJZYBNIAAEE-UHFFFAOYSA-N	8.3×10^{-2}		Govers and Krop (1998)	Q	
2-chlorodibenzofuran $C_{12}H_7ClO$ (PCDF-2) [51230-49-0] PRKTYWJFCODJOA-UHFFFAOYSA-N	1.1×10^{-1}		Govers and Krop (1998)	Q	
3-chlorodibenzofuran $C_{12}H_7ClO$ (PCDF-3) [25074-67-3] BBOZMMAURMEVAR-UHFFFAOYSA-N	1.3×10^{-1}		Govers and Krop (1998)	Q	
4-chlorodibenzofuran $C_{12}H_7ClO$ (PCDF-4) [74992-96-4] RHRYBWFAHXCUCR-UHFFFAOYSA-N	8.9×10^{-2}		Govers and Krop (1998)	Q	
1,2-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-12) [64126-85-8] QVAPRJWSOUITIF-UHFFFAOYSA-N	1.5×10^{-1}		Govers and Krop (1998)	Q	
1,3-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-13) [94538-00-8] VKIBKEFGJSPRJC-UHFFFAOYSA-N	2.0×10^{-1}		Govers and Krop (1998)	Q	
1,4-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-14) [94538-01-9] VHQCMZLPHWGUDB-UHFFFAOYSA-N	1.5×10^{-1}		Govers and Krop (1998)	Q	
1,6-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-16) [74992-97-5] JRSRWACZUFLWKF-UHFFFAOYSA-N	1.4×10^{-1}		Govers and Krop (1998)	Q	

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,7-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-17) [94538-02-0] XRQNHPGZRFKBJW-UHFFFAOYSA-N	1.9×10^{-1}		Govers and Krop (1998)	Q	
1,8-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-18) [81638-37-1] UAFNQQBPUWFPGC-UHFFFAOYSA-N	2.5×10^{-1}		Govers and Krop (1998)	Q	
1,9-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-19) [70648-14-5] AEKSGHBVWJHELW-UHFFFAOYSA-N	2.0×10^{-1}		Govers and Krop (1998)	Q	
2,3-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-23) [64126-86-9] GETJJZZRPQFSFM-UHFFFAOYSA-N	2.3×10^{-1}		Govers and Krop (1998)	Q	
2,4-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-24) [24478-74-8] LHTCKMYRNOGUOA-UHFFFAOYSA-N	1.9×10^{-1}		Govers and Krop (1998)	Q	
2,6-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-26) [60390-27-4] XVLCNKFGFHUQNL-UHFFFAOYSA-N	1.8×10^{-1}		Govers and Krop (1998)	Q	
2,7-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-27) [74992-98-6] DOZUTNBCPVUMPY-UHFFFAOYSA-N	2.0×10^{-1}		Govers and Krop (1998)	Q	
2,8-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-28) [5409-83-6] IVVRJIDVYSPKFZ-UHFFFAOYSA-N	1.6×10^{-1} 1.6×10^{-1} 1.6×10^{-1} 4.2×10^{-1} 2.6×10^{-1} 2.2×10^{-1}		Duchowicz et al. (2020) Mackay et al. (2006b) Govers and Krop (1998) Duchowicz et al. (2020) Saçan et al. (2005) Govers and Krop (1998)	V V V Q Q Q	186

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-34) [94570-83-9] HYQGGNWDPQZLGX-UHFFFAOYSA-N	1.9×10^{-1}		Govers and Krop (1998)	Q	
3,6-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-36) [74918-40-4] DMOBGFAKTSXOHG-UHFFFAOYSA-N	2.2×10^{-1}		Govers and Krop (1998)	Q	
3,7-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-37) [58802-21-4] OLTYAGNRSNFHLK-UHFFFAOYSA-N	3.0×10^{-1}		Govers and Krop (1998)	Q	
4,6-dichlorodibenzofuran $C_{12}H_6Cl_2O$ (PCDF-46) [64560-13-0] BZFIZJNKNCJEAD-UHFFFAOYSA-N	2.2×10^{-1}		Govers and Krop (1998)	Q	
1,2,3-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-123) [83636-47-9] LADSWAAWPMGHBE-UHFFFAOYSA-N	2.9×10^{-1}		Govers and Krop (1998)	Q	
1,2,4-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-124) [24478-73-7] RQIWKWHVZLDXEJ-UHFFFAOYSA-N	2.5×10^{-1}		Govers and Krop (1998)	Q	
1,2,6-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-126) [64560-15-2] CYRZCBUWRUACKJ-UHFFFAOYSA-N	2.3×10^{-1}		Govers and Krop (1998)	Q	
1,2,7-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-127) [83704-37-4] AFOVQGPNOZDUEP-UHFFFAOYSA-N	2.3×10^{-1}		Govers and Krop (1998)	Q	

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,8-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-128) [83704-34-1] UYIGPSPCOXGBCS-UHFFFAOYSA-N	3.9×10^{-1}		Govers and Krop (1998)	Q	
1,2,9-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-129) [83704-38-5] ICTXINQOXPMQPM-UHFFFAOYSA-N	4.8×10^{-1}		Govers and Krop (1998)	Q	
1,3,4-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-134) [82911-61-3] FIPOITUDJFQRRN-UHFFFAOYSA-N	2.8×10^{-1}		Govers and Krop (1998)	Q	
1,3,6-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-136) [83704-39-6] AGPTXRLVBIRYLV-UHFFFAOYSA-N	3.3×10^{-1}		Govers and Krop (1998)	Q	
1,3,7-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-137) [64560-16-3] INRBXOGZPDFCLQ-UHFFFAOYSA-N	4.1×10^{-1}		Govers and Krop (1998)	Q	
1,3,8-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-138) [76621-12-0] PHFSTDOPTZHECA-UHFFFAOYSA-N	4.2×10^{-1}		Govers and Krop (1998)	Q	
1,3,9-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-139) [83704-40-9] SPPGDLROKBFNNO-UHFFFAOYSA-N	4.4×10^{-1}		Govers and Krop (1998)	Q	
1,4,6-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-146) [82911-60-2] XDQRWSUJOURTHK-UHFFFAOYSA-N	3.5×10^{-1}		Govers and Krop (1998)	Q	

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
1,4,7-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-147) [83704-41-0] XTLMVJUSIANHND-UHFFFAOYSA-N	3.2×10^{-1}		Govers and Krop (1998)	Q	
1,4,8-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-148) [64560-14-1] PCQCYDNFBUADOK-UHFFFAOYSA-N	3.9×10^{-1}		Govers and Krop (1998)	Q	
1,4,9-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-149) [70648-13-4] NVYUPBVXKLTYHV-UHFFFAOYSA-N	3.5×10^{-1}		Govers and Krop (1998)	Q	
1,6,7-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-167) [83704-46-5] HEWLCNCSWBMZHG-UHFFFAOYSA-N	2.7×10^{-1}		Govers and Krop (1998)	Q	
1,6,8-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-168) [82911-59-9] ZOBVYDQWZXUJNO-UHFFFAOYSA-N	4.1×10^{-1}		Govers and Krop (1998)	Q	
1,7,8-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-178) [58802-18-9] YNMCXGLWHTVMQO-UHFFFAOYSA-N	4.6×10^{-1}		Govers and Krop (1998)	Q	
2,3,4-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-234) [57117-34-7] YDLADWPBKZODCJ-UHFFFAOYSA-N	3.1×10^{-1}		Govers and Krop (1998)	Q	
2,3,6-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-236) [57117-33-6] CPMGJTLNRBIKQM-UHFFFAOYSA-N	3.4×10^{-1}		Govers and Krop (1998)	Q	

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,7-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-237) [58802-17-8] CKXMNTLGGAOERF-UHFFFAOYSA-N	3.5×10^{-1}		Govers and Krop (1998)	Q	
2,3,8-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-238) [57117-32-5] NUNSNNOYACKRIK-UHFFFAOYSA-N	3.1×10^{-1}		Govers and Krop (1998)	Q	
2,4,6-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-246) [58802-14-5] GTKURBTWZFQHHY-UHFFFAOYSA-N	4.2×10^{-1}		Govers and Krop (1998)	Q	
2,4,7-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-247) [83704-42-1] SZBZRVJHPZIGAY-UHFFFAOYSA-N	3.1×10^{-1}		Govers and Krop (1998)	Q	
2,4,8-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-248) [54589-71-8] WJURXKWTCOMRCE-UHFFFAOYSA-N	3.2×10^{-1}		Govers and Krop (1998)	Q	
3,4,6-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-346) [83704-43-2] XEUHBCMRIXEBTD-UHFFFAOYSA-N	4.3×10^{-1}		Govers and Krop (1998)	Q	
3,4,7-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-347) [83704-44-3] RPJJBTSXPNFUTA-UHFFFAOYSA-N	3.9×10^{-1}		Govers and Krop (1998)	Q	
3,4,8-trichlorodibenzofuran $C_{12}H_5Cl_3O$ (PCDF-348) [83704-45-4] YTZWNIQGGIJHJX-UHFFFAOYSA-N	2.5×10^{-1}		Govers and Krop (1998)	Q	

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,4-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1234) [24478-72-6] AETAPIFVELRIDN-UHFFFAOYSA-N	3.6×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,6-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1236) [83704-21-6] BBAXFLIBRPXRBP-UHFFFAOYSA-N	4.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1237) [83704-22-7] MDNZFYGATDCKRB-UHFFFAOYSA-N	3.9×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1238) [62615-08-1] KFQRHGKKSHJMCO-UHFFFAOYSA-N	5.0×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1239) [83704-23-8] GNQHLJHTOATTOJ-UHFFFAOYSA-N	7.9×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,6-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1246) [71998-73-7] NLVWEKPJFUPVMZ-UHFFFAOYSA-N	5.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1247) [83719-40-8] MFURKMJLDQBHRA-UHFFFAOYSA-N	3.5×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1248) [64126-87-0] BFTASCFRRBHFFK-UHFFFAOYSA-N	5.5×10^{-1}		Govers and Krop (1998)	Q	

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,4,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1249) [83704-24-9] ZUYYTCCHKQGGOV-UHFFFAOYSA-N	7.4×10^{-1}		Govers and Krop (1998)	Q	
1,2,6,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1267) [83704-25-0] AUEWYHHKDYUYMI-UHFFFAOYSA-N	2.8×10^{-1}		Govers and Krop (1998)	Q	
1,2,6,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1268) [83710-07-0] KCVGVSIBBGIJNZ-UHFFFAOYSA-N	5.5×10^{-1}		Govers and Krop (1998)	Q	
1,2,6,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1269) [70648-18-9] IEPGLLVEBKXASE-UHFFFAOYSA-N	7.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,7,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1278) [58802-20-3] JODWPAQNABOHDG-UHFFFAOYSA-N	1.1 4.8×10^{-1}		Saçan et al. (2005) Govers and Krop (1998)	Q Q	
1,2,7,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1279) [83704-26-1] PDMFRPIFZAKMLH-UHFFFAOYSA-N	6.9×10^{-1}		Govers and Krop (1998)	Q	
1,2,8,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1289) [70648-22-5] OHYCQUKMNPHFPT-UHFFFAOYSA-N	9.5×10^{-1}		Govers and Krop (1998)	Q	
1,3,4,6-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1346) [83704-27-2] CBBDONKZEJKFJP-UHFFFAOYSA-N	6.3×10^{-1}		Govers and Krop (1998)	Q	

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3,4,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1347) [70648-16-7] UMKCVDZTSZNWRH-UHFFFAOYSA-N	5.1×10^{-1}		Govers and Krop (1998)	Q	
1,3,4,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1348) [92341-04-3] XWKRJSMNDOXIHS-UHFFFAOYSA-N	5.0×10^{-1}		Govers and Krop (1998)	Q	
1,3,4,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1349) [83704-28-3] PNCYJHOTZSKZPA-UHFFFAOYSA-N	5.8×10^{-1}		Govers and Krop (1998)	Q	
1,3,6,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1367) [57117-36-9] PITDPGCTIMCYEZ-UHFFFAOYSA-N	5.1×10^{-1}		Govers and Krop (1998)	Q	
1,3,6,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1368) [71998-72-6] BDXKVABZWRZKOS-UHFFFAOYSA-N	6.2×10^{-1}		Govers and Krop (1998)	Q	
1,3,6,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1369) [83690-98-6] NJQQZRLWVLWNGD-UHFFFAOYSA-N	6.8×10^{-1}		Govers and Krop (1998)	Q	
1,3,7,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1378) [57117-35-8] CSXDVUGDFSYXTD-UHFFFAOYSA-N	6.5×10^{-1}		Govers and Krop (1998)	Q	
1,3,7,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1379) [64560-17-4] IEMJMCVYAORWJV-UHFFFAOYSA-N	7.9×10^{-1}		Govers and Krop (1998)	Q	

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,4,6,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1467) [66794-59-0] RBFNYMHNIOKXLA-UHFFFAOYSA-N	5.9×10^{-1}		Govers and Krop (1998)	Q	
1,4,6,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1468) [82911-58-8] VHOBVPNETFRJED-UHFFFAOYSA-N	8.5×10^{-1}		Govers and Krop (1998)	Q	
1,4,6,9-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1469) [70648-19-0] JAYSBJFHDJOMGZ-UHFFFAOYSA-N	7.9×10^{-1}		Govers and Krop (1998)	Q	
1,4,7,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1478) [83704-29-4] IVRDRRWQABCXLY-UHFFFAOYSA-N	6.5×10^{-1}		Govers and Krop (1998)	Q	
1,6,7,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-1678) [83704-33-0] KOJMOXYETDLOPN-UHFFFAOYSA-N	5.8×10^{-1}		Govers and Krop (1998)	Q	
2,3,4,6-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-2346) [83704-30-7] JNVHSHPAAMRSKK-UHFFFAOYSA-N	6.2×10^{-1}		Govers and Krop (1998)	Q	
2,3,4,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-2347) [83704-31-8] BROFYOSLFHTGCQ-UHFFFAOYSA-N	4.4×10^{-1}		Govers and Krop (1998)	Q	
2,3,4,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-2348) [83704-32-9] IIKXRERKNIJJQY-UHFFFAOYSA-N	3.5×10^{-1}		Govers and Krop (1998)	Q	

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,6,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-2367) [57117-39-2] MJCNKMDTLRSHNK-UHFFFAOYSA-N	4.1×10^{-1}		Govers and Krop (1998)	Q	
2,3,6,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-2368) [57117-37-0] SPMZHWVRMWWTSY-UHFFFAOYSA-N	4.2×10^{-1}		Govers and Krop (1998)	Q	
2,3,7,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-2378) [51207-31-9] KSMVNVHUTQZITP-UHFFFAOYSA-N	5.9×10^{-1}		Friesen et al. (1993)	M	
	6.8×10^{-1}		Mackay et al. (2006b)	V	
	8.5×10^{-1}		Govers and Krop (1998)	V	
	2.2×10^{-3}	3700	Paasivirta et al. (1999)	T	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	1.2		Duchowicz et al. (2020)	Q	
	6.4×10^{-1}		HSDB (2015)	Q	99
	7.2×10^{-1}		Saçan et al. (2005)	Q	
	3.7×10^{-1}		Govers and Krop (1998)	Q	
	5.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,4,6,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-2467) [57117-38-1] NSDXKMRVQOSASS-UHFFFAOYSA-N	5.4×10^{-1}		Govers and Krop (1998)	Q	
2,4,6,8-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-2468) [58802-19-0] ZSPJEACWUWSAGS-UHFFFAOYSA-N	6.6×10^{-1}		Govers and Krop (1998)	Q	
3,4,6,7-tetrachlorodibenzofuran $C_{12}H_4Cl_4O$ (PCDF-3467) [57117-40-5] LMJLCLBSUNZLNW-UHFFFAOYSA-N	7.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,4,6-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12346) [83704-47-6] LIQJBAPSLUZUTB-UHFFFAOYSA-N	7.1×10^{-1}		Govers and Krop (1998)	Q	

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,4,7-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12347) [83704-48-7] DOJZTBGOWIYFAC-UHFFFAOYSA-N	4.5×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,4,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12348) [67517-48-0] ZCTNDJSCLPJCRA-UHFFFAOYSA-N	5.5×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,4,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12349) [83704-49-8] IQSZNZVZXOFRJS-UHFFFAOYSA-N	9.8×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,6,7-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12367) [57117-42-7] NZUPQBVDIWCPBX-UHFFFAOYSA-N	4.2×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,6,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12368) [83704-51-2] VHQJZOFUPXEZQZ-UHFFFAOYSA-N	6.5×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,6,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12369) [83704-52-3] IPSFQAKXDJVQOX-UHFFFAOYSA-N	1.1		Govers and Krop (1998)	Q	
1,2,3,7,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12378) [57117-41-6] SBMIVUVRFPGOEB-UHFFFAOYSA-N	8.7×10^{-4} 5.2×10^{-1}	3000	Paasivirta et al. (1999) Govers and Krop (1998)	T Q	
1,2,3,7,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12379) [83704-53-4] JVUSEQPOWCBYNG-UHFFFAOYSA-N	1.0		Govers and Krop (1998)	Q	

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,8,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12389) [83704-54-5] NKGLWUJPCTUDEH-UHFFFAOYSA-N	2.0 1.1		Saçan et al. (2005) Govers and Krop (1998)	Q Q	
1,2,4,6,7-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12467) [83704-50-1] BQTCODOVGXJHRB-UHFFFAOYSA-N	5.8×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,6,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12468) [69698-57-3] JDTUAYPJSSXDNO-UHFFFAOYSA-N	1.0		Govers and Krop (1998)	Q	
1,2,4,6,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12469) [70648-24-7] QDQFGVXGPSYEJU-UHFFFAOYSA-N	1.5		Govers and Krop (1998)	Q	
1,2,4,7,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12478) [58802-15-6] GCFDWHIKRXCUPJ-UHFFFAOYSA-N	6.2×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,7,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12479) [71998-74-8] IYGVHNHWORPMFU-UHFFFAOYSA-N	9.8×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,8,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12489) [70648-23-6] ZSPAPWGNAGTCCA-UHFFFAOYSA-N	1.3		Govers and Krop (1998)	Q	
1,2,6,7,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12678) [69433-00-7] ZAAVDGLJEOXCMV-UHFFFAOYSA-N	5.2×10^{-1}		Govers and Krop (1998)	Q	

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,6,7,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-12679) [70872-82-1] QQRRQEVOSMEVQB-UHFFFAOYSA-N	7.9×10^{-1}		Govers and Krop (1998)	Q	
1,3,4,6,7-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-13467) [83704-36-3] JVYYDUWJIJMOGW-UHFFFAOYSA-N	8.9×10^{-1}		Govers and Krop (1998)	Q	
1,3,4,6,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-13468) [83704-55-6] COKIAYPRHYHYCH-UHFFFAOYSA-N	1.0		Govers and Krop (1998)	Q	
1,3,4,6,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-13469) [70648-15-6] MYSAFUYQSBEEDR-UHFFFAOYSA-N	1.2		Govers and Krop (1998)	Q	
1,3,4,7,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-13478) [58802-16-7] ORSUQGVCWLXKLZ-UHFFFAOYSA-N	7.1×10^{-1}		Govers and Krop (1998)	Q	
1,3,4,7,9-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-13479) [70648-20-3] GFXPLABVZOBCCW-UHFFFAOYSA-N	9.5×10^{-1}		Govers and Krop (1998)	Q	
1,3,6,7,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-13678) [70648-21-4] FRLMQDUYUJIHCZ-UHFFFAOYSA-N	7.6×10^{-1}		Govers and Krop (1998)	Q	
1,4,6,7,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-14678) [83704-35-2] VANGHZRYKXDPRR-UHFFFAOYSA-N	1.1		Govers and Krop (1998)	Q	

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4,6,7-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-23467) [57117-43-8] SJFBZRQKGOGHEV-UHFFFAOYSA-N	6.9×10^{-1}		Govers and Krop (1998)	Q	
2,3,4,6,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-23468) [67481-22-5] MKRFORPSRBMAIP-UHFFFAOYSA-N	6.6×10^{-1}		Govers and Krop (1998)	Q	
2,3,4,7,8-pentachlorodibenzofuran $C_{12}H_3Cl_5O$ (PCDF-23478) [57117-31-4] OGBQILNBLMPPDP-UHFFFAOYSA-N	2.0 2.0 2.0 1.7 2.3×10^{-3} 1.6 1.6 3.9×10^{-1}	 2900 	Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006b) Govers and Krop (1998) Paasivirta et al. (1999) Duchowicz et al. (2020) Saçan et al. (2005) Govers and Krop (1998)	V V V V T Q Q Q	186
1,2,3,4,6,7-hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123467) [79060-60-9] SNWFMKXFMVHBKD-UHFFFAOYSA-N	6.8×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,4,6,8-hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123468) [69698-60-8] UCFGNWHERVQWMZ-UHFFFAOYSA-N	2.4×10^{-4} 9.8×10^{-1}	2300 	Paasivirta et al. (1999) Govers and Krop (1998)	T Q	
1,2,3,4,6,9-hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123469) [91538-83-9] KFFUZIROJGXTQH-UHFFFAOYSA-N	1.8		Govers and Krop (1998)	Q	
1,2,3,4,7,8-hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123478) [70648-26-9] LVYBAQIVPKCOEE-UHFFFAOYSA-N	6.9×10^{-1} 3.8×10^{-1} 4.1×10^{-4} 2.0 5.2×10^{-1}	 2400 	Mackay et al. (2006b) Govers and Krop (1998) Paasivirta et al. (1999) Saçan et al. (2005) Govers and Krop (1998)	V V T Q Q	

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,4,7,9- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123479) [91538-84-0] BKIXWRBZCQEZAQ-UHFFFAOYSA-N	1.1		Govers and Krop (1998)	Q	
1,2,3,4,8,9- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123489) [92341-07-6] VSDUQUBUJRNREH-UHFFFAOYSA-N	2.7 1.1		Saçan et al. (2005) Govers and Krop (1998)	Q Q	
1,2,3,6,7,8- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123678) [57117-44-9] JEYJJJXOFWNEHN-UHFFFAOYSA-N	9.1×10^{-1} 1.1×10^{-3} 2.2 5.2×10^{-1}	 3300 	Govers and Krop (1998) Paasivirta et al. (1999) Saçan et al. (2005) Govers and Krop (1998)	V T Q Q	
1,2,3,6,7,9- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123679) [92341-06-5] JZVOLXQREJNTTL-UHFFFAOYSA-N	1.0		Govers and Krop (1998)	Q	
1,2,3,6,8,9- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123689) [75198-38-8] WLGQZUOHEXTWFH-UHFFFAOYSA-N	1.3		Govers and Krop (1998)	Q	
1,2,3,7,8,9- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-123789) [72918-21-9] PYUSJFJVDVSXIU-UHFFFAOYSA-N	6.3×10^{-4} 2.6 1.0	2600 	Paasivirta et al. (1999) Saçan et al. (2005) Govers and Krop (1998)	T Q Q	
1,2,4,6,7,8- hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-124678) [67562-40-7] CKDDYGBBKXIHRY-UHFFFAOYSA-N	3.2×10^{-4} 9.3×10^{-1}	2300 	Paasivirta et al. (1999) Govers and Krop (1998)	T Q	

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,4,6,7,9-hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-124679) [75627-02-0] FAHIPPHRJJJQOG-UHFFFAOYSA-N	1.5		Govers and Krop (1998)	Q	
1,2,4,6,8,9-hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-124689) [69698-59-5] FGZCXIPKUCJGHW-UHFFFAOYSA-N	2.2×10^{-4}	2600	Paasivirta et al. (1999)	T	
	2.4		Govers and Krop (1998)	Q	
1,3,4,6,7,8-hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-134678) [71998-75-9] OGTZINCGZYXZCR-UHFFFAOYSA-N	1.1		Govers and Krop (1998)	Q	
1,3,4,6,7,9-hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-134679) [92341-05-4] TURXXOIFVABBPW-UHFFFAOYSA-N	1.6		Govers and Krop (1998)	Q	
2,3,4,6,7,8-hexachlorodibenzofuran $C_{12}H_2Cl_6O$ (PCDF-234678) [60851-34-5] XTAHLACQOVXINQ-UHFFFAOYSA-N	3.6×10^{-4}	2600	Paasivirta et al. (1999)	T	
	3.1		Saçan et al. (2005)	Q	
	5.6×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,4,6,7,8-heptachlorodibenzofuran $C_{12}HCl_7O$ (PCDF-1234678) [67562-39-4] WDMKCPIVJOGHBF-UHFFFAOYSA-N	7.0×10^{-1}		Duchowicz et al. (2020)	V	186
	7.0×10^{-1}		Mackay et al. (2006b)	V	
	2.9×10^{-1}		Govers and Krop (1998)	V	
	5.4×10^{-5}	1600	Paasivirta et al. (1999)	T	
	2.1		Duchowicz et al. (2020)	Q	
	3.9		Saçan et al. (2005)	Q	
	7.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,4,6,7,9-heptachlorodibenzofuran $C_{12}HCl_7O$ (PCDF-1234679) [70648-25-8] JWXWOEUKHXOUSK-UHFFFAOYSA-N	1.5		Govers and Krop (1998)	Q	

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Table A6.6: Polychlorinated dibenzofuranes (PCDFs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,4,6,8,9-heptachlorodibenzofuran $C_{12}HCl_7O$ (PCDF-1234689) [69698-58-4] BADFHCOLISGRRW-UHFFFAOYSA-N	3.4×10^{-4}	1800	Paasivirta et al. (1999)	T	
	1.9		Govers and Krop (1998)	Q	
1,2,3,4,7,8,9-heptachlorodibenzofuran $C_{12}HCl_7O$ (PCDF-1234789) [55673-89-7] VEZCTZWLJYWARH-UHFFFAOYSA-N	5.5×10^{-4}	2100	Paasivirta et al. (1999)	T	
	3.2		Saçan et al. (2005)	Q	
	1.0		Govers and Krop (1998)	Q	
octachlorodibenzofuran $C_{12}Cl_8O$ (PCDF-12346789) [39001-02-0] RHIROFAGUQOFLU-UHFFFAOYSA-N	5.2		Duchowicz et al. (2020)	V	186
			Mackay et al. (2006b)	V	683
	7.6×10^{-1}		Govers and Krop (1998)	V	
	2.3×10^{-4}	2400	Paasivirta et al. (1999)	T	
	1.7		Duchowicz et al. (2020)	Q	
	4.9		Saçan et al. (2005)	Q	
	1.3		Govers and Krop (1998)	Q	

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A6.7 Polychlorinated dibenzo-*p*-dioxins (PCDDs)

Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chlorodibenzo-*p*-dioxin	1.6×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{12}H_7ClO_2$	1.6×10^{-1}		Mackay et al. (2006b)	V	
(PCDD-1)	2.5×10^{-2}		Saçan et al. (2005)	V	
[39227-53-7]	1.6×10^{-1}		Govers and Krop (1998)	V	
VGGGRWRBGXENKI-UHFFFAOYSA-N	1.2×10^{-1}		Shiu et al. (1988)	V	
	2.1		Duchowicz et al. (2020)	Q	
		7100	Kühne et al. (2005)	Q	
	6.8×10^{-2}		Saçan et al. (2005)	Q	
	1.3×10^{-1}		Wang and Wong (2002)	Q	535
	1.7×10^{-1}		Govers and Krop (1998)	Q	
		6500	Kühne et al. (2005)	?	
2-chlorodibenzo-*p*-dioxin	8.6×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{12}H_7ClO_2$	7.9×10^{-2}		Mackay et al. (2006b)	V	
(PCDD-2)	7.9×10^{-2}		Govers and Krop (1998)	V	
[39227-54-8]	6.7×10^{-2}		Shiu et al. (1988)	V	
GIUGGRUEPHPVNR-UHFFFAOYSA-N	1.1		Duchowicz et al. (2020)	Q	
	9.8×10^{-2}		Saçan et al. (2005)	Q	
	1.3×10^{-1}		Wang and Wong (2002)	Q	535
	2.2×10^{-1}		Govers and Krop (1998)	Q	
1,2-dichlorodibenzo-*p*-dioxin	2.8×10^{-1}		Wang and Wong (2002)	Q	535
$C_{12}H_6Cl_2O_2$	3.2×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-12)					
[54536-18-4]					
DFGDMWHUCCHXIF-UHFFFAOYSA-N					
1,3-dichlorodibenzo-*p*-dioxin	2.2×10^{-1}		Wang and Wong (2002)	Q	535
$C_{12}H_6Cl_2O_2$	3.8×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-13)					
[50585-39-2]					
AZYJYMAKTBXNSX-UHFFFAOYSA-N					
1,4-dichlorodibenzo-*p*-dioxin	2.4×10^{-1}		Wang and Wong (2002)	Q	535
$C_{12}H_6Cl_2O_2$	3.2×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-14)					
[54536-19-5]					
MBMUPQZSDWVPQU-UHFFFAOYSA-N					
1,6-dichlorodibenzo-*p*-dioxin	2.5×10^{-1}		Wang and Wong (2002)	Q	535
$C_{12}H_6Cl_2O_2$	3.2×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-16)					
[38178-38-0]					
MAWMBEVNJGEDAD-UHFFFAOYSA-N					

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Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,7-dichlorodibenzo-*p*-dioxin $C_{12}H_6Cl_2O_2$ (PCDD-17) [82291-26-7] IJUWLAFPPVRYGY-UHFFFAOYSA-N	2.6×10^{-1}		Wang and Wong (2002)	Q	535
	3.6×10^{-1}		Govers and Krop (1998)	Q	
1,8-dichlorodibenzo-*p*-dioxin $C_{12}H_6Cl_2O_2$ (PCDD-18) [82291-27-8] PLZYIHQBHROTFD-UHFFFAOYSA-N	2.6×10^{-1}		Wang and Wong (2002)	Q	535
	3.8×10^{-1}		Govers and Krop (1998)	Q	
1,9-dichlorodibenzo-*p*-dioxin $C_{12}H_6Cl_2O_2$ (PCDD-19) [82291-28-9] JZDVJXBKJDADAY-UHFFFAOYSA-N	2.6×10^{-1}		Wang and Wong (2002)	Q	535
	5.4×10^{-1}		Govers and Krop (1998)	Q	
2,3-dichlorodibenzo-*p*-dioxin $C_{12}H_6Cl_2O_2$ (PCDD-23) [29446-15-9] YCIYTXRUZSDMRZ-UHFFFAOYSA-N	1.5×10^{-1}		Duchowicz et al. (2020)	V	186
	1.5×10^{-1}		Mackay et al. (2006b)	V	
	1.5×10^{-1}		Saçan et al. (2005)	V	
	1.5×10^{-1}		Govers and Krop (1998)	V	
	1.5×10^{-1}		Shiu et al. (1988)	V	
	8.5×10^{-1}		Duchowicz et al. (2020)	Q	
	2.5×10^{-1}		Saçan et al. (2005)	Q	
	2.6×10^{-1}		Wang and Wong (2002)	Q	535
	4.0×10^{-1}		Govers and Krop (1998)	Q	
2,7-dichlorodibenzo-*p*-dioxin $C_{12}H_6Cl_2O_2$ (PCDD-27) [33857-26-0] NBFMTHWVRBOVPE-UHFFFAOYSA-N	1.7×10^{-1}		Santl et al. (1994)	M	733
			Mackay et al. (2006b)	V	683
	1.2×10^{-1}		Govers and Krop (1998)	V	
	1.2×10^{-1}		Shiu et al. (1988)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	6.6×10^{-1}		Duchowicz et al. (2020)	Q	299
	7.3×10^{-1}		Hilal et al. (2008)	Q	
	5.0		Modarresi et al. (2007)	Q	67
	1.0×10^{-1}		Saçan et al. (2005)	Q	
	2.6×10^{-1}		Wang and Wong (2002)	Q	535
	3.5×10^{-1}		Govers and Krop (1998)	Q	
	1.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
2,8-dichlorodibenzo-*p*-dioxin $C_{12}H_6Cl_2O_2$ (PCDD-28) [38964-22-6] WMWJCKBJUQDYLM-UHFFFAOYSA-N	4.7×10^{-1}		Duchowicz et al. (2020)	V	186
	4.7×10^{-1}		Mackay et al. (2006b)	V	
	4.7×10^{-1}		Govers and Krop (1998)	V	
	4.7×10^{-1}		Shiu et al. (1988)	V	
	1.2		Duchowicz et al. (2020)	Q	
	1.7×10^{-1}		Saçan et al. (2005)	Q	
	2.6×10^{-1}		Wang and Wong (2002)	Q	535
	4.4×10^{-1}		Govers and Krop (1998)	Q	

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Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-123) [54536-17-3] SKMFBGZVVNDVFR-UHFFFAOYSA-N	5.0×10^{-1}		Wang and Wong (2002)	Q	535
	5.6×10^{-1}		Govers and Krop (1998)	Q	
1,2,4-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-124) [39227-58-2] HRVUKLBFRPWXPJ-UHFFFAOYSA-N	2.7×10^{-1}		Santl et al. (1994)	M	733
	2.9×10^{-1}		Mackay et al. (2006b)	V	
	2.6×10^{-1}		Govers and Krop (1998)	V	
	2.6×10^{-1}		Shiu et al. (1988)	V	
	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
	9.1×10^{-1}		Duchowicz et al. (2020)	Q	
	1.3		Hilal et al. (2008)	Q	
	1.1×10^{1}		Modarresi et al. (2007)	Q	67
	3.0×10^{-1}		Saçan et al. (2005)	Q	
	4.4×10^{-1}		Wang and Wong (2002)	Q	535
	5.5×10^{-1}		Govers and Krop (1998)	Q	
	2.7×10^{-1}		Duchowicz et al. (2020)	?	185, 21
			Fogg and Sangster (2003)	W	734
1,2,6-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-126) [69760-96-9] XQBPVWBIUBCJJO-UHFFFAOYSA-N	5.0×10^{-1}		Wang and Wong (2002)	Q	535
	5.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,7-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-127) [82291-30-3] TXJMXDWFPQSYEQ-UHFFFAOYSA-N	5.1×10^{-1}		Wang and Wong (2002)	Q	535
	4.6×10^{-1}		Govers and Krop (1998)	Q	
1,2,8-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-128) [82291-31-4] QBEOCKSANJLBAE-UHFFFAOYSA-N	5.1×10^{-1}		Wang and Wong (2002)	Q	535
	6.0×10^{-1}		Govers and Krop (1998)	Q	
1,2,9-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-129) [82291-32-5] DQLRDBDQLSIOIX-UHFFFAOYSA-N	5.2×10^{-1}		Wang and Wong (2002)	Q	535
	9.1×10^{-1}		Govers and Krop (1998)	Q	
1,3,6-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-136) [82291-33-6] LNPVMVSAUXUGHH-UHFFFAOYSA-N	4.2×10^{-1}		Wang and Wong (2002)	Q	535
	6.3×10^{-1}		Govers and Krop (1998)	Q	

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Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3,7-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-137) [67028-17-5] RPKWIXFZKMDPMH-UHFFFAOYSA-N	4.3×10^{-1} 6.8×10^{-1}		Wang and Wong (2002) Govers and Krop (1998)	Q Q	535
1,3,8-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-138) [82306-61-4] FJAKCOBYQSEWMT-UHFFFAOYSA-N	4.3×10^{-1} 5.6×10^{-1}		Wang and Wong (2002) Govers and Krop (1998)	Q Q	535
1,3,9-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-139) [82306-62-5] DGDADRUTFAIIQQ-UHFFFAOYSA-N	4.4×10^{-1} 1.0		Wang and Wong (2002) Govers and Krop (1998)	Q Q	535
1,4,6-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-146) [82306-63-6] UTTYFTWIJLRXKB-UHFFFAOYSA-N	4.4×10^{-1} 9.3×10^{-1}		Wang and Wong (2002) Govers and Krop (1998)	Q Q	535
1,4,7-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-147) [82306-64-7] NBWAQBGJBSYXHV-UHFFFAOYSA-N	4.5×10^{-1} 6.0×10^{-1}		Wang and Wong (2002) Govers and Krop (1998)	Q Q	535
1,7,8-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-178) [82306-65-8] CAPCTZJHYADFNX-UHFFFAOYSA-N	4.9×10^{-1} 6.2×10^{-1}		Wang and Wong (2002) Govers and Krop (1998)	Q Q	535
2,3,7-trichlorodibenzo-*p*-dioxin $C_{12}H_5Cl_3O_2$ (PCDD-237) [33857-28-2] ZSIZNEVHVVRPFF-UHFFFAOYSA-N	4.9×10^{-1} 5.6×10^{-1}		Wang and Wong (2002) Govers and Krop (1998)	Q Q	535
1,2,3,4-tetrachlorodibenzo-*p*-dioxin $C_{12}H_4Cl_4O_2$ (PCDD-1234) [30746-58-8] DJHHDLMTUOLVHY-UHFFFAOYSA-N	5.0×10^{-1} 2.7×10^{-1} 1.4 3.3×10^{-1} 2.7×10^{-1} 2.4×10^{-1} 7.0×10^{-1} 1.4		Santl et al. (1994) Mackay et al. (2006b) Mackay et al. (2006b) Govers and Krop (1998) Shiu et al. (1988) Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008)	M V V V V Q Q Q	733 184

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Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{1}		Modarresi et al. (2007)	Q	67
	6.3×10^{-1}		Saçan et al. (2005)	Q	
	8.7×10^{-1}		Wang and Wong (2002)	Q	535
	7.4×10^{-1}		Govers and Krop (1998)	Q	
	4.9×10^{-1}		Duchowicz et al. (2020)	?	185, 21
1,2,3,6-tetrachlorodibenzo-*p*-dioxin	8.7×10^{-1}		Wang and Wong (2002)	Q	535
$C_{12}H_4Cl_4O_2$ (PCDD-1236) [71669-25-5] XEZBZSVTUSXISZ-UHFFFAOYSA-N	8.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,7-tetrachlorodibenzo-*p*-dioxin	1.3		Mackay et al. (2006b)	V	
$C_{12}H_4Cl_4O_2$	1.7		Govers and Krop (1998)	V	
(PCDD-1237)	1.3		Shiu et al. (1988)	V	
[67028-18-6]	2.4×10^{-1}		Keshavarz et al. (2022)	Q	
SKGXYFVQZVPEFP-UHFFFAOYSA-N	5.7×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.7		Hilal et al. (2008)	Q	
	2.1×10^{1}		Modarresi et al. (2007)	Q	67
	4.3×10^{-1}		Saçan et al. (2005)	Q	
	8.7×10^{-1}		Wang and Wong (2002)	Q	535
	6.8×10^{-1}		Govers and Krop (1998)	Q	
	1.3		Duchowicz et al. (2020)	?	185, 21
1,2,3,8-tetrachlorodibenzo-*p*-dioxin	8.7×10^{-1}		Wang and Wong (2002)	Q	535
$C_{12}H_4Cl_4O_2$ (PCDD-1238) [53555-02-5] BXKLTNKYLCZOHF-UHFFFAOYSA-N	7.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,9-tetrachlorodibenzo-*p*-dioxin	9.1×10^{-1}		Wang and Wong (2002)	Q	535
$C_{12}H_4Cl_4O_2$ (PCDD-1239) [71669-26-6] CMVHZKSHSHQJHS-UHFFFAOYSA-N	1.4		Govers and Krop (1998)	Q	
1,2,4,6-tetrachlorodibenzo-*p*-dioxin	8.1×10^{-1}		Wang and Wong (2002)	Q	535
$C_{12}H_4Cl_4O_2$ (PCDD-1246) [71669-27-7] KQNBZUDHTCXCNA-UHFFFAOYSA-N	1.4		Govers and Krop (1998)	Q	

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Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,4,7-tetrachlorodibenzo-*p*-dioxin $C_{12}H_4Cl_4O_2$ (PCDD-1247) [71669-28-8] SMPHQCMJQUBTFZ-UHFFFAOYSA-N	7.8×10^{-1}		Wang and Wong (2002)	Q	535
	7.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,8-tetrachlorodibenzo-*p*-dioxin $C_{12}H_4Cl_4O_2$ (PCDD-1248) [71669-29-9] XGIKODBWQSAEFQ-UHFFFAOYSA-N	7.8×10^{-1}		Wang and Wong (2002)	Q	535
	8.9×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,9-tetrachlorodibenzo-*p*-dioxin $C_{12}H_4Cl_4O_2$ (PCDD-1249) [71665-99-1] WDAHVJCSSYOALR-UHFFFAOYSA-N	8.1×10^{-1}		Wang and Wong (2002)	Q	535
	1.5		Govers and Krop (1998)	Q	
1,2,6,7-tetrachlorodibenzo-*p*-dioxin $C_{12}H_4Cl_4O_2$ (PCDD-1267) [40581-90-6] SAMLAWFHXZIRMP-UHFFFAOYSA-N	9.5×10^{-1}		Wang and Wong (2002)	Q	535
	5.8×10^{-1}		Govers and Krop (1998)	Q	
1,2,6,8-tetrachlorodibenzo-*p*-dioxin $C_{12}H_4Cl_4O_2$ (PCDD-1268) [67323-56-2] YYUFYZDSYHKVDP-UHFFFAOYSA-N	8.1×10^{-1}		Wang and Wong (2002)	Q	535
	8.9×10^{-1}		Govers and Krop (1998)	Q	
1,2,6,9-tetrachlorodibenzo-*p*-dioxin $C_{12}H_4Cl_4O_2$ (PCDD-1269) [40581-91-7] ZKMXKYXNLFLUCD-UHFFFAOYSA-N	8.7×10^{-1}		Wang and Wong (2002)	Q	535
	1.4		Govers and Krop (1998)	Q	
1,2,7,8-tetrachlorodibenzo-*p*-dioxin $C_{12}H_4Cl_4O_2$ (PCDD-1278) [34816-53-0] YDZCLBKUTXYYKS-UHFFFAOYSA-N	7.8×10^{-1}		Wang and Wong (2002)	Q	535
	6.8×10^{-1}		Govers and Krop (1998)	Q	

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Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,7,9-tetrachlorodibenzo-*p*-dioxin	8.3×10^{-1}		Wang and Wong (2002)	Q	535
$C_{12}H_4Cl_4O_2$	1.2		Govers and Krop (1998)	Q	
(PCDD-1279)					
[71669-23-3]					
QIKHBBZEUNSCAF-UHFFFAOYSA-N					
1,2,8,9-tetrachlorodibenzo-*p*-dioxin	9.8×10^{-1}		Wang and Wong (2002)	Q	535
$C_{12}H_4Cl_4O_2$	1.3		Govers and Krop (1998)	Q	
(PCDD-1289)					
[62470-54-6]					
WELWFAGPAZKSBG-UHFFFAOYSA-N					
1,3,6,8-tetrachlorodibenzo-*p*-dioxin	1.4×10^{-1}		Webster et al. (1985)	M	
$C_{12}H_4Cl_4O_2$	1.4		Govers and Krop (1998)	V	
(PCDD-1368)	1.4		Shiu et al. (1988)	V	
[33423-92-6]	1.2		Hilal et al. (2008)	Q	
OTQFXRBLGNEOGH-UHFFFAOYSA-N	2.9×10^{-1}		Saçan et al. (2005)	Q	
	6.8×10^{-1}		Wang and Wong (2002)	Q	535
	8.7×10^{-1}		Govers and Krop (1998)	Q	
1,3,6,9-tetrachlorodibenzo-*p*-dioxin	7.4×10^{-1}		Wang and Wong (2002)	Q	535
$C_{12}H_4Cl_4O_2$	1.7		Govers and Krop (1998)	Q	
(PCDD-1369)					
[71669-24-4]					
QAUIRDIJIUMMEP-UHFFFAOYSA-N					
1,3,7,8-tetrachlorodibenzo-*p*-dioxin	7.8×10^{-1}		Wang and Wong (2002)	Q	535
$C_{12}H_4Cl_4O_2$	7.9×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-1378)					
[50585-46-1]					
VPTDIAYLYJBYQG-UHFFFAOYSA-N					
1,3,7,9-tetrachlorodibenzo-*p*-dioxin	7.1×10^{-1}		Wang and Wong (2002)	Q	535
$C_{12}H_4Cl_4O_2$	1.7		Govers and Krop (1998)	Q	
(PCDD-1379)					
[62470-53-5]					
JMGYHLJVDHUACM-UHFFFAOYSA-N					
1,4,6,9-tetrachlorodibenzo-*p*-dioxin	7.9×10^{-1}		Wang and Wong (2002)	Q	535
$C_{12}H_4Cl_4O_2$	2.6		Govers and Krop (1998)	Q	
(PCDD-1469)					
[40581-93-9]					
QTIIAIRUSSSOHT-UHFFFAOYSA-N					

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Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,4,7,8-tetrachlorodibenzo-*p*-dioxin	8.1×10^{-1}		Wang and Wong (2002)	Q	535
$C_{12}H_4Cl_4O_2$	9.1×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-1478)					
[40581-94-0]					
FCRXUTCUWCJZJI-UHFFFAOYSA-N					
2,3,7,8-tetrachlorodibenzo-*p*-dioxin	2.0×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{12}H_4Cl_4O_2$	2.0×10^{-1}		HSDB (2015)	V	
(PCDD-2378; TCDD)	3.0×10^{-1}		Mackay et al. (2006b)	V	
[1746-01-6]	3.0×10^{-1}		Govers and Krop (1998)	V	
HGUFODBRKLSHSI-UHFFFAOYSA-N	5.8×10^{-1}		McLachlan et al. (1990)	V	373
	6.1×10^{-1}		Shiu et al. (1988)	V	
	3.0×10^{-1}		Shiu et al. (1988)	V	
	9.7×10^{-2}		Shiu et al. (1988)	V	
	6.3×10^{-1}		Podoll et al. (1986)	V	
	4.7		Schroy et al. (1985)	V	
	2.6×10^{-4}	3600	Paasivirta et al. (1999)	T	
	4.1×10^{-1}		Duchowicz et al. (2020)	Q	
	3.3×10^{-1}		Saçan et al. (2005)	Q	
	8.9×10^{-1}		Wang and Wong (2002)	Q	535
	6.2×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,4,6-pentachlorodibenzo-*p*-dioxin	1.5		Wang and Wong (2002)	Q	535
$C_{12}H_3Cl_5O_2$	1.8		Govers and Krop (1998)	Q	
(PCDD-12346)					
[67028-19-7]					
LNWDBNKKBLRAMH-UHFFFAOYSA-N					
1,2,3,4,7-pentachlorodibenzo-*p*-dioxin	3.8		Duchowicz et al. (2020)	V	186
$C_{12}H_3Cl_5O_2$	3.8		Mackay et al. (2006b)	V	
(PCDD-12347)	4.5		Govers and Krop (1998)	V	
[39227-61-7]	3.8		Shiu et al. (1988)	V	
WRNGAZFESPEMCN-UHFFFAOYSA-N	4.5×10^{-1}		Duchowicz et al. (2020)	Q	
	7.0×10^{-1}		Saçan et al. (2005)	Q	
	1.4		Wang and Wong (2002)	Q	535
	8.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,6,7-pentachlorodibenzo-*p*-dioxin	1.5		Wang and Wong (2002)	Q	535
$C_{12}H_3Cl_5O_2$	7.8×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-12367)					
[71925-15-0]					
RLGWDUHOIIWPGN-UHFFFAOYSA-N					

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Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,6,8-pentachlorodibenzo-*p*-dioxin	1.3		Wang and Wong (2002)	Q	535
$C_{12}H_3Cl_5O_2$	9.5×10^{-1}		Govers and Krop (1998)	Q	
(PCDD-12368)					
[71925-16-1]					
VKDGHBBUEIIEHL-UHFFFAOYSA-N					
1,2,3,6,9-pentachlorodibenzo-*p*-dioxin	1.4		Wang and Wong (2002)	Q	535
$C_{12}H_3Cl_5O_2$	1.9		Govers and Krop (1998)	Q	
(PCDD-12369)					
[82291-34-7]					
NWKWRHSKKNELND-UHFFFAOYSA-N					
1,2,3,7,8-pentachlorodibenzo-*p*-dioxin	5.2×10^{-5}	2500	Paasivirta et al. (1999)	T	
$C_{12}H_3Cl_5O_2$	6.4×10^{-1}		Saçan et al. (2005)	Q	
(PCDD-12378)	1.5		Wang and Wong (2002)	Q	535
[40321-76-4]	6.8×10^{-1}		Govers and Krop (1998)	Q	
FSPZPQQWDODWAU-UHFFFAOYSA-N					
1,2,3,7,9-pentachlorodibenzo-*p*-dioxin	1.3		Wang and Wong (2002)	Q	535
$C_{12}H_3Cl_5O_2$	1.5		Govers and Krop (1998)	Q	
(PCDD-12379)					
[71925-17-2]					
UAOYHTXYVWEPIB-UHFFFAOYSA-N					
1,2,3,8,9-pentachlorodibenzo-*p*-dioxin	1.5		Wang and Wong (2002)	Q	535
$C_{12}H_3Cl_5O_2$	1.4		Govers and Krop (1998)	Q	
(PCDD-12389)					
[71925-18-3]					
VUMZAVNIADYKFC-UHFFFAOYSA-N					
1,2,4,6,7-pentachlorodibenzo-*p*-dioxin	1.4		Wang and Wong (2002)	Q	535
$C_{12}H_3Cl_5O_2$	1.4		Govers and Krop (1998)	Q	
(PCDD-12467)					
[82291-35-8]					
SEKDDGLKEYEVQK-UHFFFAOYSA-N					
1,2,4,6,8-pentachlorodibenzo-*p*-dioxin	1.2		Wang and Wong (2002)	Q	535
$C_{12}H_3Cl_5O_2$	2.1		Govers and Krop (1998)	Q	
(PCDD-12468)					
[71998-76-0]					
SJJWALZHAWITMS-UHFFFAOYSA-N					

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Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,4,6,9-pentachlorodibenzo-*p*-dioxin	1.3		Wang and Wong (2002)	Q	535
$C_{12}H_3Cl_5O_2$ (PCDD-12469) [82291-36-9] GNQVSAMSAKZLKE-UHFFFAOYSA-N	3.6		Govers and Krop (1998)	Q	
1,2,4,7,8-pentachlorodibenzo-*p*-dioxin	1.3		Wang and Wong (2002)	Q	535
$C_{12}H_3Cl_5O_2$ (PCDD-12478) [58802-08-7] QUPLGUUISJOUPJ-UHFFFAOYSA-N	9.1×10^{-1}		Govers and Krop (1998)	Q	
1,2,4,7,9-pentachlorodibenzo-*p*-dioxin	1.2		Wang and Wong (2002)	Q	535
$C_{12}H_3Cl_5O_2$ (PCDD-12479) [82291-37-0] QLBBXWPVEFJZEC-UHFFFAOYSA-N	1.8		Govers and Krop (1998)	Q	
1,2,4,8,9-pentachlorodibenzo-*p*-dioxin	1.4		Wang and Wong (2002)	Q	535
$C_{12}H_3Cl_5O_2$ (PCDD-12489) [82291-38-1] KLLFLRKEOJCTGC-UHFFFAOYSA-N	1.9		Govers and Krop (1998)	Q	
1,2,3,4,6,7-hexachlorodibenzo-*p*-dioxin	2.5		Wang and Wong (2002)	Q	535
$C_{12}H_2Cl_6O_2$ (PCDD-123467) [58200-66-1] NLBQVWJHLWAFGJ-UHFFFAOYSA-N	1.5		Govers and Krop (1998)	Q	
1,2,3,4,6,8-hexachlorodibenzo-*p*-dioxin	2.2		Wang and Wong (2002)	Q	535
$C_{12}H_2Cl_6O_2$ (PCDD-123468) [58200-67-2] IMALTUQZEIFHJW-UHFFFAOYSA-N	1.8		Govers and Krop (1998)	Q	
1,2,3,4,6,9-hexachlorodibenzo-*p*-dioxin	2.3		Wang and Wong (2002)	Q	535
$C_{12}H_2Cl_6O_2$ (PCDD-123469) [58200-68-3] UDYXCMRDCOVQLG-UHFFFAOYSA-N	4.0		Govers and Krop (1998)	Q	

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Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,3,4,7,8-hexachlorodibenzo-*p*-dioxin	2.5		Duchowicz et al. (2020)	V	186
$C_{12}H_2Cl_6O_2$	3.0		Mackay et al. (2006b)	V	
(PCDD-123478)	1.6		Govers and Krop (1998)	V	
[39227-28-6]	2.2×10^{-1}		Shiu et al. (1988)	V	
WCYYQNSQJHPVMG-UHFFFAOYSA-N	1.2×10^{-4}	2900	Paasivirta et al. (1999)	T	
	3.7×10^{-1}		Duchowicz et al. (2020)	Q	
		8800	Kühne et al. (2005)	Q	
	7.7×10^{-1}		Saçan et al. (2005)	Q	
	2.3		Wang and Wong (2002)	Q	535
	6.9×10^{-1}		Govers and Krop (1998)	Q	
		9400	Kühne et al. (2005)	?	
1,2,3,6,7,8-hexachlorodibenzo-*p*-dioxin	6.2×10^{-5}	2800	Paasivirta et al. (1999)	T	
$C_{12}H_2Cl_6O_2$	5.2		HSDB (2015)	Q	99
(PCDD-123678)	7.4×10^{-1}		Saçan et al. (2005)	Q	
[57653-85-7]	2.4		Wang and Wong (2002)	Q	535
YCLUIPQDHHPDJJ-UHFFFAOYSA-N	6.9×10^{-1}		Govers and Krop (1998)	Q	
1,2,3,6,7,9-hexachlorodibenzo-*p*-dioxin	2.2		Wang and Wong (2002)	Q	535
$C_{12}H_2Cl_6O_2$ (PCDD-123679) [64461-98-9] BQOHWGKNRKCEFT-UHFFFAOYSA-N	1.7		Govers and Krop (1998)	Q	
1,2,3,6,8,9-hexachlorodibenzo-*p*-dioxin	2.2		Wang and Wong (2002)	Q	535
$C_{12}H_2Cl_6O_2$ (PCDD-123689) [58200-69-4] GZRQZUFXVFRKBI-UHFFFAOYSA-N	1.8		Govers and Krop (1998)	Q	
1,2,3,7,8,9-hexachlorodibenzo-*p*-dioxin	2.5×10^{-4}	2700	Paasivirta et al. (1999)	T	
$C_{12}H_2Cl_6O_2$	5.2		HSDB (2015)	Q	99
(PCDD-123789)	1.1		Saçan et al. (2005)	Q	
[19408-74-3]	2.4		Wang and Wong (2002)	Q	535
LGIRBUBHIWTVCK-UHFFFAOYSA-N	1.2		Govers and Krop (1998)	Q	
1,2,4,6,7,9-hexachlorodibenzo-*p*-dioxin	2.1		Wang and Wong (2002)	Q	535
$C_{12}H_2Cl_6O_2$ (PCDD-124679) [39227-62-8] BSJDQMWAWFTDGD-UHFFFAOYSA-N	3.5		Govers and Krop (1998)	Q	

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Table A6.7: Polychlorinated dibenzo-*p*-dioxins (PCDDs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,4,6,8,9-hexachlorodibenzo-*p*-dioxin	2.0		Wang and Wong (2002)	Q	535
$C_{12}H_2Cl_6O_2$	4.4		Govers and Krop (1998)	Q	
(PCDD-124689)					
[58802-09-8]					
URELDHWUZUWPIU-UHFFFAOYSA-N					
1,2,3,4,6,7,8-heptachlorodibenzo-*p*-dioxin	5.6×10^{-2}		Duchowicz et al. (2020)	V	186
$C_{12}HCl_7O_2$	7.5		Mackay et al. (2006b)	V	
(PCDD-1234678)	2.3		Govers and Krop (1998)	V	
[35822-46-9]	7.5		Shiu et al. (1988)	V	
WCLNVRQZUKYVAI-UHFFFAOYSA-N	7.5×10^{-5}	2400	Paasivirta et al. (1999)	T	
	4.5×10^{-1}		Duchowicz et al. (2020)	Q	
	4.5×10^{-1}		HSDB (2015)	Q	545
	1.4		Saçan et al. (2005)	Q	
	3.6		Wang and Wong (2002)	Q	535
	1.2		Govers and Krop (1998)	Q	
1,2,3,4,6,7,9-heptachlorodibenzo-*p*-dioxin	3.4		Wang and Wong (2002)	Q	535
$C_{12}HCl_7O_2$	3.2		Govers and Krop (1998)	Q	
(PCDD-1234679)					
[58200-70-7]					
KTJJIBIRZGQFQZ-UHFFFAOYSA-N					
octachlorodibenzo-*p*-dioxin	1.5		Duchowicz et al. (2020)	V	186
$C_{12}Cl_8O_2$	1.5		HSDB (2015)	V	
(PCDD-12346789)	1.5		Mackay et al. (2006b)	V	
[3268-87-9]	7.6×10^{-1}		Govers and Krop (1998)	V	
FOIBFBMSLDGNHL-UHFFFAOYSA-N	1.5		Shiu et al. (1988)	V	
	1.1×10^{-5}	2300	Paasivirta et al. (1999)	T	
	3.8×10^{-1}		Duchowicz et al. (2020)	Q	
		9600	Kühne et al. (2005)	Q	
	1.7		Saçan et al. (2005)	Q	
	5.2		Wang and Wong (2002)	Q	535
	1.9		Govers and Krop (1998)	Q	
		9500	Kühne et al. (2005)	?	

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A6.8 Chlorocarbons with nitrogen (C, H, O, N, Cl)

Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyanogen chloride NCCl [506-77-4] QPJDMGCKMHUXFD-UHFFFAOYSA-N	1.2×10^{-2} 5.1×10^{-3}		Hilal et al. (2008) Yaws (1999)	Q ?	 21
N,N-dichloromethylamine CH_3NCl_2 [7651-91-4] DWEYPOWXNBAIDU-UHFFFAOYSA-N	3.3×10^{-3} 3.3×10^{-3} 3.3×10^{-3}	4300 4300 4300	Burkholder et al. (2019) Burkholder et al. (2015) Cimetiere and de Laat (2009)	L L M	
chloroacetonitrile C_2H_2ClN [107-14-2] RENMDAKOXSCIGH-UHFFFAOYSA-N	9.1×10^{-1}	 4600 5400	HSDB (2015) Kühne et al. (2005) Kühne et al. (2005)	Q Q ?	447
dichloroacetonitrile C_2HCl_2N [3018-12-0] STZZWJCGRKXEFF-UHFFFAOYSA-N	2.6		HSDB (2015)	Q	99
trichloroacetonitrile C_2Cl_3N [545-06-2] DRUIESSIVFYOMK-UHFFFAOYSA-N	7.6 7.3 1.9×10^{-2} 3.9×10^{-3} 1.0×10^{-2}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	99 287, 288 287, 289 287, 290 287, 291
tetramethylammonium chloride $C_4H_{12}ClN$ [75-57-0] OKIZCWYLBDKLSU-UHFFFAOYSA-M	2.3×10^{6}		HSDB (2015)	Q	99
metformin hydrochloride $C_4H_{12}ClN_5$ [1115-70-4] OETHQSJEHLVLGH-UHFFFAOYSA-N	1.3×10^{10}		HSDB (2015)	Q	99
bis(2-chloroethyl)methylamine $C_5H_{11}Cl_2N$ [51-75-2] HAWPXGHAZFHHAD-UHFFFAOYSA-N	3.4 8.5×10^{-1}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
chlormequat chloride $C_5H_{13}Cl_2N$ [999-81-5] OLQFELZRGYJRAZ-UHFFFAOYSA-N	$>3.2\times10^{9}$		Maniere et al. (2011)	?	241, 165

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tris(2-chloroethyl)amine	5.3×10^{-1}		Duchowicz et al. (2020)	V	186
$C_6H_{12}Cl_3N$	5.3×10^{-1}		HSDB (2015)	V	
[555-77-1]	7.3×10^{-1}		Duchowicz et al. (2020)	Q	
FDAYLTPAFBGXAB-UHFFFAOYSA-N					
bis(2-chloroethyl)ethylamine	2.8×10^{-2}		Duchowicz et al. (2020)	V	186
$C_6H_{13}Cl_2N$	2.9×10^{-2}		HSDB (2015)	V	
(ethylbis(2-chloroethyl)amine)	3.0×10^{-1}		Duchowicz et al. (2020)	Q	
[538-07-8]					
UQZPGHOJMQTOHB-UHFFFAOYSA-N					
cetrimonium chloride	3.4×10^{4}		HSDB (2015)	Q	99
$C_{19}H_{42}ClN$					
(trimethylhexadecylammonium chloride)					
[112-02-7]					
WOWHHFRSBJGXCM-UHFFFAOYSA-M					
dimethyldioctadecylammonium chloride	1.5×10^{2}		HSDB (2015)	Q	99
$C_{38}H_{80}ClN$					
[107-64-2]					
REZZEXDLIUJMMS-UHFFFAOYSA-M					
1-amino-2-chlorobenzene	1.9	7900	Brockbank (2013)	L	1, 735
C_6H_6ClN	7.8×10^{-1}		Chao et al. (2017)	M	
(o-chloroaniline)	1.8		Duchowicz et al. (2020)	V	186
[95-51-2]	7.6×10^{-1}		Chao et al. (2017)	V	
AKCRQHGQIJBRMN-UHFFFAOYSA-N	1.8		HSDB (2015)	V	
	1.3		Mackay et al. (2006d)	V	
	1.3		Lide and Frederikse (1995)	V	
	1.3		Mackay et al. (1995)	V	
	2.4		Meylan and Howard (1991)	V	
	1.6		Abraham et al. (1994a)	R	
	7.4		Duchowicz et al. (2020)	Q	
	2.3		Hilal et al. (2008)	Q	
	9.6×10^{1}		Modarresi et al. (2007)	Q	67
	2.8		English and Carroll (2001)	Q	230, 231
	1.1×10^{1}		Katritzky et al. (1998)	Q	
	5.4		Nirmalakhandan et al. (1997)	Q	
	7.0		Meylan and Howard (1991)	Q	
	1.1		Yaws (1999)	?	21, 12
1-amino-3-chlorobenzene	4.7		Chao et al. (2017)	M	
C_6H_6ClN	9.8		Altschuh et al. (1999)	M	
(m-chloroaniline)	2.7		Chao et al. (2017)	V	
[108-42-9]	4.5		Mackay et al. (2006d)	V	
PNPCRKVUWYDDST-UHFFFAOYSA-N	4.5		Mackay et al. (1995)	V	
	7.5		Abraham et al. (1994a)	R	
	7.5		Yaws (2003)	X	237, 12

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	9.1		Keshavarz et al. (2022)	Q	
	8.8		Duchowicz et al. (2020)	Q	
	4.9		Gharagheizi et al. (2010)	Q	246
	7.7		Hilal et al. (2008)	Q	
	3.1×10^{1}		Modarresi et al. (2007)	Q	67
	4.6		Yao et al. (2002)	Q	229
	4.1		English and Carroll (2001)	Q	230, 274
	1.5×10^{1}		Katritzky et al. (1998)	Q	
	5.3		Nirmalakhandan et al. (1997)	Q	
	9.9		Duchowicz et al. (2020)	?	185, 21
	4.9		Yaws (1999)	?	21, 12
1-amino-4-chlorobenzene C_6H_6ClN (*p*-chloroaniline) [106-47-8] QSNSCYSYFYORTR-UHFFFAOYSA-N	8.5		Duchowicz et al. (2020)	V	186
	3.2		HSDB (2015)	V	
	1.0×10^{1}		Mackay et al. (2006d)	V	
	9.1×10^{-1}		Lide and Frederikse (1995)	V	
	1.0×10^{1}		Mackay et al. (1995)	V	
	2.5×10^{1}		Meylan and Howard (1991)	V	
	8.6		Abraham et al. (1994a)	R	
	3.4		Yaws (2003)	X	237, 12
	9.2×10^{-1}		Howard (1989)	X	412
	8.3		Duchowicz et al. (2020)	Q	
	4.9		Gharagheizi et al. (2010)	Q	246
	8.6		Hilal et al. (2008)	Q	
	1.6×10^{1}		Modarresi et al. (2007)	Q	67
	8.8		Yaffe et al. (2003)	Q	248, 249
	5.4		English and Carroll (2001)	Q	230, 260
	1.5×10^{1}		Katritzky et al. (1998)	Q	
	5.3		Nirmalakhandan et al. (1997)	Q	
	7.0		Meylan and Howard (1991)	Q	
2,3-dichlorobenzenamine $C_6H_5Cl_2N$ (2,3-dichloroaniline) [608-27-5] BRPSAOUFIJSKOT-UHFFFAOYSA-N	6.2		HSDB (2015)	Q	99
2,4-dichlorobenzenamine $C_6H_5Cl_2N$ (2,4-dichloroaniline) [554-00-7] KQCMTOWTPBNWDB-UHFFFAOYSA-N	6.2		HSDB (2015)	Q	99
3,4-dichlorobenzenamine $C_6H_5Cl_2N$ (3,4-dichloroaniline) [95-76-1] SDYWXFYBZPNOFX-UHFFFAOYSA-N	6.8×10^{-1}		Duchowicz et al. (2020)	V	186
	6.8×10^{-1}		HSDB (2015)	V	
	4.4×10^{-1}		Mackay et al. (2006d)	V	
	4.4×10^{-1}		Mackay et al. (1995)	V	
	1.8×10^{1}		Duchowicz et al. (2020)	Q	
	2.0×10^{1}		Katritzky et al. (1998)	Q	

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,5-dichlorobenzenamine $C_6H_5Cl_2N$ (3,5-dichloroaniline) [626-43-7] UQRLKWGPEVNVHT-UHFFFAOYSA-N	6.2		HSDB (2015)	Q	99
2,5-dichlorobenzenamine	6.2		HSDB (2015)	Q	99
$C_6H_5Cl_2N$	9.5		Zhang et al. (2010)	Q	287, 288
(2,5-dichloroaniline)	2.6		Zhang et al. (2010)	Q	287, 289
[95-82-9]	2.7		Zhang et al. (2010)	Q	287, 290
AVYGCQXNNJPXSS-UHFFFAOYSA-N	1.9×10^{1}		Zhang et al. (2010)	Q	287, 291
2,4,5-trichlorobenzenamine	1.3×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_6H_4Cl_3N$	2.4		Zhang et al. (2010)	Q	287, 289
[636-30-6]	9.5		Zhang et al. (2010)	Q	287, 290
GUMCAKKKNKYFEB-UHFFFAOYSA-N	1.8×10^{1}		Zhang et al. (2010)	Q	287, 291
2,4,6-trichlorobenzenamine	7.4		HSDB (2015)	V	
$C_6H_4Cl_3N$	1.3×10^{1}		Zhang et al. (2010)	Q	287, 288
[634-93-5]	6.2×10^{-1}		Zhang et al. (2010)	Q	287, 289
NATVSFWWYVJTAZ-UHFFFAOYSA-N	4.1×10^{-1}		Zhang et al. (2010)	Q	287, 290
	1.5×10^{1}		Zhang et al. (2010)	Q	287, 291
2,3,4,5,6-pentachloroaniline $C_6H_2Cl_5N$ [527-20-8] KHCZSJXTDDHLGJ-UHFFFAOYSA-N	2.3×10^{1}		HSDB (2015)	Q	99
2,6-dichlorobenzenenitrile	4.8×10^{-1}	5400	Schoene and Steinhanses (1985)	M	
$C_6H_3Cl_2CN$	9.8×10^{-1}		Duchowicz et al. (2020)	V	186
(dichlobenil)	9.9×10^{-1}		HSDB (2015)	V	
[1194-65-6]	1.5		Mackay et al. (2006d)	V	
YOYAIZYFCNQIRF-UHFFFAOYSA-N	1.4		Schüürmann (2000)	V	
	1.5		Suntio et al. (1988)	V	12
	1.4		Burkhard and Guth (1981)	V	
	1.5×10^{-2}		Barcelo and Hennion (1997)	X	567
	3.5×10^{-1}		Duchowicz et al. (2020)	Q	
	1.5×10^{-2}		Goodarzi et al. (2010)	Q	568, 569
	3.6×10^{-1}		Modarresi et al. (2007)	Q	67
		6000	Kühne et al. (2005)	Q	
		5500	Kühne et al. (2005)	?	
(2,4,6-trichlorophenyl)hydrazine	3.1×10^{3}		Zhang et al. (2010)	Q	287, 288
$C_6H_5Cl_3N_2$	3.7×10^{1}		Zhang et al. (2010)	Q	287, 289
[5329-12-4]	1.1×10^{1}		Zhang et al. (2010)	Q	287, 290
MULHANRBCQBHII-UHFFFAOYSA-N	5.4×10^{3}		Zhang et al. (2010)	Q	287, 291

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-chlorobenzonitrile C_7H_4ClN [623-03-0] GJNGXPDXRVXSEH-UHFFFAOYSA-N	2.5×10^{-1} 3.8×10^{-1} 1.6 4.5×10^{-1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
3-chloro-2-methylbenzenamine C_7H_8ClN [87-60-5] ZUVPLKVDZNDZCM-UHFFFAOYSA-N	6.3		HSDB (2015)	Q	99
3-chloro-4-methylbenzenamine C_7H_8ClN [95-74-9] RQKFYFNZSHWXAW-UHFFFAOYSA-N	4.9		HSDB (2015)	Q	99
4-chloro-2-methylbenzenamine C_7H_8ClN [95-69-2] CXNVOWPRHWWCQR-UHFFFAOYSA-N	4.9		HSDB (2015)	Q	99
5-chloro-2-methylbenzenamine C_7H_8ClN [95-79-4] WRZOMWDJOLIVQP-UHFFFAOYSA-N	6.3		HSDB (2015)	Q	545
2,4,5,6-tetrachloro-1,3-dicyanobenzene $C_8Cl_4N_2$ (chlorothalonil) [1897-45-6] CRQQGFGUEAVUIL-UHFFFAOYSA-N	5.0×10^{1} 1.7×10^{-2} 3.9×10^{1} 4.5×10^{1} 4.1×10^{-1} 1.8×10^{1} 6.5×10^{1} 1.5 6.9×10^{1} 2.7×10^{1} 5.8 2.4×10^{1} 6.5×10^{1} 4.9		Kawamoto and Urano (1989) Mackay et al. (2006d) MacBean (2012b) Armbrust (2000) Keshavarz et al. (2022) Duchowicz et al. (2020) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Meylan and Howard (1991) Duchowicz et al. (2020)	M V X C Q Q Q Q Q Q Q Q Q ?	 350 287, 288 287, 289 287, 290 287, 291 67 185, 21
2-chlorobenzalmalononitrile $C_{10}H_5ClN_2$ [2698-41-1] JJNZXLAFIPKXIG-UHFFFAOYSA-N	9.9×10^{2}		HSDB (2015)	Q	99

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benzyltrimethylammonium chloride $C_{10}H_{16}ClN$ [56-93-9] KXHPPCXNWTUNSB-UHFFFAOYSA-M	2.9×10^{8}		HSDB (2015)	Q	99
chlordimeform $C_{10}H_{13}ClN_2$ [6164-98-3] STUSTWKEFDQFFZ-UHFFFAOYSA-N	2.9×10^{1} 2.6×10^{1}		HSDB (2015) MacBean (2012a)	V ?	 12
4,4'-dichloroazobenzene $C_{12}H_8Cl_2N_2$ [1602-00-2] XHQLXCFUPJSGOE-UHFFFAOYSA-N	1.2		HSDB (2015)	Q	99
bis(3,4-dichlorophenyl)diazene $C_{12}H_6Cl_4N_2$ (3,4,3',4'-tetrachloroazobenzene) [14047-09-7] SOBGIMQKWDUEPY-UHFFFAOYSA-N	2.2		HSDB (2015)	Q	447
2-(*p*-chlorophenyl)-3-methylbutyronitrile $C_{11}H_{12}ClN$ [2012-81-9] RBGSZIRWNWQDOK-UHFFFAOYSA-N	2.3 4.4 3.9 2.9×10^{-1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
3,3'-dichloro-(1,1'-biphenyl)-4,4'-diamine $C_{12}H_{10}Cl_2N_2$ (3,3'-dichlorobenzidine) [91-94-1] HUWXDEQWWKGHRV-UHFFFAOYSA-N	2.0×10^{2} 2.0×10^{2} 1.2×10^{1} 3.5×10^{5}		Mackay et al. (2006d) Mackay et al. (1995) Mackay et al. (1995) HSDB (2015)	V V C Q	 99
4-chloroazobenzene $C_{12}H_9ClN_2$ [4340-77-6] NJFDMENHTAYHMA-UHFFFAOYSA-N	7.4 2.2		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
4,4'-methylenebis(2-chlorobenzenamine) $C_{13}H_{12}Cl_2N_2$ [101-14-4] IBOFVQJTBBUKMU-UHFFFAOYSA-N	9.0×10^{5} 3.0×10^{5} 3.4×10^{4} 2.9×10^{4} 9.7×10^{5}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	99 287, 288 287, 289 287, 290 287, 291
clofentezine $C_{14}H_8N_4Cl_2$ [74115-24-5] UXADOQPNKNTIHB-UHFFFAOYSA-N	2.5×10^{4} 1.7×10^{4}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
aniline, 4,4'-(imidocarbonyl)bis-(N,N-dimethyl)-, hydrochloride $C_{17}H_{22}ClN_3$ (auramine hydrochloride) [2465-27-2] KSCQDDRPFHTIRL-UHFFFAOYSA-N	3.5×10^{10}		HSDB (2015)	Q	99
amitriptyline hydrochloride $C_{20}H_{24}ClN$ [549-18-8] KFYRPLNVJVHZGT-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	99
chlorhexidine $C_{22}H_{30}Cl_2N_{10}$ [55-56-1] GHXZTYHSJHQHIJ-UHFFFAOYSA-N	9.0×10^{24}		HSDB (2015)	Q	99
malachite green $C_{23}H_{25}ClN_2$ [569-64-2] FDZZZRQASAIRJF-UHFFFAOYSA-M	5.2×10^{8}		HSDB (2015)	Q	99
tetradecylbenzyldimethyl ammonium chloride $C_{23}H_{42}ClN$ [139-08-2] OCBHHZMJRVXXQK-UHFFFAOYSA-M	7.6×10^{5}		HSDB (2015)	Q	99
stearyldimethylbenzylammonium chloride $C_{27}H_{50}ClN$ (benzyldimethylstearylammonium chloride) [122-19-0] SFVFIFLLYFPGHH-UHFFFAOYSA-M	2.3×10^{5}		HSDB (2015)	Q	99
2,4,6-trichloro-1,3,5-triazine $C_3Cl_3N_3$ [108-77-0] MGNCLNQXLYJVJD-UHFFFAOYSA-N	2.0×10^{1} 2.0×10^{1} 2.4×10^{1} 3.1×10^{-1} 7.9		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	99 287, 288 287, 289 287, 290 287, 291
2-chloropyridine C_5H_4ClN [109-09-1] OKDGRDCXVWSXDC-UHFFFAOYSA-N	7.4×10^{-1} 6.1×10^{-1} 1.9×10^{-1} 5.8×10^{-1} 1.1 6.7×10^{-1}	5900 6100 	Arnett and Chawla (1979) Duchowicz et al. (2020) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Kühne et al. (2005) Yaffe et al. (2003)	M V Q Q Q Q Q	559 186 67 248, 249

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.9×10^{-1}		English and Carroll (2001)	Q	230, 274
	8.0×10^{-2}		Katritzky et al. (1998)	Q	
	1.5×10^{1}		Nirmalakhandan et al. (1997)	Q	
		6600	Kühne et al. (2005)	?	
3-chloropyridine	3.5×10^{-1}	5600	Arnett and Chawla (1979)	M	559
C_5H_4ClN	4.1×10^{-1}		Hilal et al. (2008)	Q	
[626-60-8]	8.3×10^{-1}		Modarresi et al. (2007)	Q	67
PWRBCZZQRRPXAB-UHFFFAOYSA-N	3.7×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.9×10^{-1}		English and Carroll (2001)	Q	230, 231
	1.5×10^{1}		Nirmalakhandan et al. (1997)	Q	
2,3,4,6-tetrachloropyridine	1.2×10^{-3}		Zhang et al. (2010)	Q	287, 288
C_5HCl_4N	1.1×10^{-1}		Zhang et al. (2010)	Q	287, 289
[14121-36-9]	7.9×10^{-2}		Zhang et al. (2010)	Q	287, 290
FZFNDUTVMQOPCT-UHFFFAOYSA-N	2.9×10^{-1}		Zhang et al. (2010)	Q	287, 291
2,3,5,6-tetrachloropyridine	1.2×10^{-3}		HSDB (2015)	Q	99
C_5HCl_4N	1.2×10^{-3}		Zhang et al. (2010)	Q	287, 288
[2402-79-1]	3.4×10^{-2}		Zhang et al. (2010)	Q	287, 289
FATBKZJZAHWCSL-UHFFFAOYSA-N	8.4×10^{-2}		Zhang et al. (2010)	Q	287, 290
	1.9×10^{-1}		Zhang et al. (2010)	Q	287, 291
pentachloropyridine	1.6×10^{-3}		HSDB (2015)	Q	99
C_5Cl_5N	1.6×10^{-3}		Zhang et al. (2010)	Q	287, 288
[2176-62-7]	1.3×10^{-2}		Zhang et al. (2010)	Q	287, 289
DNDPLEAVNVOOQZ-UHFFFAOYSA-N	2.5×10^{-2}		Zhang et al. (2010)	Q	287, 290
	1.8×10^{-1}		Zhang et al. (2010)	Q	287, 291
desethylatrazine $C_6H_{10}ClN_5$ [6190-65-4] DFWFIQKMSFGDCQ-UHFFFAOYSA-N	6.6×10^{3}		HSDB (2015)	Q	99
2-chloro-6-(trichloromethyl)-pyridine	6.2×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_6H_3Cl_4N$	1.8		Zhang et al. (2010)	Q	287, 289
[1929-82-4]	2.7		Zhang et al. (2010)	Q	287, 290
DCUJJWWUNKIJPH-UHFFFAOYSA-N	4.2×10^{-1}		Zhang et al. (2010)	Q	287, 291
	1.8		Hilal et al. (2008)	Q	
	5.9×10^{-1}		Modarresi et al. (2007)	Q	67
2,3,4,5-tetrachloro-6-methylpyridine	6.7×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_6H_3Cl_4N$	3.6×10^{-2}		Zhang et al. (2010)	Q	287, 289
[10469-02-0]	3.6×10^{-2}		Zhang et al. (2010)	Q	287, 290
OZLPEWBQZDDFCQ-UHFFFAOYSA-N	1.1×10^{-1}		Zhang et al. (2010)	Q	287, 291

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-chloro-5- (trichloromethyl)pyridine	6.2×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_6H_3Cl_4N$	2.2		Zhang et al. (2010)	Q	287, 289
[69045-78-9]	7.7×10^{-1}		Zhang et al. (2010)	Q	287, 290
VLJIVLGVKMTBOD-UHFFFAOYSA-N	4.2×10^{-1}		Zhang et al. (2010)	Q	287, 291
2,3-dichloro-5- (trichloromethyl)pyridine	8.4×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_6H_2Cl_5N$	4.1×10^{-1}		Zhang et al. (2010)	Q	287, 289
[69045-83-6]	1.8×10^{-1}		Zhang et al. (2010)	Q	287, 290
XVBWGQSXLITICX-UHFFFAOYSA-N	6.1×10^{-1}		Zhang et al. (2010)	Q	287, 291
2,5-dichloro-6- (trichloromethyl)pyridine	8.4×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_6H_2Cl_5N$	1.2		Zhang et al. (2010)	Q	287, 289
[1817-13-6]	9.9×10^{-1}		Zhang et al. (2010)	Q	287, 290
MWFCRQNUHFSUNY-UHFFFAOYSA-N	5.7×10^{-1}		Zhang et al. (2010)	Q	287, 291
3,4,5-trichloro-2- (trichloromethyl)pyridine	7.2×10^{1}		Zhang et al. (2010)	Q	287, 288
C_6HCl_6N	9.0×10^{-2}		Zhang et al. (2010)	Q	287, 289
[1201-30-5]	1.0×10^{-1}		Zhang et al. (2010)	Q	287, 290
YWSFDYUMEBEQNZ-UHFFFAOYSA-N	4.1×10^{-1}		Zhang et al. (2010)	Q	287, 291
2,3,4,5-tetrachloro-6- (trichloromethyl)pyridine	1.5		Zhang et al. (2010)	Q	287, 288
C_6Cl_7N	6.7×10^{-2}		Zhang et al. (2010)	Q	287, 289
[1134-04-9]	7.0×10^{-2}		Zhang et al. (2010)	Q	287, 290
YMBFWRZKTZICHS-UHFFFAOYSA-N	2.3×10^{-1}		Zhang et al. (2010)	Q	287, 291
3,4,5,6-tetrachloropyridine-2- carbonitrile	7.5		Zhang et al. (2010)	Q	287, 288
$C_6Cl_4N_2$	1.7		Zhang et al. (2010)	Q	287, 289
[17824-83-8]	8.0×10^{-1}		Zhang et al. (2010)	Q	287, 290
KFPBGJYBKSQIAI-UHFFFAOYSA-N	1.5×10^{1}		Zhang et al. (2010)	Q	287, 291
4-amino-3,5,6-trichloropyridine-2- carbonitrile	1.6×10^{4}		Zhang et al. (2010)	Q	287, 288
$C_6H_2Cl_3N_3$	1.1×10^{3}		Zhang et al. (2010)	Q	287, 289
[14143-60-3]	9.0×10^{3}		Zhang et al. (2010)	Q	287, 290
AZYYQVGBVUCIEO-UHFFFAOYSA-N	1.0×10^{5}		Zhang et al. (2010)	Q	287, 291
crimidine $C_7H_{10}ClN_3$ [535-89-7] HJIUPFPIEBPYIE-UHFFFAOYSA-N	2.6×10^{2}		HSDB (2015)	Q	99

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
simazine	1.0×10^{4}		HSDB (2015)	V	
$C_7H_{12}ClN_5$	2.9×10^{3}		Mackay et al. (2006d)	V	
[122-34-9]	2.9×10^{3}		Suntio et al. (1988)	V	12
ODCWYMIRDDJXKW-UHFFFAOYSA-N	1.6×10^{4}		Glotfelty et al. (1987)	V	
	2.9×10^{1}		Barcelo and Hennion (1997)	X	567
	6.2×10^{7}		Delgado and Alderete (2003)	C	
	1.1×10^{4}		Delgado and Alderete (2003)	C	
	9.1×10^{1}		Goodarzi et al. (2010)	Q	568
	1.7×10^{3}		Hilal et al. (2008)	Q	
	7.2×10^{3}		Abraham et al. (2007)	Q	
	5.5×10^{5}		Delgado and Alderete (2003)	Q	
	4.0×10^{6}		Delgado and Alderete (2003)	Q	
desethylterbuthylazine	2.2×10^{3}		Otto et al. (1997)	V	
$C_7H_{12}ClN_5$					
[30125-63-4]					
LMKQNTMFZLAJDV-UHFFFAOYSA-N					
mepiquat chloride	3.3×10^{11}		Maniere et al. (2011)	?	241, 165
$C_7H_{16}NCl$					
[24307-26-4]					
VHOVSQVSAAQANU-UHFFFAOYSA-M					
atrazine	1.9×10^{3}		Muir et al. (2004)	L	367
$C_8H_{14}ClN_5$	3.5×10^{3}		Mackay et al. (2006d)	V	
[1912-24-9]	1.0×10^{3}		Siebers et al. (1994)	V	
MXWJVTOOROXGIU-UHFFFAOYSA-N	3.3×10^{3}		Riederer (1990)	V	
	3.4×10^{3}		Suntio et al. (1988)	V	12
	2.0×10^{3}		Glotfelty et al. (1987)	V	
	3.4×10^{1}		Barcelo and Hennion (1997)	X	567
	8.3×10^{6}		Delgado and Alderete (2003)	C	
	4.3×10^{3}		Delgado and Alderete (2003)	C	
	7.2×10^{1}		Goodarzi et al. (2010)	Q	568
	7.2×10^{2}		Hilal et al. (2008)	Q	
	5.1×10^{3}		Abraham et al. (2007)	Q	
	2.8×10^{4}		Delgado and Alderete (2003)	Q	
	4.0×10^{5}		Delgado and Alderete (2003)	Q	
clonidine	6.6×10^{5}		HSDB (2015)	Q	99
$C_9H_9Cl_2N_3$					
[4205-90-7]					
GJSURZIOUXUGAL-UHFFFAOYSA-N					
cyprazine	7.6×10^{3}		Duchowicz et al. (2020)	V	186
$C_9H_{12}ClN_5$	7.7×10^{4}		Duchowicz et al. (2020)	Q	
[22936-86-3]	3.8×10^{3}		HSDB (2015)	Q	99
OOHIAOSLOGDBCE-UHFFFAOYSA-N					

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
propazine	2.1×10^{3}		HSDB (2015)	V	
$C_9H_{16}ClN_5$			Mackay et al. (2006d)	V	558
[139-40-2]	1.0×10^{4}		Suntio et al. (1988)	V	12
WJNRPILHGGKWCK-UHFFFAOYSA-N	9.9×10^{1}		Barcelo and Hennion (1997)	X	567
	1.7×10^{2}		Goodarzi et al. (2010)	Q	568, 571
	3.6×10^{2}		Hilal et al. (2008)	Q	
	4.0×10^{3}		Abraham et al. (2007)	Q	
sebuthylazine	8.4×10^{2}		Ebert et al. (2023)	?	318
$C_9H_{16}ClN_5$					
[7286-69-3]					
BZRUVKZGXNSXMB-UHFFFAOYSA-N					
terbuthylazine	4.3×10^{2}		HSDB (2015)	V	
$C_9H_{16}ClN_5$	2.5×10^{2}		Mackay et al. (2006d)	V	
[5915-41-3]	2.5×10^{2}		Otto et al. (1997)	V	
FZXISNSWEXTPMF-UHFFFAOYSA-N	2.4×10^{2}		Siebers et al. (1994)	V	
	2.9×10^{2}		Hilal et al. (2008)	Q	
	9.0×10^{2}		Abraham et al. (2007)	Q	
	4.3×10^{2}		Maniere et al. (2011)	?	241, 165
cyanazine	3.3×10^{6}		Mackay et al. (2006d)	V	
$C_9H_{13}ClN_6$	3.3×10^{4}		Barcelo and Hennion (1997)	X	567
[21725-46-2]	8.3×10^{9}		Delgado and Alderete (2003)	C	
MZZBPDKVEFVLFF-UHFFFAOYSA-N	3.9×10^{6}		Delgado and Alderete (2003)	C	
	9.6×10^{1}		Goodarzi et al. (2010)	Q	568
	6.4×10^{5}		Hilal et al. (2008)	Q	
	2.0×10^{6}		Abraham et al. (2007)	Q	
	4.5×10^{6}		Delgado and Alderete (2003)	Q	
	1.0×10^{9}		Delgado and Alderete (2003)	Q	
anilazine	3.5×10^{4}		HSDB (2015)	V	
$C_9H_5Cl_3N_4$	3.5×10^{4}		Mackay et al. (2006d)	V	
[101-05-3]	2.9×10^{1}		Zhang et al. (2010)	Q	287, 288
IMHBYKMAHXWHRP-UHFFFAOYSA-N	1.2×10^{3}		Zhang et al. (2010)	Q	287, 289
	9.5		Zhang et al. (2010)	Q	287, 290
	5.4×10^{3}		Zhang et al. (2010)	Q	287, 291
	3.5×10^{4}		MacBean (2012a)	?	
4,7-dichloroquinoline	2.6×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_9H_5Cl_2N$	6.9		Zhang et al. (2010)	Q	287, 289
[86-98-6]	1.5		Zhang et al. (2010)	Q	287, 290
HXEWMTXDBOQQKO-UHFFFAOYSA-N	7.0		Zhang et al. (2010)	Q	287, 291
fenclorim	5.6×10^{-1}		Ebert et al. (2023)	?	318
$C_{10}H_6Cl_2N_2$					
[3740-92-9]					
NRFQZTCQAYEXEE-UHFFFAOYSA-N					

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
acetamiprid	1.4×10^{2}		HSDB (2015)	Q	99
$C_{10}H_{11}ClN_4$	$>1.9\times10^{7}$		Maniere et al. (2011)	?	165
[135410-20-7]					
WCXDHFDTOYPNIE-UHFFFAOYSA-N					
pyrimethamine	9.1×10^{4}		HSDB (2015)	Q	447
$C_{12}H_{13}ClN_4$					
[58-14-0]					
WKSAUQYGYAYLPV-UHFFFAOYSA-N					
penconazole	6.9×10^{2}		Duchowicz et al. (2020)	V	186
$C_{13}H_{15}Cl_2N_3$	1.2×10^{3}		Mackay et al. (2006d)	V	
[66246-88-6]	2.1		Duchowicz et al. (2020)	Q	
WKBPZYKAUNRMKP-UHFFFAOYSA-N	1.5×10^{3}		Maniere et al. (2011)	?	12, 165
myclobutanil	2.3×10^{3}		Duchowicz et al. (2020)	V	186
$C_{15}H_{17}ClN_4$	2.3×10^{3}		HSDB (2015)	V	
[88671-89-0]	2.2×10^{2}		Duchowicz et al. (2020)	Q	
HZJKXKUJVSEEFU-UHFFFAOYSA-N	2.3×10^{3}		Maniere et al. (2011)	?	12, 165
2-chloro-4,6-bis(2,4- dimethylphenyl)-1,3,5-triazine	1.2×10^{3}		Zhang et al. (2010)	Q	287, 288
$C_{19}H_{18}N_3Cl$	1.3×10^{3}		Zhang et al. (2010)	Q	287, 289
[1237-53-2]	7.0		Zhang et al. (2010)	Q	287, 290
LVWOBZPDFCTAOU-UHFFFAOYSA-N	1.2×10^{3}		Zhang et al. (2010)	Q	287, 291
fenbuconazole	3.3×10^{4}		Maniere et al. (2011)	?	241, 165
$C_{19}H_{17}ClN_4$					
[114369-43-6]					
RQDJADAKIFFEKQ-UHFFFAOYSA-N					
trichloronitromethane	4.7×10^{-3}		Burkholder et al. (2019)	L	
CCl_3NO_2	4.7×10^{-3}		Burkholder et al. (2015)	L	
(chloropicrin)	4.7×10^{-3}		Sander et al. (2011)	L	
[76-06-2]	4.7×10^{-3}		Worthington and Wade (2007)	M	
LFHISGNCFUNFFM-UHFFFAOYSA-N	4.0×10^{-3}		Welke et al. (1998)	M	
	4.8×10^{-3}		Kawamoto and Urano (1989)	M	
			Mackay et al. (2006d)	V	558
	5.1×10^{-3}		Suntio et al. (1988)	V	12
	5.0×10^{-2}		Keshavarz et al. (2022)	Q	
	2.6×10^{-2}		Duchowicz et al. (2020)	Q	184
	2.5×10^{-3}		Hilal et al. (2008)	Q	
	3.0×10^{-2}		Modarresi et al. (2007)	Q	67
	4.8×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.3×10^{-2}		Katritzky et al. (1998)	Q	
	4.8×10^{-3}		Duchowicz et al. (2020)	?	185, 21

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
phosgene oxime $CHCl_2NO$ [1794-86-1] JIRJHEXNDQBKRZ-UHFFFAOYSA-N	1.8×10^{1}		HSDB (2015)	Q	99
1,1-dichloro-1-nitroethane	7.7×10^{-3}		Duchowicz et al. (2020)	V	186
$C_2H_3Cl_2NO_2$	1.3×10^{-1}		Duchowicz et al. (2020)	Q	
[594-72-9]	7.7×10^{-3}		HSDB (2015)	Q	99
OQOGEOLRYAOSKO-UHFFFAOYSA-N	2.0×10^{-2}		Hilal et al. (2008)	Q	
	1.1×10^{-1}		Modarresi et al. (2007)	Q	67
2-chloroacetamide C_2H_4ClNO [79-07-2] VXIVSQZSERGHQP-UHFFFAOYSA-N	2.5×10^{3}		HSDB (2015)	Q	99
MCM:CCL3PAN	1.0×10^{1}		Wang et al. (2017)	Q	80, 238
$C_2NO_5Cl_3$	7.3×10^{-1}		Wang et al. (2017)	Q	80, 239
LLOMRHYBAIQQGH-UHFFFAOYSA-N	3.6×10^{-5}		Wang et al. (2017)	Q	80, 240
MCM:CCLNO3COOH	2.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_2H_4NO_5Cl$	2.6×10^{3}		Wang et al. (2017)	Q	80, 239
GVGGZHVOOFUNFY-UHFFFAOYSA-N	4.2		Wang et al. (2017)	Q	80, 240
MCM:CHCL2PAN	2.2×10^{1}		Wang et al. (2017)	Q	80, 238
$C_2HNO_5Cl_2$	1.6×10^{1}		Wang et al. (2017)	Q	80, 239
BORKLXDOXKHVRO-UHFFFAOYSA-N	4.9×10^{-4}		Wang et al. (2017)	Q	80, 240
MCM:CLETPAN	9.8		Wang et al. (2017)	Q	80, 238
$C_2H_2NO_5Cl$	3.3×10^{1}		Wang et al. (2017)	Q	80, 239
IEQWXJNETVFAEB-UHFFFAOYSA-N	4.2×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:CNO3CLOOH	2.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_2H_4NO_5Cl$	3.0×10^{3}		Wang et al. (2017)	Q	80, 239
FBIXZLOOAAICML-UHFFFAOYSA-N	8.3		Wang et al. (2017)	Q	80, 240
MCM:CCLNO3COH	1.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_4NO_4Cl$	7.1×10^{2}		Wang et al. (2017)	Q	80, 239
PMLDKFZZOPGPNK-UHFFFAOYSA-N	7.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:CL2OHPAN	3.8×10^{3}		Wang et al. (2017)	Q	80, 238
$C_2HNO_6Cl_2$	1.5×10^{2}		Wang et al. (2017)	Q	80, 239
YJZUCQDIDXVPNP-UHFFFAOYSA-N	1.4×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:CLOHPAN	4.2×10^{3}		Wang et al. (2017)	Q	80, 238
$C_2H_2NO_6Cl$	1.0×10^{4}		Wang et al. (2017)	Q	80, 239
ZNYKQWDXHYNGTP-UHFFFAOYSA-N	8.9×10^{-2}		Wang et al. (2017)	Q	80, 240
1-chloro-1-nitroethane $C_2H_4ClNO_2$ [598-92-5] LPIWIOBGUAPNQW-UHFFFAOYSA-N	2.0×10^{-2}		Ebert et al. (2023)	?	316

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:CNO3CLOH	2.8×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_4NO_4Cl$	1.4×10^{3}		Wang et al. (2017)	Q	80, 239
OUFVLIWCNZOATK-UHFFFAOYSA-N	1.4×10^{2}		Wang et al. (2017)	Q	80, 240
MCM:CCLCONO3	2.6×10^{1}		Wang et al. (2017)	Q	80, 238
$C_2H_2NO_4Cl$	1.6×10^{2}		Wang et al. (2017)	Q	80, 239
XDEFPIDZLAIVCM-UHFFFAOYSA-N	2.5×10^{-3}		Wang et al. (2017)	Q	80, 240
MCM:CNO3OCL	1.7×10^{1}		Wang et al. (2017)	Q	80, 238
$C_2H_2NO_4Cl$	1.1×10^{1}		Wang et al. (2017)	Q	80, 239
ODQFUUDIEKKDDJ-UHFFFAOYSA-N	4.4×10^{-3}		Wang et al. (2017)	Q	80, 240
symclosene $C_3Cl_3N_3O_3$ (trichloroisocyanuric acid) [87-90-1] YRIZYWQGELRKNT-UHFFFAOYSA-N	1.6×10^{5}		HSDB (2015)	Q	99
MCM:CL12PAN	6.2×10^{1}		Wang et al. (2017)	Q	80, 238
$C_3H_3NO_5Cl_2$	4.9×10^{1}		Wang et al. (2017)	Q	80, 239
MSMFQRZPTBDNBF-UHFFFAOYSA-N	2.5×10^{-3}		Wang et al. (2017)	Q	80, 240
1-chloro-1-nitropropane $C_3H_6ClNO_2$ [600-25-9] XEKUXTMJEFPWCG-UHFFFAOYSA-N	4.6×10^{-2}		Ebert et al. (2023)	?	316
1,3-dichloro-5,5-dimethylhydantoin $C_5H_6Cl_2N_2O_2$ [118-52-5] KEQGZUUPPQEDPF-UHFFFAOYSA-N	9.9		HSDB (2015)	Q	99
carmustine $C_5H_9Cl_2N_3O_2$ [154-93-8] DLGOEMSEDOSKAD-UHFFFAOYSA-N	2.1×10^{5}		HSDB (2015)	Q	99
2-chloro-N,N-di-2-propenylacetamide	9.2×10^{1}		Duchowicz et al. (2020)	V	186
$C_8H_{12}ClNO$	9.2×10^{1}		HSDB (2015)	V	
[93-71-0]	9.5		Duchowicz et al. (2020)	Q	
MDBGGTQNNUOQRC-UHFFFAOYSA-N	9.7×10^{1}		Hilal et al. (2008)	Q	
	1.9×10^{1}		Modarresi et al. (2007)	Q	67
2,2-dichloro-N,N-di-2-propenylacetamide	3.1×10^{1}		Hilal et al. (2008)	Q	
$C_8H_{11}Cl_2NO$	2.7×10^{1}		Modarresi et al. (2007)	Q	67
(dichlormid) [37764-25-3] YRMLFORXOOIJDR-UHFFFAOYSA-N					

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
lomustine $C_9H_{16}ClN_3O_2$ [13010-47-4] GQYIWUVLTXOXAJ-UHFFFAOYSA-N	5.5×10^{4}		HSDB (2015)	Q	99
semustine $C_{10}H_{18}ClN_3O_2$ [13909-09-6] FVLVBPDQNARYJU-UHFFFAOYSA-N	3.9×10^{4}		HSDB (2015)	Q	99
furilazole $C_{11}H_{13}Cl_2NO_3$ [121776-33-8] MCNOFYBITGAAGM-UHFFFAOYSA-N	1.1×10^{5} 1.3×10^{3}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
dimethazone $C_{12}H_{14}ClNO_2$ (clomazone) [81777-89-1] KIEDNEWSYUYDSN-UHFFFAOYSA-N	2.4×10^{2} 2.4×10^{2} 4.5 2.4×10^{2}		Duchowicz et al. (2020) MacBean (2012b) Duchowicz et al. (2020) Maniere et al. (2011)	V X Q ?	186 350 241, 165
2-chloronitrobenzene $C_6H_4ClNO_2$ (*o*-chloronitrobenzene) [88-73-3] BFCFYVKQTRLZHA-UHFFFAOYSA-N	1.1 2.2×10^{-1} 2.8×10^{-1} 1.1 3.1 6.2×10^{-1} 1.5×10^{-1} 1.2 4.6×10^{-1} 3.1×10^{-1} 1.8×10^{-1} 2.3×10^{-1} 8.1×10^{-1} 7.5×10^{-1} 1.1 9.7×10^{-1}	 4700 6000 	Altschuh et al. (1999) Hellmann (1987) Lide and Frederikse (1995) Keshavarz et al. (2022) Duchowicz et al. (2020) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) Kühne et al. (2005) Yaffe et al. (2003) Yao et al. (2002) Katritzky et al. (1998) Duchowicz et al. (2020) Kühne et al. (2005) Yaws (1999)	M M V Q Q Q Q Q Q Q Q Q Q Q Q ? ? ?	 87 184 287, 288 287, 289 287, 290 287, 291 67 248, 249 229 185, 21 21, 12
3-chloronitrobenzene $C_6H_4ClNO_2$ (*m*-chloronitrobenzene) [121-73-3] KMAQZIILEGKYQZ-UHFFFAOYSA-N	1.4 7.3×10^{-1} 1.1×10^{-1} 1.1 1.8 6.2×10^{-1} 2.8×10^{-1} 2.8×10^{-1} 4.6×10^{-1} 2.1×10^{-1}		Chao et al. (2017) Altschuh et al. (1999) Schüürmann (2000) Keshavarz et al. (2022) Duchowicz et al. (2020) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Hilal et al. (2008)	M M V Q Q Q Q Q Q Q	 287, 288 287, 289 287, 290 287, 291

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.7×10^{-1}		Modarresi et al. (2007)	Q	67
	7.3×10^{-1}		Duchowicz et al. (2020)	?	185, 21
	3.4×10^{-1}		Yaws (1999)	?	21, 12
4-chloronitrobenzene	6.4×10^{-1}	5900	Brockbank (2013)	L	1
$C_6H_4ClNO_2$	1.4		Chao et al. (2017)	M	
(p-chloronitrobenzene)	2.0		Altschuh et al. (1999)	M	
[100-00-5]	1.8×10^{-1}		Hellmann (1987)	M	87
CZGCEKJOLUNIFY-UHFFFAOYSA-N	2.8×10^{-1}		Lide and Frederikse (1995)	V	
	1.1		Keshavarz et al. (2022)	Q	
	1.7		Duchowicz et al. (2020)	Q	184
	6.2×10^{-1}		Zhang et al. (2010)	Q	287, 288
	3.0×10^{-1}		Zhang et al. (2010)	Q	287, 289
	6.1×10^{-1}		Zhang et al. (2010)	Q	287, 290
	4.6×10^{-1}		Zhang et al. (2010)	Q	287, 291
	2.3×10^{-1}		Hilal et al. (2008)	Q	
	2.3×10^{-1}		Hilal et al. (2008)	Q	
	1.4×10^{-1}		Modarresi et al. (2007)	Q	67
		4700	Kühne et al. (2005)	Q	
	1.9×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	1.6		Katritzky et al. (1998)	Q	
	2.0		Duchowicz et al. (2020)	?	185, 21
		4000	Kühne et al. (2005)	?	
1,2-dichloro-4-nitrobenzene	1.2		Altschuh et al. (1999)	M	
$C_6H_3Cl_2NO_2$	1.1		Keshavarz et al. (2022)	Q	
[99-54-7]	1.8		Duchowicz et al. (2020)	Q	
NTBYINQTYWZXLH-UHFFFAOYSA-N	2.1×10^{-1}		Abraham et al. (2019)	Q	
	8.4×10^{-1}		Zhang et al. (2010)	Q	287, 288
	3.1×10^{-1}		Zhang et al. (2010)	Q	287, 289
	4.6×10^{-1}		Zhang et al. (2010)	Q	287, 290
	6.7×10^{-1}		Zhang et al. (2010)	Q	287, 291
	2.7×10^{-1}		Hilal et al. (2008)	Q	
	2.3×10^{-1}		Modarresi et al. (2007)	Q	67
	1.2		Duchowicz et al. (2020)	?	185, 21
1,4-dichloro-2-nitrobenzene	8.2×10^{-1}		Altschuh et al. (1999)	M	
$C_6H_3Cl_2NO_2$	1.1		Keshavarz et al. (2022)	Q	
[89-61-2]	1.8		Duchowicz et al. (2020)	Q	184
RZKKOBGFCAHLCZ-UHFFFAOYSA-N	3.2×10^{-1}		Abraham et al. (2019)	Q	
	8.4×10^{-1}		Zhang et al. (2010)	Q	287, 288
	1.5×10^{-1}		Zhang et al. (2010)	Q	287, 289
	7.3×10^{-1}		Zhang et al. (2010)	Q	287, 290
	6.1×10^{-1}		Zhang et al. (2010)	Q	287, 291
	3.1×10^{-1}		Hilal et al. (2008)	Q	
	2.2×10^{-1}		Modarresi et al. (2007)	Q	67
	8.2×10^{-1}		Duchowicz et al. (2020)	?	185, 21

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3-dichloronitrobenzene	5.0×10^{-1}		Abraham et al. (2019)	Q	
$C_6H_3Cl_2NO_2$	8.2×10^{-1}		HSDB (2015)	Q	99
[3209-22-1]	8.4×10^{-1}		Zhang et al. (2010)	Q	287, 288
CMVQZRLQEOAYSW-UHFFFAOYSA-N	1.4×10^{-1}		Zhang et al. (2010)	Q	287, 289
	9.7×10^{-1}		Zhang et al. (2010)	Q	287, 290
	6.7×10^{-1}		Zhang et al. (2010)	Q	287, 291
2,4-dichloronitrobenzene	3.1×10^{-1}		HSDB (2015)	Q	99
$C_6H_3Cl_2NO_2$	8.4×10^{-1}		Zhang et al. (2010)	Q	287, 288
[611-06-3]	1.6×10^{-1}		Zhang et al. (2010)	Q	287, 289
QUIMTLZDMCNYGY-UHFFFAOYSA-N	8.4×10^{-1}		Zhang et al. (2010)	Q	287, 290
	2.9×10^{-1}		Zhang et al. (2010)	Q	287, 291
3,5-dichloronitrobenzene	8.4×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_6H_3Cl_2NO_2$	2.0×10^{-1}		Zhang et al. (2010)	Q	287, 289
[618-62-2]	1.1×10^{-1}		Zhang et al. (2010)	Q	287, 290
RNABGKOKSBUFHW-UHFFFAOYSA-N	2.9×10^{-1}		Zhang et al. (2010)	Q	287, 291
pentachloronitrobenzene	2.7		Kawamoto and Urano (1989)	M	
$C_6Cl_5NO_2$	2.2×10^{-1}		Duchowicz et al. (2020)	V	186
(quintozene)	2.2×10^{-1}		HSDB (2015)	V	
[82-68-8]	2.3×10^{-1}		Mackay et al. (2006d)	V	
LKPLKUMXSAEKID-UHFFFAOYSA-N	2.1×10^{-1}		Howard and Meylan (1997)	X	446
	1.1		Duchowicz et al. (2020)	Q	
	2.1		Zhang et al. (2010)	Q	287, 288
	2.3×10^{-2}		Zhang et al. (2010)	Q	287, 289
	2.2×10^{-2}		Zhang et al. (2010)	Q	287, 290
	2.2×10^{-1}		Zhang et al. (2010)	Q	287, 291
	6.9×10^{-2}		Hilal et al. (2008)	Q	
	2.1		Meylan and Howard (1991)	Q	
4-chloro-2-nitrophenol	7.8×10^{-1}		Duchowicz et al. (2020)	V	186
$C_6H_4ClNO_3$	7.8×10^{-1}		Schwarzenbach et al. (1988)	V	12
[89-64-5]	1.6×10^{1}		Duchowicz et al. (2020)	Q	
NWSIFTLPLKCTSX-UHFFFAOYSA-N	7.9×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	3.6×10^{1}		Katritzky et al. (1998)	Q	
2-chloro-4-nitrobenzenamine	1.0×10^{3}		Altschuh et al. (1999)	M	
$C_6H_5ClN_2O_2$	4.2×10^{3}		Keshavarz et al. (2022)	Q	
[121-87-9]	1.3×10^{3}		Duchowicz et al. (2020)	Q	184
LOCWBQIWHWIRGN-UHFFFAOYSA-N	1.8×10^{3}		Zhang et al. (2010)	Q	287, 288
	1.3×10^{3}		Zhang et al. (2010)	Q	287, 289
	6.7×10^{4}		Zhang et al. (2010)	Q	287, 290
	2.1×10^{3}		Zhang et al. (2010)	Q	287, 291
	4.6×10^{2}		Hilal et al. (2008)	Q	
	6.4×10^{2}		Modarresi et al. (2007)	Q	67
	1.0×10^{3}		Duchowicz et al. (2020)	?	185, 21

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-chloro-5-nitrobenzenamine $C_6H_5ClN_2O_2$ [6283-25-6] KWIXNFOTNVKIGM-UHFFFAOYSA-N	1.8×10^{3}		HSDB (2015)	Q	99
4-chloro-2,6-dinitrobenzenamine $C_6H_4ClN_3O_4$ [5388-62-5] CLMQUEQFVUMDPC-UHFFFAOYSA-N	7.6×10^{1}		HSDB (2015)	Q	99
1-chloro-2,4-dinitrobenzene $C_6H_3ClN_2O_4$ [97-00-7] VYZAHLCBVHPDDF-UHFFFAOYSA-N	3.5		Duchowicz et al. (2020)	V	186
	4.0		HSDB (2015)	V	
	1.1×10^{1}		Yaws (2003)	X	237, 80
	1.8×10^{2}		Duchowicz et al. (2020)	Q	
	1.6×10^{2}		Zhang et al. (2010)	Q	287, 288
	6.0		Zhang et al. (2010)	Q	287, 289
	5.3		Zhang et al. (2010)	Q	287, 290
	3.9×10^{1}		Zhang et al. (2010)	Q	287, 291
	1.0×10^{1}		Gharagheizi et al. (2010)	Q	246
1-chloro-2,6-dinitrobenzene $C_6H_3ClN_2O_4$ [606-21-3] BPPMIQPXQVIZNJ-UHFFFAOYSA-N	1.6×10^{2}		Zhang et al. (2010)	Q	287, 288
	4.3		Zhang et al. (2010)	Q	287, 289
	7.2		Zhang et al. (2010)	Q	287, 290
	3.9×10^{1}		Zhang et al. (2010)	Q	287, 291
2-chloro-1,3,5-trinitrobenzene $C_6H_2ClN_3O_6$ [88-88-0] HJRJRUMKQCMYDL-UHFFFAOYSA-N	3.9×10^{4}		HSDB (2015)	Q	99
2,3,4-trichloronitrobenzene $C_6H_2Cl_3NO_2$ [17700-09-3] BGKIECJVXXHLDP-UHFFFAOYSA-N	1.1		Zhang et al. (2010)	Q	287, 288
	1.3×10^{-1}		Zhang et al. (2010)	Q	287, 289
	2.0×10^{-1}		Zhang et al. (2010)	Q	287, 290
	4.0×10^{-1}		Zhang et al. (2010)	Q	287, 291
2,3,4,5-tetrachloronitrobenzene $C_6HCl_4NO_2$ [879-39-0] MTBYTWZDRVOMBR-UHFFFAOYSA-N	4.3×10^{-1}		HSDB (2015)	Q	99
1,2,4,5-tetrachloronitrobenzene $C_6HCl_4NO_2$ (tecnazene) [117-18-0] XQTLDIFVVHJORV-UHFFFAOYSA-N	4.3×10^{-1}		HSDB (2015)	Q	99
4-chloro-2-nitrobenzenamine $C_6H_5ClN_2O_2$ [89-63-4] PBGKNXWGYQPUJK-UHFFFAOYSA-N	8.2×10^{1}		HSDB (2015)	Q	99
	8.0×10^{1}		Zhang et al. (2010)	Q	287, 288
	1.7×10^{2}		Zhang et al. (2010)	Q	287, 289
	2.2×10^{3}		Zhang et al. (2010)	Q	287, 290
	2.9×10^{2}		Zhang et al. (2010)	Q	287, 291

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-chloro-3-nitrobenzenamine	1.8×10^{3}		HSDB (2015)	Q	99
$C_6H_5ClN_2O_2$	1.8×10^{3}		Zhang et al. (2010)	Q	287, 288
[635-22-3]	1.1×10^{3}		Zhang et al. (2010)	Q	287, 289
FOHHWGVAOVDVLP-UHFFFAOYSA-N	2.4×10^{3}		Zhang et al. (2010)	Q	287, 290
	3.5×10^{3}		Zhang et al. (2010)	Q	287, 291
botran	1.2×10^{2}		HSDB (2015)	V	
$C_6H_4Cl_2N_2O_2$	2.4×10^{3}		Zhang et al. (2010)	Q	287, 288
[99-30-9]	6.9×10^{1}		Zhang et al. (2010)	Q	287, 289
BIXZHMJUSMUDOQ-UHFFFAOYSA-N	1.7×10^{3}		Zhang et al. (2010)	Q	287, 290
	1.4×10^{3}		Zhang et al. (2010)	Q	287, 291
3,5-dichlorophenyl isocyanate	7.7×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_7H_3Cl_2NO$	2.8		Zhang et al. (2010)	Q	287, 289
[34893-92-0]	8.2×10^{-3}		Zhang et al. (2010)	Q	287, 290
XEFUJGURFLOFAN-UHFFFAOYSA-N	7.2×10^{-1}		Zhang et al. (2010)	Q	287, 291
2-chloro-5-nitrobenzoic acid $C_7H_4ClNO_4$ [2516-96-3] QUEKGYQTRJVEQC-UHFFFAOYSA-N	6.5×10^{3}		Abraham et al. (2019)	Q	
4-chloro-3-nitrobenzoic acid	3.6×10^{3}		Abraham et al. (2019)	Q	
$C_7H_4ClNO_4$	3.1×10^{4}		Zhang et al. (2010)	Q	287, 288
[96-99-1]	2.1×10^{3}		Zhang et al. (2010)	Q	287, 289
DFXQXFGFOLXAPO-UHFFFAOYSA-N	1.6×10^{3}		Zhang et al. (2010)	Q	287, 290
	9.2×10^{4}		Zhang et al. (2010)	Q	287, 291
1-chloro-4-isocyanatobenzene	5.7×10^{-2}		Zhang et al. (2010)	Q	287, 288
C_7H_4ClNO	4.1		Zhang et al. (2010)	Q	287, 289
[104-12-1]	9.7×10^{-3}		Zhang et al. (2010)	Q	287, 290
ADAKRBAJFHTIEW-UHFFFAOYSA-N	3.4		Zhang et al. (2010)	Q	287, 291
1,2-dichloro-4-isocyanatobenzene	7.7×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_7H_3Cl_2NO$	4.5		Zhang et al. (2010)	Q	287, 289
[102-36-3]	1.6×10^{-2}		Zhang et al. (2010)	Q	287, 290
MFUVCHZWGSJKEQ-UHFFFAOYSA-N	2.2		Zhang et al. (2010)	Q	287, 291
2-chloro-1-methyl-4-nitrobenzene	2.4×10^{-1}		HSDB (2015)	Q	545
$C_7H_6ClNO_2$	5.7×10^{-1}		Zhang et al. (2010)	Q	287, 288
[121-86-8]	3.4×10^{-1}		Zhang et al. (2010)	Q	287, 289
LLYXJBROWQDVMI-UHFFFAOYSA-N	3.7×10^{-1}		Zhang et al. (2010)	Q	287, 290
	2.5×10^{-1}		Zhang et al. (2010)	Q	287, 291
2,4-dichloro-3-methyl-6-nitrophenol	2.3		Zhang et al. (2010)	Q	287, 288
$C_7H_5Cl_2NO_3$	2.9		Zhang et al. (2010)	Q	287, 289
[39549-27-4]	9.5×10^{1}		Zhang et al. (2010)	Q	287, 290
VMBRJHMTAZXHES-UHFFFAOYSA-N	3.3×10^{-1}		Zhang et al. (2010)	Q	287, 291

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Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-chloro-5-methyl-2-nitrophenol $C_7H_6ClNO_3$ (4-chloro-6-nitro-*m*-cresol) [7147-89-9] JBMGJOKJUYGIJH-UHFFFAOYSA-N	3.6×10^{-1}		Schwarzenbach et al. (1988)	V	12
3-amino-2,5-dichlorobenzoic acid $C_7H_5Cl_2NO_2$ [133-90-4] HSSBORCLYSCBJR-UHFFFAOYSA-N	2.6×10^{5} 3.6 4.5×10^{5}		Duchowicz et al. (2020) Mackay et al. (2006d) Duchowicz et al. (2020)	V V Q	186
2,3,5,6-tetrachloro-4-nitroanisole $C_7H_3Cl_4NO_3$ (TCNA) [2438-88-2] BGPPUXMKKQMWLV-UHFFFAOYSA-N	5.2×10^{-1}		HSDB (2015)	Q	99
2,6-dichlorobenzamide $C_7H_5Cl_2NO$ [2008-58-4] JHSPCUHPSIUQRB-UHFFFAOYSA-N	8.2×10^{3}		HSDB (2015)	Q	99
swep $C_8H_7Cl_2NO$ [1918-18-9] WOZQBERUBLYCEG-UHFFFAOYSA-N	8.2×10^{2}		HSDB (2015)	Q	99
N-(4-chlorophenyl)acetamide C_8H_8ClNO (*p*-chloroacetanilide) [539-03-7] GGUOCFNAWIODMF-UHFFFAOYSA-N	2.1		HSDB (2015)	Q	99
methyl 5-chloro-2-nitrobenzoate $C_8H_6ClNO_4$ [51282-49-6] JGBJHRKCUKTQOE-UHFFFAOYSA-N	9.7×10^{1} 1.2×10^{2} 3.7×10^{3} 6.7×10^{1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
4-chloro-2,5-dimethoxynitrobenzene $C_8H_8ClNO_4$ [6940-53-0] ORLPGMKKCAEWOW-UHFFFAOYSA-N	1.8×10^{2} 1.6×10^{1} 2.0×10^{2} 3.9×10^{1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
chloraniformethan $C_9H_7Cl_5N_2O$ [20856-57-9] REEFSLKDEDEWAO-UHFFFAOYSA-N	$>2.3\times10^{10}$		MacBean (2012a)	?	

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monuron	1.7×10^{4}		HSDB (2015)	V	
$C_9H_{11}ClN_2O$	1.5×10^{4}		Mackay et al. (2006d)	V	
[150-68-5]	3.3×10^{2}		Suntio et al. (1988)	V	12
BMLIZLVNXIYGCK-UHFFFAOYSA-N	1.7×10^{4}		Burkhard and Guth (1981)	V	
	1.7×10^{4}		Abraham et al. (2019)	Q	
	1.7×10^{4}		MacBean (2012a)	?	
monolinuron	2.1×10^{2}		HSDB (2015)	V	
$C_9H_{11}ClN_2O_2$	1.7×10^{2}		Mackay et al. (2006d)	V	
[1746-81-2]					
LKJPSUCKSLORMF-UHFFFAOYSA-N					
diuron	3.5×10^{1}		Chao et al. (2017)	M	
$C_9H_{10}Cl_2N_2O$	2.0×10^{4}		HSDB (2015)	V	
[330-54-1]			Mackay et al. (2006d)	V	558
XMTQQYYKAHVGBJ-UHFFFAOYSA-N	8.3×10^{2}		Suntio et al. (1988)	V	12
	8.2		Barcelo and Hennion (1997)	X	567
	4.0×10^{4}		Abraham et al. (2019)	Q	
	5.2×10^{1}		Goodarzi et al. (2010)	Q	568
linuron	1.6×10^{3}		Duchowicz et al. (2020)	V	186
$C_9H_{10}Cl_2N_2O_2$			Mackay et al. (2006d)	V	558
[330-55-2]	1.9×10^{2}		Suntio et al. (1988)	V	12
XKJMBINCVNINCA-UHFFFAOYSA-N	5.0×10^{3}		MacBean (2012b)	X	350
	1.8		Barcelo and Hennion (1997)	X	567
	6.5		Duchowicz et al. (2020)	Q	
	2.2×10^{1}		Goodarzi et al. (2010)	Q	568, 571
propanil	1.3×10^{1}		Chao et al. (2017)	M	
$C_9H_9Cl_2NO$	5.8×10^{3}		Duchowicz et al. (2020)	V	186
[709-98-8]	5.8×10^{3}		HSDB (2015)	V	
LFULEKSKNZEWOE-UHFFFAOYSA-N	1.8×10^{2}		Mackay et al. (2006d)	V	
	2.8×10^{2}		Suntio et al. (1988)	V	12
	2.7		Barcelo and Hennion (1997)	X	567
	2.8		Duchowicz et al. (2020)	Q	
	2.2×10^{3}		Zhang et al. (2010)	Q	287, 288
	8.0×10^{2}		Zhang et al. (2010)	Q	287, 289
	3.8×10^{3}		Zhang et al. (2010)	Q	287, 290
	8.4×10^{3}		Zhang et al. (2010)	Q	287, 291
	1.2×10^{-1}		Goodarzi et al. (2010)	Q	568, 571
methazole	4.3×10^{1}		HSDB (2015)	V	
$C_9H_6Cl_2N_2O_3$	4.8×10^{4}		Hilal et al. (2008)	Q	
[20354-26-1]	4.3×10^{1}		MacBean (2012a)	?	
LRUUNMYPIBZBQH-UHFFFAOYSA-N					

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1,4-naphthalenedione, 2-amino-3-chloro- $C_{10}H_6ClNO_2$ (quinoclamine) [2797-51-5] OBLNWSCLAYSJJR-UHFFFAOYSA-N	3.3×10^{4}		Maniere et al. (2011)	?	241, 165
chlortoluron $C_{10}H_{13}ClN_2O$ (chlorotoluron) [15545-48-9] JXCGFZXSOMJFOA-UHFFFAOYSA-N	7.0×10^{4} 1.9×10^{4} 1.9×10^{2} 3.4×10^{1}		HSDB (2015) Mackay et al. (2006d) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V X Q	 567 568, 571
metoxuron $C_{10}H_{13}ClN_2O_2$ [19937-59-8] DSRNRYQBBJQVCW-UHFFFAOYSA-N	6.9×10^{2} 6.9×10^{2} 6.6 2.0×10^{2} 1.2×10^{1}		Duchowicz et al. (2020) Mackay et al. (2006d) Barcelo and Hennion (1997) Duchowicz et al. (2020) Goodarzi et al. (2010)	V V X Q Q	186 567 568
chlorpropham $C_{10}H_{12}ClNO_2$ [101-21-3] CWJSHJJYOPWUGX-UHFFFAOYSA-N	2.3×10^{1} 1.7×10^{1} 1.7×10^{1} 4.8×10^{2} 4.7×10^{1} 5.4×10^{-2} 2.9		Watanabe (1993) Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Duchowicz et al. (2020) Goodarzi et al. (2010)	M V V V V X Q Q	 186 558 12 567 568, 571
pyrazon $C_{10}H_8ClN_3O$ [1698-60-8] WYKYKTKDBLFHCY-UHFFFAOYSA-N	3.0×10^{4} 3.0×10^{4} 2.3×10^{-1} 2.3×10^{-1} 8.3×10^{4} 1.9×10^{9}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Duchowicz et al. (2020) Maniere et al. (2011)	V V V V Q ?	186 12 12, 165
2,4-D dimethylamine $C_{10}H_{13}Cl_2NO_3$ ((2,4-dichlorophenoxy)acetic acid dimethylamine) [2008-39-1] IUQJDHJVPLLKFL-UHFFFAOYSA-N	2.1×10^{10} 4.9×10^{1} 7.0×10^{10}		Duchowicz et al. (2020) Duchowicz et al. (2020) HSDB (2015)	V Q Q	186 99
3',4'- dichlorocyclopropanecarboxanilide $C_{10}H_9Cl_2NO$ (cypromid) [2759-71-9] PLQDLOBGKJCDSZ-UHFFFAOYSA-N	3.8×10^{3}		HSDB (2015)	Q	99

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Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
triazoxide $C_{10}H_6N_5OCl$ [72459-58-6] IQGKIPDJXCAMSM-UHFFFAOYSA-N	4.6×10^{5} 7.9×10^{5}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
chlorbufam $C_{11}H_{10}ClNO_2$ [1967-16-4] ULBXWWGWDPVHAO-UHFFFAOYSA-N	1.1×10^{3} 1.1×10^{3}		HSDB (2015) MacBean (2012a)	V ?	
zarilamid $C_{11}H_{11}N_2O_2Cl$ [84527-51-5] VLBZAQJMGULJIU-UHFFFAOYSA-N	1.5×10^{5}		MacBean (2012a)	?	
chloramphenicol $C_{11}H_{12}Cl_2N_2O_5$ [56-75-7] WIIZWVCIJKGZOK-IUCAKERBSA-N	4.3×10^{12}		HSDB (2015)	Q	99
cloethocarb $C_{11}H_{14}ClNO_4$ [51487-69-5] PITWUHDDNUVBPT-UHFFFAOYSA-N	5.0×10^{5}		MacBean (2012a)	?	
formetanate hydrochloride $C_{11}H_{16}ClN_3O_2$ [23422-53-9] MYPKGPZHHQEODQ-UHFFFAOYSA-N	4.3×10^{13} 2.0×10^{9}		HSDB (2015) Maniere et al. (2011)	Q ?	99 241, 165
cyclanilide $C_{11}H_9Cl_2NO_3$ [113136-77-9] GLWWLNJJJCTFMZ-UHFFFAOYSA-N	1.4×10^{4} 1.2×10^{4} 1.2×10^{5} 1.4×10^{4}		MacBean (2012b) Keshavarz et al. (2022) Duchowicz et al. (2020) Duchowicz et al. (2020)	X Q Q ?	350 185, 21
propachlor $C_{11}H_{14}ClNO$ [1918-16-7] MFOUDYKPLGXPGO-UHFFFAOYSA-N	2.7×10^{1} 9.1×10^{1} 9.1×10^{1} 9.0×10^{-1} 3.7×10^{-1}		HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V V X Q	 12 567 568
barban $C_{11}H_9Cl_2NO_2$ [101-27-9] MCOQHIWZJUDQIC-UHFFFAOYSA-N	8.4×10^{2} 8.2×10^{2} 8.5×10^{2} 3.3×10^{-1} 8.5×10^{2}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Duchowicz et al. (2020) MacBean (2012a)	V V V Q ?	186
aclonifen $C_{12}H_9ClN_2O_3$ [74070-46-5] DDBMQDADIHOWIC-UHFFFAOYSA-N	5.9×10^{2} 7.1×10^{3} 3.3×10^{2}		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	186 12, 165

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
propyzamide	1.0×10^{3}		Duchowicz et al. (2020)	V	186
$C_{12}H_{11}Cl_2NO$	5.2		HSDB (2015)	V	
(pronamide)	5.2×10^{-2}		Barcelo and Hennion (1997)	X	567
[23950-58-5]	1.5×10^{2}		Duchowicz et al. (2020)	Q	
PHNUZKMIPFFYSO-UHFFFAOYSA-N	6.6×10^{-2}		Goodarzi et al. (2010)	Q	568
	1.3×10^{8}		Maniere et al. (2011)	?	12, 165
			Mackay et al. (2006d)	W	736
2,4,6-trichlorophenyl 4-nitrophenyl ether	>8.1		Kawamoto and Urano (1989)	M	
$C_{12}H_6Cl_3NO_3$					
(chlornitrofen)					
[1836-77-7]					
XQNAUQUKWRBODG-UHFFFAOYSA-N					
nitrofen	3.3		HSDB (2015)	V	
$C_{12}H_7Cl_2NO_3$	3.9×10^{1}		Zhang et al. (2010)	Q	287, 288
[1836-75-5]	2.8×10^{1}		Zhang et al. (2010)	Q	287, 289
XITQUSLLOSKDTB-UHFFFAOYSA-N	1.2×10^{2}		Zhang et al. (2010)	Q	287, 290
	1.1×10^{2}		Zhang et al. (2010)	Q	287, 291
buturon	1.3×10^{4}		MacBean (2012a)	?	
$C_{12}H_{13}ClN_2O$					
[3766-60-7]					
BYYMILHAKOURNM-UHFFFAOYSA-N					
triclocarban	2.2×10^{5}		HSDB (2015)	Q	99
$C_{13}H_9Cl_3N_2O$	2.2×10^{5}		Zhang et al. (2010)	Q	287, 288
[101-20-2]	5.0×10^{3}		Zhang et al. (2010)	Q	287, 289
ICUTUKXCWQYESQ-UHFFFAOYSA-N	7.2×10^{7}		Zhang et al. (2010)	Q	287, 290
	1.8×10^{7}		Zhang et al. (2010)	Q	287, 291
dimethachlor	5.9×10^{3}		Maniere et al. (2011)	?	165
$C_{13}H_{18}ClNO_2$					
[50563-36-5]					
SCCDDNKJYDZXMM-UHFFFAOYSA-N					
3,5-dichloro-N-(3,4-dichlorophenyl)-2-hydroxybenzamide	2.1×10^{5}		HSDB (2015)	Q	99
$C_{13}H_7Cl_4NO_2$	2.1×10^{5}		Zhang et al. (2010)	Q	287, 288
[1154-59-2]	2.3×10^{5}		Zhang et al. (2010)	Q	287, 289
SJQBHPJLLIJASD-UHFFFAOYSA-N	3.9×10^{6}		Zhang et al. (2010)	Q	287, 290
	1.6×10^{5}		Zhang et al. (2010)	Q	287, 291
procymidone	8.5×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{13}H_{11}Cl_2NO_2$	8.5×10^{-1}		Mackay et al. (2006d)	V	
[32809-16-8]	9.0×10^{-3}		Barcelo and Hennion (1997)	X	567
QXJKBPAVAHBARF-UHFFFAOYSA-N	9.7×10^{-1}		Duchowicz et al. (2020)	Q	
	1.4×10^{-2}		Goodarzi et al. (2010)	Q	568

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
melphalan $C_{13}H_{18}Cl_2N_2O_2$ [148-82-3] SGDBTWWWUNNDEQ-LBPRGKRZSA-N	2.3×10^{7}		HSDB (2015)	Q	99
niclosamide $C_{13}H_8Cl_2N_2O_4$ [50-65-7] RJMUSRYZPJIFPJ-UHFFFAOYSA-N	1.5×10^{4}		HSDB (2015)	V	
iprodione $C_{13}H_{13}Cl_2N_3O_3$ [36734-19-7] ONUFESLQCSAYKA-UHFFFAOYSA-N	7.1×10^{2}		Barcelo and Hennion (1997)	X	567
	4.0×10^{4}		Keshavarz et al. (2022)	Q	
	9.5×10^{3}		Duchowicz et al. (2020)	Q	
	2.0×10^{1}		Goodarzi et al. (2010)	Q	568, 569
	3.2×10^{3}		Duchowicz et al. (2020)	?	185, 21
zoxamide $C_{14}H_{16}Cl_3NO_2$ [156052-68-5] SOUGWDPPRBKJEX-UHFFFAOYSA-N	4.9×10^{3}		HSDB (2015)	Q	99
	$>1.5\times10^{2}$		Maniere et al. (2011)	?	241, 165
fenhexamid $C_{14}H_{17}Cl_2NO_2$ [126833-17-8] VDLGAVXLJYLFDH-UHFFFAOYSA-N	2.0×10^{5}		MacBean (2012b)	X	350
	2.0×10^{5}		Maniere et al. (2011)	?	12, 493, 165
	3.3×10^{6}		Maniere et al. (2011)	?	12, 573, 165
	1.1×10^{5}		Maniere et al. (2011)	?	12, 570, 165
chlorambucil $C_{14}H_{19}Cl_2NO_2$ [305-03-3] JCKYGMPEJWAADB-UHFFFAOYSA-N	3.7×10^{4}		HSDB (2015)	Q	99
2-chloro-N-(ethoxymethyl)-N-(2-ethyl-6-methylphenyl)acetamide $C_{14}H_{20}ClNO_2$ (acetochlor) [34256-82-1] VTNQPKFIQCLBDU-UHFFFAOYSA-N	3.7×10^{4}		HSDB (2015)	V	
alachlor $C_{14}H_{20}ClNO_2$ [15972-60-8] XCSGPAVHZFQHGE-UHFFFAOYSA-N	6.7×10^{2}		Muir et al. (2004)	L	367
	9.9×10^{2}		Muir et al. (2004)	L	366
	7.4		Chao et al. (2017)	M	
	1.4×10^{2}	9200	Gautier et al. (2003)	M	
	9.0×10^{2}		Fendinger et al. (1989)	M	72
	1.2×10^{3}		Fendinger and Glotfelty (1988)	M	72
	4.5×10^{2}		Mackay et al. (2006d)	V	
	1.6×10^{2}		Suntio et al. (1988)	V	12
	3.1×10^{2}		Glotfelty et al. (1987)	V	
	1.6		Barcelo and Hennion (1997)	X	567

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.6×10^{-2}		Goodarzi et al. (2010)	Q	568, 569
	3.1×10^{3}		Hilal et al. (2008)	Q	
	4.5×10^{1}		Modarresi et al. (2007)	Q	67
		11000	Kühne et al. (2005)	Q	
	8.2×10^{4}		Meylan and Howard (1991)	Q	
		9300	Kühne et al. (2005)	?	
	3.1×10^{2}		Chesters et al. (1989)	?	
bifenox $C_{14}H_9Cl_2NO_3$ [42576-02-3] SUSRORUBZHMPCO-UHFFFAOYSA-N	9.1×10^{1}		Duchowicz et al. (2020)	V	186
	3.7		HSDB (2015)	V	
	3.2		Mackay et al. (2006d)	V	
	3.3×10^{-2}		Barcelo and Hennion (1997)	X	567
	6.2×10^{3}		Duchowicz et al. (2020)	Q	
	3.5×10^{-2}		Goodarzi et al. (2010)	Q	568, 571
	$<6.2\times10^{3}$		Maniere et al. (2011)	?	12, 165
S-metolachlor $C_{15}H_{22}ClNO_2$ [87392-12-9] WVQBLGZPHOPPFO-LBPRGKRZSA-N	4.5×10^{2}		Maniere et al. (2011)	?	165
metolachlor $C_{15}H_{22}ClNO_2$ [51218-45-2] WVQBLGZPHOPPFO-UHFFFAOYSA-N	7.5×10^{2}		Muir et al. (2004)	L	367
	7.2×10^{2}		Muir et al. (2004)	L	366
	6.2×10^{2}	15000	Fogg and Sangster (2003)	L	
	2.1×10^{2}	10000	Feigenbrugel et al. (2004a)	M	
	1.3×10^{2}		Rice et al. (1997b)	M	12
	5.7×10^{2}	15000	Lau et al. (1995)	M	737
	4.3×10^{2}		Mackay et al. (2006d)	V	
	4.1×10^{2}		Otto et al. (1997)	V	
	1.1×10^{3}		Glotfelty et al. (1987)	V	
	1.1×10^{3}		Burkhard and Guth (1981)	V	
	1.1×10^{1}		Barcelo and Hennion (1997)	X	567
	1.2×10^{3}		Rice et al. (1997b)	C	
	7.9×10^{-2}		Goodarzi et al. (2010)	Q	568
	6.2×10^{3}		Hilal et al. (2008)	Q	
	1.7×10^{2}		Modarresi et al. (2007)	Q	67
		12000	Kühne et al. (2005)	Q	
		10000	Kühne et al. (2005)	?	
	1.1×10^{3}		Chesters et al. (1989)	?	12
clonitralid $C_{15}H_{15}Cl_2N_3O_5$ [1420-04-8] XYCDHXSQODHSLG-UHFFFAOYSA-N	$>2.6\times10^{4}$		HSDB (2015)	V	
chloroxuron $C_{15}H_{15}ClN_2O_2$ [1982-47-4] IVUXTESCPZUGJC-UHFFFAOYSA-N	2.4×10^{4}		HSDB (2015)	V	
	5.3×10^{4}		MacBean (2012a)	?	

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Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
CGA 80000 $C_{15}H_{18}ClNO_4$ [67932-85-8] FHZMAAGOSXDIBJ-UHFFFAOYSA-N	4.4×10^{6}		MacBean (2012a)	?	
oxadiargyl $C_{15}H_{14}N_2O_3Cl_2$ [39807-15-3] DVOODWOZJVJKQR-UHFFFAOYSA-N	4.3×10^{2} 8.2×10^{1}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
diniconazole $C_{15}H_{17}Cl_2N_3O$ [83657-24-3] FBOUIAKEJMZPQG-UHFFFAOYSA-N	2.5×10^{1} 2.8×10^{2}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
pethoxamid $C_{16}H_{22}ClNO_2$ [106700-29-2] CSWIKHNSBZVWNQ-UHFFFAOYSA-N	8.5×10^{2}		Maniere et al. (2011)	?	12, 165
pigment red 4 $C_{16}H_{10}ClN_3O_3$ [2814-77-9] XLTMWFMRJZDFFD-VHEBQXMUSA-N	1.1×10^{7}		HSDB (2015)	Q	99
darendoside b $C_{17}H_{15}Cl_2N_5O_2$ [13301-61-6] KHZRTXVUEZJYNE-UHFFFAOYSA-N	2.7×10^{7} 5.0×10^{6} 2.5×10^{7} 7.3×10^{4}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
butenachlor $C_{17}H_{24}NO_2Cl$ [87310-56-3] HZDIJTXDRLNTIS-DAXSKMNVSA-N	1.0×10^{2}		MacBean (2012a)	?	
butachlor $C_{17}H_{26}ClNO_2$ [23184-66-9] HKPHPIREJKHECO-UHFFFAOYSA-N	1.6×10^{2} 1.2×10^{2} 6.9×10^{2} 1.7×10^{2}		Watanabe (1993) Mackay et al. (2006d) Hilal et al. (2008) Modarresi et al. (2007)	M V Q Q	 67
pretilachlor $C_{17}H_{26}ClNO_2$ [51218-49-6] YLPGTOIOYRQOHV-UHFFFAOYSA-N	4.5×10^{3} 1.8×10^{2}		Hilal et al. (2008) Modarresi et al. (2007)	Q Q	 67
halofenozide $C_{18}H_{19}ClN_2O_2$ [112226-61-6] CNKHSLKYRMDDNQ-UHFFFAOYSA-N	2.7×10^{5}		HSDB (2015)	Q	99

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Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
benzoximate $C_{18}H_{18}ClNO_5$ [29104-30-1] BZMIHNKNQJJVRO-UHFFFAOYSA-N	1.8×10^2 1.5×10^5		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
pencycuron $C_{19}H_{21}ClN_2O$ [66063-05-6] OGYFATSSENRIKG-UHFFFAOYSA-N	2.0×10^6		Maniere et al. (2011)	?	12, 165
valifenalate $C_{19}H_{27}ClN_2O_5$ [283159-90-0] DBXFMOWZRXXBRN-LWKPJOBUSA-N	6.2×10^5		Maniere et al. (2011)	?	12, 738, 165
pyrazoxyfen $C_{20}H_{16}Cl_2N_2O_3$ [71561-11-0] FKERUJTUOYLBKB-UHFFFAOYSA-N	4.7×10^4 1.9×10^4		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
α-cypermethrin $C_{22}H_{19}Cl_2NO_3$ [67375-30-8] KAATUXNTWXVJKI-DXCJPMOASA-N	1.0 1.0×10^2 1.9×10^1		HSDB (2015) Mackay et al. (2006d) Maniere et al. (2011)	V V ?	 12, 165
cypermethrin-β $C_{22}H_{19}Cl_2NO_3$ [1224510-29-5] KAATUXNTWXVJKI-FLXSOZOKSA-N	5.6×10^1		Ebert et al. (2023)	?	318
β-cypermethrin $C_{22}H_{19}Cl_2NO_3$ [65731-84-2] KAATUXNTWXVJKI-NSHGMRRFSA-N			Mackay et al. (2006d)	V	558
δ-cypermethrin $C_{22}H_{19}Cl_2NO_3$ (cypermethrin; alphamethrin) [52315-07-8] KAATUXNTWXVJKI-UHFFFAOYSA-N	4.1×10^1 4.3×10^2 1.2×10^1 2.5×10^1 1.0×10^1 4.2×10^1 5.0×10^7		HSDB (2015) Mackay et al. (2006d) Siebers and Mattusch (1996) Barcelo and Hennion (1997) Goodarzi et al. (2010) Maniere et al. (2011) Maniere et al. (2011)	V V V X Q ? ?	 12 567 568, 569 12, 165 241, 165
θ-cypermethrin $C_{22}H_{19}Cl_2NO_3$ [71697-59-1] KAATUXNTWXVJKI-GGPKGHCWSA-N	6.1×10^2		Ebert et al. (2023)	?	318

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ζ-cypermethrin $C_{22}H_{19}Cl_2NO_3$ [1315501-18-8] KAATUXNTWXVJKI-QPIRBTGLSA-N	4.3×10^{2}		Ebert et al. (2023)	?	365
ochratoxin C $C_{22}H_{22}ClNO_6$ [4865-85-4] BPZZWRPHVVDAPT-PXAZEXFGSA-N	7.6×10^{8}		HSDB (2015)	Q	99
quizalofop-p-tefuryl $C_{22}H_{21}N_2O_5Cl$ [119738-06-6] BBKDWPHJZANJGB-UHFFFAOYSA-N	1.8×10^{4} 3.4×10^{6}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
mandipropamid $C_{23}H_{22}ClNO_4$ [374726-62-2] KWLVWJPJKJMCSH-UHFFFAOYSA-N	1.1×10^{4} $>1.1\times10^{4}$		HSDB (2015) Maniere et al. (2011)	V ?	 165
fenvalerate $C_{25}H_{22}ClNO_3$ [51630-58-1] NYPJDWWKZLNGGM-UHFFFAOYSA-N	2.9×10^{2} 2.9×10^{2} 4.7×10^{1} 7.0×10^{1} 3.2×10^{3}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Cotham and Bidleman (1989) Duchowicz et al. (2020)	V V V V Q	186
esfenvalerate $C_{25}H_{22}ClNO_3$ [66230-04-4] NYPJDWWKZLNGGM-ZEQRLZLVSA-N	2.4×10^{1} 2.4×10^{1} 3.2×10^{3} 2.0×10^{3}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Maniere et al. (2011)	V V Q ?	186 241, 165
clopyralid $C_6H_3Cl_2NO_2$ [1702-17-6] HUBANNPOLNYSAD-UHFFFAOYSA-N	3.3×10^{3} 3.2×10^{2} 1.8×10^{3} 3.6×10^{1} 3.0×10^{9} 4.5×10^{10} 6.2×10^{10} 5.6×10^{10}		Duchowicz et al. (2020) Barcelo and Hennion (1997) Duchowicz et al. (2020) Goodarzi et al. (2010) Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011)	V X Q Q ? ? ? ?	186 567 568 12, 165 12, 570, 165 12, 573, 165 12, 493, 165
picloram $C_6H_3Cl_3N_2O_2$ [1918-02-1] NQQVFXUMIDALNH-UHFFFAOYSA-N	3.0×10^{4} 2.9×10^{4} 2.9×10^{2} 7.7×10^{6} 2.5 9.0×10^{4} 1.6×10^{8} 1.1×10^{3}		Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Goodarzi et al. (2010)	V V X Q Q Q Q Q	 12 567 287, 288 287, 289 287, 290 287, 291 568, 571

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.1×10^4		Maniere et al. (2011)	?	241, 165
aminopyralid $C_6H_4Cl_2N_2O_2$ [150114-71-9] NIXXQNOQHKNPEJ-UHFFFAOYSA-N	5.8×10^6 1.0×10^{11}		HSDB (2015) Maniere et al. (2011)	Q ?	99 241, 493, 165
3,4,5,6-tetrachloropyridine-2-carboxylic acid $C_6HCl_4NO_2$ [10469-09-7] GXFRQLQUKBSYQL-UHFFFAOYSA-N	3.7×10^3 2.4 1.2×10^2 4.1×10^4		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
[(3,5,6-trichloro-2-pyridinyl)oxy]-acetic acid $C_7H_4Cl_3NO_3$ (triclopyr) [55335-06-3] REEQLXCGVXDJSQ-UHFFFAOYSA-N	1.0×10^4 1.0×10^4 1.2×10^4 3.2×10^3 1.1×10^4 2.1×10^5 2.3×10^5		Duchowicz et al. (2020) HSDB (2015) Armbrust (2000) Duchowicz et al. (2020) Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011)	V V C Q ? ? ?	186 12, 165 12, 570, 165 12, 493, 165
clopidol $C_7H_7Cl_2NO$ [2971-90-6] ZDPIZLCVJAAHHR-UHFFFAOYSA-N	9.9×10^3		HSDB (2015)	Q	99
[(3,5,6-trichloro-2-pyridinyl)oxy]-acetic acid, methyl ester $C_8H_6Cl_3NO_3$ [60825-26-5] MNYBZEHWPRTNJY-UHFFFAOYSA-N	6.0 3.1×10^1 4.6×10^3 3.5×10^2		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
aminocyclopyrachlor $C_8H_8ClN_3O_2$ [858956-08-8] KWAIHLIXESXTJL-UHFFFAOYSA-N	1.3×10^7		Ebert et al. (2023)	?	318
uracil mustard $C_8H_{11}Cl_2N_3O_2$ [66-75-1] IDPUKCWIGUEADI-UHFFFAOYSA-N	2.5×10^7		HSDB (2015)	Q	99

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
imidacloprid $C_9H_{10}ClN_5O_2$ [138261-41-3] YWTYJOPNNQFBPC-UHFFFAOYSA-N	4.9×10^9 5.9×10^9		Armbrust (2000) Maniere et al. (2011)	C ?	 12, 165
ethyl [(3,5,6-trichloro-2-pyridinyl)oxy]acetate $C_9H_8Cl_3NO_3$ [60825-27-6] KXAVVWXJUDQGDA-UHFFFAOYSA-N	4.5 1.7×10^1 2.3×10^1 3.1×10^2		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
N-methyl-3,4,5,6-tetrachlorophthalimide $C_9H_3Cl_4NO_2$ [14737-80-5] OHCSZUQRNNNMRG-UHFFFAOYSA-N	1.5×10^3 1.2×10^3 4.1×10^1 3.1×10^3		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
terbacil $C_9H_{13}ClN_2O_2$ [5902-51-2] NBQCNZYJJMBDKY-UHFFFAOYSA-N	5.2×10^4 6.5×10^4 7.9×10^4 5.6×10^4 5.5×10^2 4.4×10^2		HSDB (2015) Mackay et al. (2006d) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V V V X Q	 12 567 568
eglinazine-ethyl $C_9H_{14}ClN_5O_2$ [6616-80-4] YESXTECNXIKUMM-UHFFFAOYSA-N	4.1×10^4		Ebert et al. (2023)	?	318
proglinazine ethyl ester $C_{10}H_{16}ClN_5O_2$ [68228-18-2] QQADVTSTCZBBOE-UHFFFAOYSA-N	1.0×10^4		Ebert et al. (2023)	?	318
triforine $C_{10}H_{14}Cl_6N_4O_2$ [26644-46-2] RROQIUMZODEXOR-UHFFFAOYSA-N	2.6×10^3 2.6×10^3		HSDB (2015) Mackay et al. (2006d)	V V	
drazoxolon $C_{10}H_8ClN_3O_2$ [5707-69-7] OOTHTARUZHONSW-UHFFFAOYSA-N	1.4×10^2		Ebert et al. (2023)	?	318
anagrelide $C_{10}H_7Cl_2N_3O$ [68475-42-3] OTBXOEAOVRKTNQ-UHFFFAOYSA-N	3.7×10^7		HSDB (2015)	Q	99

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
fenpiclonil $C_{11}H_6Cl_2N_2$ [74738-17-3] FKLFBQCQQYDUAM-UHFFFAOYSA-N	1.8×10^3 5.4×10^2 1.9×10^3		Duchowicz et al. (2020) Duchowicz et al. (2020) MacBean (2012a)	V Q ?	186
benoxacor $C_{11}H_{11}Cl_2NO_2$ [98730-04-2] PFJJMJDEVDLPNE-UHFFFAOYSA-N	1.3×10^2 2.9×10^2 1.3×10^2		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	186 12, 165
ethychlozate $C_{11}H_{11}ClN_2O_2$ [27512-72-7] GLPZEHFBLBYFHN-UHFFFAOYSA-N	1.6×10^4		Ebert et al. (2023)	?	318
quinmerac $C_{11}H_8ClNO_2$ [90717-03-6] ALZOLUNSQWINIR-UHFFFAOYSA-N	1.0×10^{10}		Maniere et al. (2011)	?	241, 165
quinonamid $C_{12}H_6Cl_3NO_3$ [27541-88-4] ZIEWAMOXCOLNSJ-UHFFFAOYSA-N	8.0×10^2		Ebert et al. (2023)	?	365
fenchlorazole-ethyl $C_{12}H_8N_3O_2Cl_5$ [103112-35-2] GMBRUAIJEFRHFQ-UHFFFAOYSA-N	2.7×10^3		MacBean (2012a)	?	12
vinclozoline $C_{12}H_9Cl_2NO_3$ (vinclozolin) [50471-44-8] FSCWZHGZWWDELK-UHFFFAOYSA-N	5.8×10^2 2.6×10^5 9.1×10^1 7.6 1.7		HSDB (2015) Mackay et al. (2006d) Siebers et al. (1994) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V V X Q	 567 568
forchlorfenuron $C_{12}H_{10}ClN_3O$ [68157-60-8] GPXLRLUVLMHHIK-UHFFFAOYSA-N	3.4×10^6 3.5×10^6 1.7×10^1 3.4×10^6		Duchowicz et al. (2020) MacBean (2012b) Duchowicz et al. (2020) Maniere et al. (2011)	V X Q ?	186 350 241, 165
azaconazole $C_{12}H_{11}Cl_2N_3O_2$ [60207-31-0] AKNQMEBLVAMSNZ-UHFFFAOYSA-N	5.1×10^4		Ebert et al. (2023)	?	318
myclozolin $C_{12}H_{11}NO_4Cl_2$ [54864-61-8] FTCOKXNKPOUEFH-UHFFFAOYSA-N	3.7×10^2		MacBean (2012a)	?	

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
triclopyr-butotyl $C_{13}H_{16}Cl_3NO_4$ [64700-56-7] IVDRCZNHVGQBHZ-UHFFFAOYSA-N	3.4×10^{2}		Maniere et al. (2011)	?	12, 165
clofencet $C_{13}H_{11}ClN_2O_3$ [129025-54-3] PIZCXVUFSNPNON-UHFFFAOYSA-N	$>1.9\times10^{8}$ $>2.3\times10^{10}$		HSDB (2015) MacBean (2012a)	V ?	
chlozolinate $C_{13}H_{11}NO_5Cl_2$ [84332-86-5] IGUYEXXAGBDLLX-UHFFFAOYSA-N	7.6×10^{3} 4.7×10^{2} 2.8×10^{1} 2.8×10^{1} 4.4×10^{2}		Duchowicz et al. (2020) Duchowicz et al. (2020) Duchowicz et al. (2020) Duchowicz et al. (2020) MacBean (2012a)	V V Q Q ?	186 186
monalide $C_{13}H_{18}ClNO$ [7287-36-7] KXGYBSNVFXBPNO-UHFFFAOYSA-N	4.0×10^{2}		MacBean (2012a)	?	
chlomethoxyfen $C_{13}H_9Cl_2NO_4$ [32861-85-1] DXXVCXKMSWHGTF-UHFFFAOYSA-N	5.1×10^{-1}		Ebert et al. (2023)	?	318
metazachlor $C_{14}H_{16}ClN_3O$ [67129-08-2] STEPQTYSZVCJPV-UHFFFAOYSA-N	1.3×10^{1} 3.5×10^{2} 7.1×10^{3} 1.7×10^{4}		Barcelo and Hennion (1997) Goodarzi et al. (2010) Modarresi et al. (2007) Maniere et al. (2011)	X Q Q ?	567 568 67 12, 165
etaconazole $C_{14}H_{15}Cl_2N_3O_2$ [60207-93-4] DWRKFAJEBUWTQM-UHFFFAOYSA-N	7.9×10^{3}		MacBean (2012a)	?	
triadimenol $C_{14}H_{18}ClN_3O_2$ [55219-65-3] BAZVSMNPJJMILC-UHFFFAOYSA-N	7.6×10^{6} 3.8×10^{6} 4.5×10^{5}		HSDB (2015) Mackay et al. (2006d) Maniere et al. (2011)	V V ?	 241, 165
hexaconazole $C_{14}H_{17}Cl_2N_3O$ [79983-71-4] STMIIPIFODONDC-UHFFFAOYSA-N	2.8×10^{1} 6.0×10^{1}		Barcelo and Hennion (1997) Goodarzi et al. (2010)	X Q	567 568
triadimefon $C_{14}H_{16}ClN_3O_2$ [43121-43-3] WURBVZBTWMNKQT-UHFFFAOYSA-N	1.2×10^{5} 1.2×10^{5} 1.2×10^{5} 1.5×10^{2}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Duchowicz et al. (2020)	V V V Q	186

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
imazalil $C_{14}H_{14}Cl_2N_2O$ [35554-44-0] PZBPKYOVPCNPJY-UHFFFAOYSA-N	3.8×10^3 5.1×10^5 9.3×10^3		HSDB (2015) Mackay et al. (2006d) Maniere et al. (2011)	V V ?	 241, 165
pyrifenox $C_{14}H_{12}Cl_2N_2O$ [88283-41-4] CKPCAYZTYMHQEX-UHFFFAOYSA-N	2.3×10^2		Ebert et al. (2023)	?	318
chlorphthalim $C_{14}H_{12}ClNO_2$ [39985-63-2] MJQBFSWPMMHVSM-UHFFFAOYSA-N	5.1×10^2		Ebert et al. (2023)	?	318
cyprofuram $C_{14}H_{14}ClNO_3$ [69581-33-5] KRZUZYJEQBXUIN-UHFFFAOYSA-N	3.1×10^5		Ebert et al. (2023)	?	316
ofurace $C_{14}H_{16}ClNO_3$ [58810-48-3] OWDLFBLNMPCXSD-UHFFFAOYSA-N	1.1×10^4		Ebert et al. (2023)	?	318
triadimenol B $C_{14}H_{18}ClN_3O_2$ [82200-72-4]	1.1×10^5		Ebert et al. (2023)	?	365
triadimenol A $C_{14}H_{18}ClN_3O_2$ [89482-17-7]	1.3×10^5		Ebert et al. (2023)	?	318
propiconazole $C_{15}H_{17}Cl_2N_3O_2$ [60207-90-1] STJLVHWMYQXCPB-UHFFFAOYSA-N	1.1×10^4 5.7×10^3 2.5×10^3 2.4×10^1 3.1×10^1		HSDB (2015) Mackay et al. (2006d) Siebers et al. (1994) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V V X Q	 567 568, 571
clonazepam $C_{15}H_{10}ClN_3O_3$ [1622-61-3] DGBIGWXXNGSACT-UHFFFAOYSA-N	1.4×10^7		HSDB (2015)	Q	99
oxazepam $C_{15}H_{12}ClN_2O_2$ [604-75-1] ADIMAYPTOBDMTL-UHFFFAOYSA-N	1.8×10^4		HSDB (2015)	Q	99

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
oxadiazon $C_{15}H_{18}Cl_2N_2O_3$ [19666-30-9] CHNUNORXWHYHNE-UHFFFAOYSA-N	1.4×10^{2} 1.4×10^{2}		HSDB (2015) Armbrust (2000)	V C	
cyproconazole $C_{15}H_{18}ClN_3O$ [94361-06-5] UFNOUKDBUJZYDE-UHFFFAOYSA-N	1.4×10^{4} 1.3×10^{2} 3.4×10^{2} 2.0×10^{4}		HSDB (2015) Barcelo and Hennion (1997) Goodarzi et al. (2010) Maniere et al. (2011)	V X Q ?	 567 568 241, 165
diclobutrazol $C_{15}H_{19}Cl_2N_3O$ [75736-33-3] URDNHJIVMYZFRT-UHFFFAOYSA-N	8.0×10^{3}		MacBean (2012a)	?	
paclobutrazol $C_{15}H_{20}ClN_3O$ [76738-62-0] RMOGWMIKYWRTKW-UHFFFAOYSA-N	4.2×10^{4}		Maniere et al. (2011)	?	241, 165
prochloraz $C_{15}H_{16}Cl_3N_3O_2$ [67747-09-5] TVLSRXXIMLFWEO-UHFFFAOYSA-N	6.0×10^{2} 5.8 6.4×10^{3} 5.9×10^{-1} 6.1×10^{2}		Duchowicz et al. (2020) Barcelo and Hennion (1997) Duchowicz et al. (2020) Goodarzi et al. (2010) Maniere et al. (2011)	V X Q Q ?	186 567 568 241, 165
cis-propiconazole $C_{15}H_{17}Cl_2N_3O_2$ [112721-87-6]	1.2×10^{4}		Ebert et al. (2023)	?	318
trans-propiconazole $C_{15}H_{17}Cl_2N_3O_2$ [120523-07-1]	7.8×10^{3}		Ebert et al. (2023)	?	318
fenoxanil $C_{15}H_{18}Cl_2N_2O_2$ [115852-48-7] IUOKJNROJISWRO-UHFFFAOYSA-N	5.0×10^{6}		Ebert et al. (2023)	?	318
carpropamid $C_{15}H_{18}Cl_3NO$ [104030-54-8] RXDMAYSSBPYBFW-UHFFFAOYSA-N	8.4×10^{2}		Ebert et al. (2023)	?	318
propisochlor $C_{15}H_{22}ClNO_2$ [86763-47-5] KZNDFYDURHAESM-UHFFFAOYSA-N	5.6×10^{1}		Ebert et al. (2023)	?	318

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
mefenpyr-diethyl $C_{16}H_{18}Cl_2N_2O_4$ [135590-91-9] OPGCOAPTHCZZIW-UHFFFAOYSA-N	3.8×10^3 8.5×10^3		Maniere et al. (2011) Maniere et al. (2011)	? ?	165 12, 165
diazepam $C_{16}H_{13}ClN_2O$ [439-14-5] AAOVKJBEBIDNHE-UHFFFAOYSA-N	2.7×10^3		HSDB (2015)	Q	99
bendamustine $C_{16}H_{21}Cl_2N_3O_2$ [16506-27-7] YTKUWDBFDASYHO-UHFFFAOYSA-N	2.5×10^7		HSDB (2015)	Q	99
fentrazamide $C_{16}H_{20}ClN_5O_2$ [158237-07-1] LLQPHQFNMLZJMP-UHFFFAOYSA-N	5.1×10^4		Ebert et al. (2023)	?	318
piperalin $C_{16}H_{21}Cl_2NO_2$ [3478-94-2] BZGLBXYQOMFXAU-UHFFFAOYSA-N	4.3×10^2		HSDB (2015)	Q	99
tebuconazole $C_{16}H_{22}ClN_3O$ [107534-96-3] PXMNMQRDXWABCY-UHFFFAOYSA-N	7.0×10^4 1.1×10^3 2.2×10^2 1.0×10^5		HSDB (2015) Barcelo and Hennion (1997) Goodarzi et al. (2010) Maniere et al. (2011)	V X Q ?	 567 568, 571 12, 165
diethatyl-ethyl $C_{16}H_{22}ClNO_3$ [38727-55-8] WFKSADNZWSKCRZ-UHFFFAOYSA-N	7.9×10^2		Ebert et al. (2023)	?	318
fenarimol $C_{17}H_{12}Cl_2N_2O$ [60168-88-9] NHOWDZOIZKMVAI-UHFFFAOYSA-N	1.4×10^3 1.4×10^3 7.8×10^5		Duchowicz et al. (2020) Mackay et al. (2006d) Duchowicz et al. (2020)	V V Q	186
cumyluron $C_{17}H_{19}ClN_2O$ [99485-76-4] VYNOULHXXDFBLU-UHFFFAOYSA-N	2.5×10^6		Ebert et al. (2023)	?	318
triticonazole $C_{17}H_{20}N_3OCl$ [131983-72-7] PPDBOQMNKNNODG-ZROIWOOFSA-N	6.6×10^4 3.3×10^4		HSDB (2015) Maniere et al. (2011)	Q ?	99 241, 165

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
furametpyr $C_{17}H_{20}ClN_3O_2$ [123572-88-3] NRTLIYOWLVMQBO-UHFFFAOYSA-N	6.0×10^6		Ebert et al. (2023)	?	318
metconazole $C_{17}H_{22}ClN_3O$ [125116-23-6] XWPZUHJBOLQNMN-UHFFFAOYSA-N	3.8×10^3 1.3×10^3 4.5×10^6		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	186 12, 165
tepraloxydim $C_{17}H_{24}ClNO_4$ [149979-41-9] IOYNQIMAUDJVEI-BMVIKAAMSA-N	5.2×10^4		Ebert et al. (2023)	?	318
cloquintocet-mexyl $C_{18}H_{22}ClNO_3$ [99607-70-2] COYBRKAVBMYYSF-UHFFFAOYSA-N	1.2×10^4 3.4×10^2 3.3×10^2		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	186 165
fenoxaprop-p-ethyl $C_{18}H_{16}ClNO_5$ [71283-80-2] PQKBPHSEKWERTG-LLVKDONJSA-N	6.2×10^2 2.3×10^3 3.7×10^3		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	186 12, 165
ipconazole $C_{18}H_{24}ClN_3O$ [125225-28-7] QTYCMDBMOLSEAM-UHFFFAOYSA-N	3.9×10^3 1.3×10^3 3.3×10^4		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	186 241, 165
pyriofenone $C_{18}H_{20}ClNO_5$ [688046-61-9] NMVCBWZLCXANER-UHFFFAOYSA-N	5.3×10^3		Maniere et al. (2011)	?	241, 165
cintofen $C_{18}H_{15}ClN_2O_5$ (sintofen) [130561-48-7] QLMNCUHSDAGQGT-UHFFFAOYSA-N	1.4×10^7 5.4×10^9 6.1×10^9		Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011)	? ? ?	12, 577, 165 12, 573, 165 12, 493, 165
boscalid $C_{18}H_{12}Cl_2N_2O$ [188425-85-6] WYEMLYFITZORAB-UHFFFAOYSA-N	1.9×10^4 1.9×10^4		MacBean (2012b) Maniere et al. (2011)	X ?	350 241, 165

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tebufenpyrad	$>8.2\times10^2$		HSDB (2015)	V	
$C_{18}H_{24}ClN_3O$	$>9.1\times10^2$		Maniere et al. (2011)	?	241, 165
[119168-77-3]					
ZZYSLNWGKKDOML-UHFFFAOYSA-N					
8,9,10,11-tetrachloro-12-phthaloperinone	4.8×10^5		Zhang et al. (2010)	Q	287, 288
$C_{18}H_6Cl_4N_2O$	7.5×10^9		Zhang et al. (2010)	Q	287, 289
[20749-68-2]	5.7×10^3		Zhang et al. (2010)	Q	287, 290
UBZVRROHBDDCQY-UHFFFAOYSA-N	1.9×10^5		Zhang et al. (2010)	Q	287, 291
pigment red 254	3.4×10^9		Zhang et al. (2010)	Q	287, 288
$C_{18}H_{10}Cl_2N_2O_2$	3.9×10^6		Zhang et al. (2010)	Q	287, 289
[84632-65-5]	1.9×10^{13}		Zhang et al. (2010)	Q	287, 290
JNNHVXMCVRYTTN-UHFFFAOYSA-N	2.2×10^{12}		Zhang et al. (2010)	Q	287, 291
fenoxaprop-ethyl	6.2×10^2		Ebert et al. (2023)	?	316
$C_{18}H_{16}ClNO_5$					
[66441-23-4]					
PQKBPHSEKWERTG-UHFFFAOYSA-N					
benzoylprop-ethyl	1.2×10^4		Ebert et al. (2023)	?	739
$C_{18}H_{17}Cl_2NO_3$					
[22212-55-1]					
SLCGUGMPSUYJAY-UHFFFAOYSA-N					
difenoconazole	1.1×10^6		Duchowicz et al. (2020)	V	186
$C_{19}H_{17}Cl_2N_3O_3$	6.6×10^3		Barcelo and Hennion (1997)	X	567
[119446-68-3]	3.1×10^4		Duchowicz et al. (2020)	Q	
BQYJATMQXGBDHF-UHFFFAOYSA-N	7.7×10^1		Goodarzi et al. (2010)	Q	568
	1.1×10^6		Maniere et al. (2011)	?	165
quizalofop ethyl	9.3×10^2		Duchowicz et al. (2020)	V	186
$C_{19}H_{17}ClN_2O_4$	9.0×10^2		HSDB (2015)	V	
[76578-14-8]	4.0×10^4		Duchowicz et al. (2020)	Q	
OSUHJPCHFDQAIT-UHFFFAOYSA-N	1.5×10^4		Maniere et al. (2011)	?	12, 165
quizalofop-p-ethyl	4.8×10^3		Ebert et al. (2023)	?	318
$C_{19}H_{17}ClN_2O_4$					
[100646-51-3]					
OSUHJPCHFDQAIT-GFCCVEGCSA-N					
pyraclostrobine	1.9×10^5		MacBean (2012b)	X	350
$C_{19}H_{18}ClN_3O_4$	1.9×10^5		Maniere et al. (2011)	?	12, 165
[175013-18-0]					
HZRSNVGNWUDEFX-UHFFFAOYSA-N					
pyrimidifen	3.6×10^4		Ebert et al. (2023)	?	318
$C_{20}H_{28}ClN_3O_2$					
[105779-78-0]					
ITKAIUGKVKDENI-UHFFFAOYSA-N					

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Table A6.8: Chlorocarbons with nitrogen (C, H, O, N, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ponsol red violet 2rnx	2.4×10^{10}		Zhang et al. (2010)	Q	287, 288
$C_{21}H_8Cl_3NO_3$	4.1×10^{7}		Zhang et al. (2010)	Q	287, 289
[6373-31-5]	9.9×10^{8}		Zhang et al. (2010)	Q	287, 290
SQAQTWYUQXFOMH-UHFFFAOYSA-N	4.6×10^{9}		Zhang et al. (2010)	Q	287, 291
dimethomorph	4.9×10^{4}		Duchowicz et al. (2020)	V	186
$C_{21}H_{22}NO_4Cl$	9.3×10^{5}		Duchowicz et al. (2020)	Q	
[110488-70-5]	9.9×10^{9}		HSDB (2015)	Q	99
QNBTYORWCCMPQP-JXAWBTAJSA-N	1.9×10^{5}		Maniere et al. (2011)	?	241, 165
	4.0×10^{4}		Maniere et al. (2011)	?	241, 165
propaquizafop	3.2×10^{6}		Duchowicz et al. (2020)	V	186
$C_{22}H_{22}ClN_3O_5$	1.1×10^{7}		Duchowicz et al. (2020)	Q	
[111479-05-1]	1.1×10^{7}		Maniere et al. (2011)	?	12, 165
FROBCXTULYFHEJ-UHFFFAOYSA-N					
aripiprazole	9.9×10^{11}		HSDB (2015)	Q	99
$C_{23}H_{27}Cl_2N_3O_2$					
[129722-12-9]					
CEUORZQYGODEFX-UHFFFAOYSA-N					
ag-g-86814	1.8×10^{14}		Zhang et al. (2010)	Q	287, 288
$C_{26}H_6Cl_8N_2O_4$	9.7×10^{12}		Zhang et al. (2010)	Q	287, 289
[30125-47-4]	1.1×10^{11}		Zhang et al. (2010)	Q	287, 290
ZEHOVWPIGREOPO-UHFFFAOYSA-N	4.1×10^{14}		Zhang et al. (2010)	Q	287, 291
8,18-dichloro-5,15-diethyl-5,15-dihydrodiindolo(3,2-b:3',2'-m)triphenodioxazine	8.0×10^{6}		Zhang et al. (2010)	Q	287, 288
$C_{34}H_{22}Cl_2N_4O_2$	1.8×10^{12}		Zhang et al. (2010)	Q	287, 289
[6358-30-1]	6.2×10^{6}		Zhang et al. (2010)	Q	287, 290
CGLVZFOCZLHKOH-UHFFFAOYSA-N	1.0×10^{10}		Zhang et al. (2010)	Q	287, 291

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A6.9 Chlorofluorocarbons (C, H, O, N, F, Cl)

Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chlorofluoromethane	1.5×10^{-3}	2600	Wilhelm et al. (1977)	L	
CH_2FCl	1.5×10^{-3}	2300	Boggs and Buck (1958)	M	
(R31)	1.5×10^{-3}		Duchowicz et al. (2020)	V	186
[593-70-4]	1.5×10^{-3}		Hine and Mookerjee (1975)	V	
XWCDCDSDNJVCLO-UHFFFAOYSA-N	1.6×10^{-3}		Yaws (2003)	X	237
	1.5×10^{-3}		Duchowicz et al. (2020)	Q	
	3.9×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{-3}		Gharagheizi et al. (2010)	Q	246
	3.4×10^{-3}		Hilal et al. (2008)	Q	
	5.9×10^{-4}		Modarresi et al. (2007)	Q	67
		2600	Kühne et al. (2005)	Q	
	6.6×10^{-4}		Yao et al. (2002)	Q	229
	1.8×10^{-3}		English and Carroll (2001)	Q	230, 231
	6.1×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	1.8×10^{-3}		Irmann (1965)	Q	
		2500	Kühne et al. (2005)	?	
	1.6×10^{-3}		Yaws (1999)	?	21
	1.5×10^{-3}		Yaws and Yang (1992)	?	21
chlorodifluoromethane	3.5×10^{-4}	2600	Burkholder et al. (2019)	L	
CHF_2Cl	3.2×10^{-4}	2700	Burkholder et al. (2019)	L	70
(R22)	3.5×10^{-4}	2600	Burkholder et al. (2015)	L	
[75-45-6]	3.2×10^{-4}	2700	Burkholder et al. (2015)	L	70
VOPWNXZWBYDODV-UHFFFAOYSA-N	3.4×10^{-4}	3400	Sander et al. (2011)	L	1
	3.4×10^{-4}	3400	Wilhelm et al. (1977)	L	
	2.9×10^{-4}	3100	Ooki and Yokouchi (2011)	M	70
	3.4×10^{-4}	3000	Zheng et al. (1997)	M	740
	3.5×10^{-4}	3100	Maaßen (1995)	M	741
	3.5×10^{-4}	3000	Reichl (1995)	M	742
	1.7×10^{-4}	3500	Chang and Criddle (1995)	M	743
	3.5×10^{-4}	2600	Boggs and Buck (1958)	M	
	3.3×10^{-4}		Mackay et al. (2006b)	V	
	3.3×10^{-4}		Mackay et al. (1993)	V	
	3.3×10^{-4}	3600	McLinden (1989)	V	744, 745
	3.4×10^{-4}		Hine and Mookerjee (1975)	V	
	3.2×10^{-4}		Irmann (1965)	V	
	3.3×10^{-4}		Yaws (2003)	X	237
			Kanakidou et al. (1995)	C	746
	3.1×10^{-4}		Hayer et al. (2022)	Q	20
	3.4×10^{-4}	3100	Li et al. (2019)	Q	1
	1.4×10^{-4}		Gharagheizi et al. (2012)	Q	
	3.9×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-5}		Raventos-Duran et al. (2010)	Q	245
	3.7×10^{-4}		Gharagheizi et al. (2010)	Q	246
	6.0×10^{-4}		Hilal et al. (2008)	Q	
	1.9×10^{-4}		Modarresi et al. (2007)	Q	67
		2600	Kühne et al. (2005)	Q	
	3.4×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	8.4×10^{-4}		English and Carroll (2001)	Q	230, 231
	1.0×10^{-4}		Katritzky et al. (1998)	Q	
	4.0×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	3.5×10^{-4}		Irmann (1965)	Q	
		3000	Kühne et al. (2005)	?	
	3.3×10^{-4}		Yaws (1999)	?	21
	2.4×10^{-4}		Abraham and Weathersby (1994)	?	21
	3.3×10^{-4}		Yaws and Yang (1992)	?	21
dichlorofluoromethane	9.1×10^{-4}		HSDB (2015)	V	
$CHFCl_2$	1.8×10^{-3}		Mackay et al. (1993)	V	
(R21)	6.8×10^{-4}		Gharagheizi et al. (2012)	Q	
[75-43-4]	1.6×10^{-3}		Hilal et al. (2008)	Q	
UMNKXPULIDJLSU-UHFFFAOYSA-N	5.9×10^{-4}		Modarresi et al. (2007)	Q	67
	9.2×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	1.5×10^{-3}		Yao et al. (2002)	Q	229
	7.2×10^{-4}		Katritzky et al. (1998)	Q	
	1.9×10^{-3}		Yaws (1999)	?	21
	3.8×10^{-5}		Mackay et al. (1993)	?	
	1.9×10^{-3}		Yaws and Yang (1992)	?	21
chlorotrifluoromethane	9.9×10^{-6}	1700	Burkholder et al. (2019)	L	747
CF_3Cl	8.0×10^{-6}	1500	Burkholder et al. (2019)	L	70
(R13)	9.9×10^{-6}	1700	Burkholder et al. (2015)	L	748
[75-72-9]	8.0×10^{-6}	1500	Burkholder et al. (2015)	L	70
AFYPFACVUDMOHA-UHFFFAOYSA-N	9.9×10^{-6}	1700	Sander et al. (2011)	L	749
	9.3×10^{-6}	1600	Wilhelm et al. (1977)	L	
	8.9×10^{-6}	1900	Reichl (1995)	M	750
	9.0×10^{-6}	2100	Scharlin and Battino (1995)	M	751
	9.0×10^{-6}	2100	Scharlin and Battino (1994)	M	752
	7.8×10^{-6}		Park et al. (1982)	M	
	1.5×10^{-4}		Mackay et al. (1993)	V	
	5.7×10^{-6}		Hine and Mookerjee (1975)	V	
	8.8×10^{-6}		Yaws (2003)	X	237
	7.2×10^{-6}		Hilal et al. (2008)	C	
	5.7×10^{-6}		Irmann (1965)	C	
	8.3×10^{-6}		Hayer et al. (2022)	Q	20
	6.4×10^{-6}		Keshavarz et al. (2022)	Q	
	4.0×10^{-5}		Duchowicz et al. (2020)	Q	
	2.3×10^{-5}		Gharagheizi et al. (2012)	Q	
	6.9×10^{-6}		Gharagheizi et al. (2010)	Q	246

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.6×10^{-5}		Hilal et al. (2008)	Q	
	2.1×10^{-5}		Modarresi et al. (2007)	Q	67
		2600	Kühne et al. (2005)	Q	
	7.7×10^{-6}		Yaffe et al. (2003)	Q	248, 249
	6.7×10^{-7}		Katritzky et al. (1998)	Q	
	1.4×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	5.1×10^{-6}		Irmann (1965)	Q	
	7.2×10^{-6}		Duchowicz et al. (2020)	?	185, 21
		2000	Kühne et al. (2005)	?	
	8.8×10^{-6}		Yaws (1999)	?	21
	8.7×10^{-6}		Yaws and Yang (1992)	?	21
dichlorodifluoromethane	3.0×10^{-5}	3500	Burkholder et al. (2019)	L	
CF_2Cl_2	2.6×10^{-5}	2100	Burkholder et al. (2019)	L	70
(R12)	3.0×10^{-5}	3500	Burkholder et al. (2015)	L	
[75-71-8]	2.6×10^{-5}	2100	Burkholder et al. (2015)	L	70
PXBRQCKWGAHEHS-UHFFFAOYSA-N	3.1×10^{-5}	3200	Brockbank (2013)	L	1
	3.0×10^{-5}	3400	Warneck and Williams (2012)	L	
	3.0×10^{-5}	3500	Sander et al. (2011)	L	
	3.0×10^{-5}	3500	Sander et al. (2006)	L	
	3.1×10^{-5}	3500	Staudinger and Roberts (2001)	L	
	2.1×10^{-5}	1800	Wilhelm et al. (1977)	L	
	1.3×10^{-4}	5500	Hiatt (2013)	M	
	3.0×10^{-5}	3000	Reichl (1995)	M	753
	2.9×10^{-5}	2900	Scharlin and Battino (1995)	M	754
	2.9×10^{-5}	2900	Scharlin and Battino (1994)	M	755
	3.1×10^{-5}	3500	Munz and Roberts (1987)	M	
	2.9×10^{-5}	3200	Warner and Weiss (1985)	M	
	2.3×10^{-5}	3400	Wisegarver and Cline (1985)	M	70
	2.9×10^{-5}		Park et al. (1982)	M	
	2.5×10^{-5}		Pearson and McConnell (1975)	M	649, 12
	2.4×10^{-5}		Mackay et al. (2006b)	V	
	2.4×10^{-5}		Mackay et al. (1993)	V	
	2.3×10^{-5}		Mackay and Shiu (1981)	V	
	2.3×10^{-5}		Hine and Mookerjee (1975)	V	
	2.5×10^{-5}		Yaws (2003)	X	237
	3.5×10^{-6}	-210	Goldstein (1982)	X	298
	3.6×10^{-5}		Hilal et al. (2008)	C	
	6.4×10^{-6}		Ryan et al. (1988)	C	
	2.3×10^{-5}		Irmann (1965)	C	
	2.4×10^{-5}		Hayer et al. (2022)	Q	20
	1.9×10^{-5}		Keshavarz et al. (2022)	Q	
	1.1×10^{-4}		Duchowicz et al. (2020)	Q	184
	2.8×10^{-5}	3300	Li et al. (2019)	Q	1
	1.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	2.4×10^{-5}		Gharagheizi et al. (2010)	Q	246
	5.4×10^{-5}		Hilal et al. (2008)	Q	
	7.7×10^{-5}		Modarresi et al. (2007)	Q	67

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
		3000	Kühne et al. (2005)	Q	
	2.5×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	1.1×10^{-5}		Katritzky et al. (1998)	Q	
	4.7×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	2.0×10^{-5}		Irmann (1965)	Q	
	2.9×10^{-5}		Duchowicz et al. (2020)	?	185, 21
		3400	Kühne et al. (2005)	?	
	2.5×10^{-5}		Yaws (1999)	?	21
	2.3×10^{-5}		Abraham and Weathersby (1994)	?	21
	2.5×10^{-5}		Yaws and Yang (1992)	?	21
trichlorofluoromethane	1.1×10^{-4}	3300	Burkholder et al. (2019)	L	
$CFCl_3$	7.3×10^{-5}	3900	Burkholder et al. (2019)	L	70
(R11)	1.1×10^{-4}	3300	Burkholder et al. (2015)	L	
[75-69-4]	7.3×10^{-5}	3900	Burkholder et al. (2015)	L	70
CYRMSUTZVYGINF-UHFFFAOYSA-N	1.0×10^{-4}	3400	Brockbank (2013)	L	1
	1.1×10^{-4}	3400	Warneck and Williams (2012)	L	
	1.1×10^{-4}	3300	Sander et al. (2011)	L	
	1.1×10^{-4}	3300	Sander et al. (2006)	L	
	1.1×10^{-4}	3300	Staudinger and Roberts (2001)	L	
	1.0×10^{-4}	3100	Staudinger and Roberts (1996)	L	
	2.8×10^{-4}	5100	Hiatt (2013)	M	
	6.0×10^{-5}	4900	Ooki and Yokouchi (2011)	M	70
	1.0×10^{-4}	3700	Maaßen (1995)	M	756
	1.5×10^{-4}	3700	Reichl (1995)	M	757
	9.8×10^{-5}	3500	Ashworth et al. (1988)	M	278
	1.0×10^{-4}	3600	Warner and Weiss (1985)	M	
	7.8×10^{-5}	3900	Wisegarver and Cline (1985)	M	70
	1.1×10^{-4}	2700	Hunter-Smith et al. (1983)	M	658
	1.1×10^{-4}		Park et al. (1982)	M	
	1.7×10^{-4}		Warner et al. (1980)	M	
	1.1×10^{-4}	2100	Balls (1980)	M	
	1.2×10^{-5}		Pearson and McConnell (1975)	M	649, 12
	7.8×10^{-5}		Mackay et al. (2006b)	V	
	9.9×10^{-5}	6100	Fogg and Sangster (2003)	V	
	7.8×10^{-5}		Mackay et al. (1993)	V	
	9.0×10^{-5}		Yoshida et al. (1983)	V	
	9.0×10^{-5}		Mackay and Shiu (1981)	V	
	9.5×10^{-5}		Warner et al. (1980)	V	
	9.8×10^{-5}		Irmann (1965)	V	
	8.0×10^{-5}		Yaws (2003)	X	237, 38
	1.7×10^{-4}	730	Goldstein (1982)	X	298
	1.0×10^{-4}		Hilal et al. (2008)	C	
	1.7×10^{-4}		Ryan et al. (1988)	C	
	1.7×10^{-4}		Shen (1982)	C	
	8.1×10^{-5}		Liss and Slater (1974)	C	
	9.4×10^{-5}		Hayer et al. (2022)	Q	20
	5.9×10^{-5}		Keshavarz et al. (2022)	Q	

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.7×10^{-4}		Duchowicz et al. (2020)	Q	299
	6.5×10^{-4}		Gharagheizi et al. (2012)	Q	
	8.4×10^{-5}		Gharagheizi et al. (2010)	Q	246
	1.7×10^{-4}		Hilal et al. (2008)	Q	
	2.5×10^{-4}		Modarresi et al. (2007)	Q	67
		3300	Kühne et al. (2005)	Q	
	1.1×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	8.6×10^{-5}		Katritzky et al. (1998)	Q	
	8.6×10^{-5}		Irmann (1965)	Q	
	1.0×10^{-4}		Duchowicz et al. (2020)	?	185, 21
	9.8×10^{-5}		Mackay et al. (2006b)	?	
		3800	Kühne et al. (2005)	?	
	8.1×10^{-5}		Yaws (1999)	?	21, 38
	8.2×10^{-5}		Abraham and Weathersby (1994)	?	21
	9.8×10^{-5}		Mackay et al. (1993)	?	
	8.1×10^{-5}		Yaws and Yang (1992)	?	21
1,1,1,2-tetrachlorodifluoroethane	6.1×10^{-5}		Duchowicz et al. (2020)	V	186
$C_2Cl_4F_2$	6.2×10^{-5}		HSDB (2015)	V	
[76-11-9]	7.3×10^{-4}		Duchowicz et al. (2020)	Q	
SLGOCMATMKJJCE-UHFFFAOYSA-N	5.1×10^{-4}		Hilal et al. (2008)	Q	
	2.8×10^{-4}		Modarresi et al. (2007)	Q	67
	2.4×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	3.2×10^{-5}		Katritzky et al. (1998)	Q	
1,1,2,2-tetrachlorodifluoroethane	9.0×10^{-5}		HSDB (2015)	V	
$C_2F_2Cl_4$	1.0×10^{-4}		Hine and Mookerjee (1975)	V	
(R112)	7.9×10^{-5}		Yaws (2003)	X	237
[76-12-0]	2.4×10^{-3}		Gharagheizi et al. (2012)	Q	
UGCSPKPEHQEOSR-UHFFFAOYSA-N	7.1×10^{-5}		Gharagheizi et al. (2010)	Q	246
	5.1×10^{-4}		Hilal et al. (2008)	Q	
	3.2×10^{-4}		Modarresi et al. (2007)	Q	67
	1.1×10^{-4}		Yao et al. (2002)	Q	229
	7.9×10^{-5}		Yaws (1999)	?	21
1,1,1-trichloro-2,2,2-trifluoroethane	3.4×10^{-5}	3200	Burkholder et al. (2019)	L	
$C_2F_3Cl_3$	3.4×10^{-5}	3200	Burkholder et al. (2015)	L	
(R113a)	3.7×10^{-5}		HSDB (2015)	Q	99
[354-58-5]	3.7×10^{-5}		Zhang et al. (2010)	Q	287, 288
BOSAWIQFTJIYIS-UHFFFAOYSA-N	2.1×10^{-4}		Zhang et al. (2010)	Q	287, 289
	5.8×10^{-5}		Zhang et al. (2010)	Q	287, 290
	3.0×10^{-5}		Zhang et al. (2010)	Q	287, 291

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1,2-trichloro-1,2,2-trifluoroethane	2.9×10^{-5}	4100	Brockbank (2013)	L	1
$C_2F_3Cl_3$	2.0×10^{-4}	5700	Hiatt (2013)	M	
(R113)	2.9×10^{-5}	4300	Dewulf et al. (1999)	M	
[76-13-1]	2.9×10^{-5}	4000	Bu and Warner (1995)	M	758
AJDIZQLSFPQPEY-UHFFFAOYSA-N	2.8×10^{-5}	6500	Reichl (1995)	M	759
	3.4×10^{-5}	3200	Ashworth et al. (1988)	M	278
	1.9×10^{-5}		HSDB (2015)	V	
			Mackay et al. (2006b)	V	683
	8.8×10^{-6}		Mackay et al. (1993)	V	
	2.0×10^{-5}		Hine and Mookerjee (1975)	V	
	2.0×10^{-5}		Yaws (2003)	X	237
	7.0×10^{-4}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-5}		Gharagheizi et al. (2010)	Q	246
	1.8×10^{-4}		Hilal et al. (2008)	Q	
	1.1×10^{-4}		Modarresi et al. (2007)	Q	67
		3700	Kühne et al. (2005)	Q	
	3.1×10^{-5}		Mackay et al. (2006b)	?	
		3800	Kühne et al. (2005)	?	
	2.1×10^{-5}		Yaws (1999)	?	21
	3.1×10^{-5}		Mackay et al. (1993)	?	
	2.0×10^{-5}		Yaws and Yang (1992)	?	21
	2.0×10^{-5}		Abraham et al. (1990)	?	
1,1-dichlorotetrafluoroethane	8.2×10^{-6}		HSDB (2015)	V	
$C_2F_4Cl_2$	5.8×10^{-6}		Hine and Mookerjee (1975)	V	
(R114a)	7.5×10^{-6}		Hilal et al. (2008)	C	
[374-07-2]	5.8×10^{-6}		Irmann (1965)	C	294
BAMUEXIPKSRTBS-UHFFFAOYSA-N	8.8×10^{-5}		Hilal et al. (2008)	Q	
	6.6×10^{-6}		Irmann (1965)	Q	
1,2-dichlorotetrafluoroethane	9.0×10^{-6}	2800	Reichl (1995)	M	760
$C_2F_4Cl_2$	7.9×10^{-6}		Mackay et al. (1993)	V	
(R114)	8.0×10^{-6}		Hine and Mookerjee (1975)	V	
[76-14-2]	8.1×10^{-6}		Yaws (2003)	X	237
DDMOUSALMHHKOS-UHFFFAOYSA-N	8.1×10^{-6}		Irmann (1965)	C	12
	7.1×10^{-4}		Hayer et al. (2022)	Q	20
	1.8×10^{-4}		Gharagheizi et al. (2012)	Q	
	8.1×10^{-6}		Gharagheizi et al. (2010)	Q	246
	8.4×10^{-5}		Hilal et al. (2008)	Q	
	2.8×10^{-5}		Modarresi et al. (2007)	Q	67
		3300	Kühne et al. (2005)	Q	
	1.1×10^{-4}		Yao et al. (2002)	Q	229
	6.6×10^{-6}		Irmann (1965)	Q	
		2700	Kühne et al. (2005)	?	
	8.2×10^{-6}		Yaws (1999)	?	21
	7.9×10^{-6}		Abraham and Weathersby (1994)	?	21
	8.1×10^{-6}		Yaws and Yang (1992)	?	21

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chloropentafluoroethane	3.4×10^{-6}	2800	Wilhelm et al. (1977)	L	
C_2F_5Cl	3.1×10^{-6}	2100	Reichl (1995)	M	761
(R115)	1.8×10^{-6}		Duchowicz et al. (2020)	V	186
[76-15-3]	1.8×10^{-6}		HSDB (2015)	V	
RFCAUADVODFSLZ-UHFFFAOYSA-N	3.8×10^{-6}		Mackay et al. (1993)	V	
	3.7×10^{-6}		Meylan and Howard (1991)	V	
	3.2×10^{-6}		Hine and Mookerjee (1975)	V	
	3.8×10^{-6}		Yaws (2003)	X	237
	3.2×10^{-6}		Irmann (1965)	C	
	3.1×10^{-6}		Hayer et al. (2022)	Q	20
	6.5×10^{-5}		Duchowicz et al. (2020)	Q	
	4.9×10^{-5}		Gharagheizi et al. (2012)	Q	
	2.5×10^{-6}		Gharagheizi et al. (2010)	Q	246
	3.4×10^{-5}		Hilal et al. (2008)	Q	
	7.6×10^{-6}		Modarresi et al. (2007)	Q	67
		2900	Kühne et al. (2005)	Q	
	2.4×10^{-5}		Yao et al. (2002)	Q	229
	1.2×10^{-6}		Meylan and Howard (1991)	Q	
	2.1×10^{-6}		Irmann (1965)	Q	
		2000	Kühne et al. (2005)	?	
	3.8×10^{-6}		Yaws (1999)	?	21
	3.8×10^{-6}		Yaws and Yang (1992)	?	21
1,1,2,2-tetrachloro-1-fluoroethane C_2HCl_4F [354-14-3] LUBCGHUOCJOIJA-UHFFFAOYSA-N	3.3×10^{-3}		HSDB (2015)	Q	99
1,1-dichloro-1,2,2-trifluoroethane $C_2HCl_2F_3$ [812-04-4] AFTSHZRGGNMLHC-UHFFFAOYSA-N	1.0×10^{-4}		HSDB (2015)	Q	99
1,2-dichloro-1,1,2-trifluoroethane $C_2HCl_2F_3$ [354-23-4] YMRMDGSNYHCUCL-UHFFFAOYSA-N	1.0×10^{-4}		HSDB (2015)	Q	99
2,2-dichloro-1,1,1-trifluoroethane	2.3×10^{-4}	2400	Kutsuna (2013)	M	
$C_2HF_3Cl_2$	3.2×10^{-4}	3100	Chang and Criddle (1995)	M	762
(R123)	2.8×10^{-4}	2600	McLinden (1989)	V	
[306-83-2]	5.0×10^{-4}		Hilal et al. (2008)	Q	
OHMHBGPWCHTMQE-UHFFFAOYSA-N	1.8×10^{-4}		Modarresi et al. (2007)	Q	67
1-chloro-1,1,2,2-tetrafluoroethane C_2HClF_4 [354-25-6] JQZFYIGAYWLRCC-UHFFFAOYSA-N	1.8×10^{-5}		HSDB (2015)	Q	99

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloro-1,2,2,2-tetrafluoroethane	1.1×10^{-4}	2800	Kutsuna (2013)	M	
C_2HF_4Cl	1.0×10^{-4}	3500	Maaßen (1995)	M	763
(R124)	1.1×10^{-4}	3400	Reichl (1995)	M	764
[2837-89-0]	1.1×10^{-4}		Duchowicz et al. (2020)	V	186
BOUGCJDAQLKBQH-UHFFFAOYSA-N	1.0×10^{-4}	3200	McLinden (1989)	V	
	1.2×10^{-4}		Hayer et al. (2022)	Q	20
	1.3×10^{-3}		Duchowicz et al. (2020)	Q	
		2900	Kühne et al. (2005)	Q	
		3400	Kühne et al. (2005)	?	
1,2-dichloro-1,1-difluoroethane	1.4×10^{-4}		Duchowicz et al. (2020)	V	186
$C_2H_2Cl_2F_2$	1.4×10^{-4}		HSDB (2015)	V	
[1649-08-7]	1.1×10^{-3}		Duchowicz et al. (2020)	Q	
SKDFWEPBABSFMG-UHFFFAOYSA-N					
2-chloro-1,1,1-trifluoroethane	3.7×10^{-4}	3600	Maaßen (1995)	M	765
$C_2H_2F_3Cl$	4.1×10^{-4}	3500	Reichl (1995)	M	766
(R133a)	3.7×10^{-4}		Hine and Mookerjee (1975)	V	
[75-88-7]	3.7×10^{-4}		Irmann (1965)	C	
CYXIKYKBLDZZNW-UHFFFAOYSA-N	4.8×10^{-4}		Hayer et al. (2022)	Q	20
	3.7×10^{-5}		HSDB (2015)	Q	99
	3.0×10^{-4}		Hilal et al. (2008)	Q	
	4.6×10^{-4}		English and Carroll (2001)	Q	230, 231
	3.9×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	2.9×10^{-4}		Irmann (1965)	Q	
	2.7×10^{-4}		Abraham and Weathersby (1994)	?	21
1,1-dichloro-1-fluoroethane	2.9×10^{-4}	2800	Kutsuna (2013)	M	
CH_3CFCl_2	2.8×10^{-4}	3700	Maaßen (1995)	M	767
(R141b)	4.5×10^{-4}		Duchowicz et al. (2020)	V	186
[1717-00-6]	4.5×10^{-4}		HSDB (2015)	V	
FRCHKSNAZZFGCA-UHFFFAOYSA-N	7.7×10^{-5}	5200	McLinden (1989)	V	
	2.9×10^{-4}		Hayer et al. (2022)	Q	20
	6.8×10^{-4}		Duchowicz et al. (2020)	Q	
	2.9×10^{-4}	3500	Li et al. (2019)	Q	1
		3300	Kühne et al. (2005)	Q	
		3700	Kühne et al. (2005)	?	
1-chloro-1,1-difluoroethane	1.5×10^{-4}	2600	Kutsuna (2013)	M	
CH_3CF_2Cl	1.4×10^{-4}	3200	Maaßen (1995)	M	768
(R142b)	1.4×10^{-4}	3200	Reichl (1995)	M	769
[75-68-3]	1.5×10^{-4}	3000	Chang and Criddle (1995)	M	770
BHNZEZWIUMJCGF-UHFFFAOYSA-N	1.4×10^{-4}	2500	McLinden (1989)	V	
	1.9×10^{-4}		Irmann (1965)	C	294
	1.6×10^{-4}		Hayer et al. (2022)	Q	20
	1.4×10^{-4}	3200	Li et al. (2019)	Q	1
	1.5×10^{-4}		Modarresi et al. (2007)	Q	67
	8.4×10^{-5}		Yaffe et al. (2003)	Q	248, 249
	1.5×10^{-3}		Katritzky et al. (1998)	Q	

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	1.5×10^{-4}		Irmann (1965)	Q	
1-chloro-1,2-difluoroethane $C_2H_3ClF_2$ [338-64-7] UOVSDUIHNGNMBZ-UHFFFAOYSA-N		2900 3200	Kühne et al. (2005) Kühne et al. (2005)	Q ?	
1-chloro-1,1,2-trifluoroethane $C_2H_2F_3Cl$ (R133b) [421-04-5] HILNUELUDBMBJQ-UHFFFAOYSA-N		2900 3500	Kühne et al. (2005) Kühne et al. (2005)	Q ?	
2-chloro-1,1-difluoroethene C_2HClF_2 (R1122) [359-10-4] HTHNTJCVPNKCPZ-UHFFFAOYSA-N	1.7×10^{-4} 1.7×10^{-4} 1.9×10^{-4} 1.1×10^{-4}	3300 3300 2800 3300 	Maaßen (1995) Reichl (1995) Hayer et al. (2022) Kühne et al. (2005) Kühne et al. (2005) Abraham and Weathersby (1994)	M M Q Q ? ?	771 772 20 21
chlorotrifluoroethene C_2ClF_3 [79-38-9] UUAGAQFQZIEFAH-UHFFFAOYSA-N	3.2×10^{-5}		HSDB (2015)	Q	99
3,3-dichloro-1,1,1,2,2-pentafluoropropane $CF_3CF_2CHCl_2$ (R225ca) [422-56-0] COAUHYBSXMIJDK-UHFFFAOYSA-N	9.8×10^{-5} 1.5×10^{-5} 8.4×10^{-4} 9.0×10^{-5} 2.0×10^{-5} 3.0×10^{-4} 1.1×10^{-4} 3.9×10^{-5} 2.0×10^{-5}	3500 	Kutsuna (2013) Keshavarz et al. (2022) Duchowicz et al. (2020) HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Duchowicz et al. (2020)	M Q Q Q Q Q Q Q ?	 99 287, 288 287, 289 287, 290 287, 291 185, 21
1,3-dichloro-1,1,2,2,3-pentafluoropropane $CClF_2CF_2CHClF$ (R225cb) [507-55-1] UJIGKESMIPTWJH-UHFFFAOYSA-N	1.1×10^{-4} 3.6×10^{-6}	3100 	Kutsuna (2013) HSDB (2015)	M Q	 99
1-chloro-2-fluorobenzene C_6H_4ClF [348-51-6] ZCJAYDKWZAWMPR-UHFFFAOYSA-N	3.1×10^{-3}		Ebert et al. (2023)	?	316

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-chloro-3-fluorobenzene C_6H_4ClF [625-98-9] VZHJIJZEOCBKRA-UHFFFAOYSA-N	1.6×10^{-3}		Ebert et al. (2023)	?	316
1-chloro-3-(trifluoromethyl)benzene $C_7H_4ClF_3$ [98-15-7] YTCGOUNVIAWCMG-UHFFFAOYSA-N	2.9×10^{-4}		Zhang et al. (2010)	Q	287, 288
	2.8×10^{-3}		Zhang et al. (2010)	Q	287, 289
	1.4×10^{-3}		Zhang et al. (2010)	Q	287, 290
	1.4×10^{-4}		Zhang et al. (2010)	Q	287, 291
1-chloro-4-(trifluoromethyl)benzene $C_7H_4ClF_3$ [98-56-6] QULYNCCPRWKEMF-UHFFFAOYSA-N	2.8×10^{-4}		HSDB (2015)	Q	99
	2.9×10^{-4}		Zhang et al. (2010)	Q	287, 288
	3.1×10^{-3}		Zhang et al. (2010)	Q	287, 289
	1.5×10^{-3}		Zhang et al. (2010)	Q	287, 290
	1.4×10^{-4}		Zhang et al. (2010)	Q	287, 291
3-chloro-4-fluorobenzotrifluoride $C_7H_3ClF_4$ [78068-85-6] BKHVEYHSOXVAOP-UHFFFAOYSA-N	2.4×10^{-4}		Zhang et al. (2010)	Q	287, 288
	2.5×10^{-3}		Zhang et al. (2010)	Q	287, 289
	8.6×10^{-4}		Zhang et al. (2010)	Q	287, 290
	1.1×10^{-4}		Zhang et al. (2010)	Q	287, 291
3,4-dichlorobenzotrifluoride $C_7H_3Cl_2F_3$ [328-84-7] XILPLWOGHPSJBK-UHFFFAOYSA-N	3.8×10^{-4}		HSDB (2015)	Q	99
	3.9×10^{-4}		Zhang et al. (2010)	Q	287, 288
	5.3×10^{-3}		Zhang et al. (2010)	Q	287, 289
	2.0×10^{-3}		Zhang et al. (2010)	Q	287, 290
	2.3×10^{-4}		Zhang et al. (2010)	Q	287, 291
chlorodifluoroethanoic acid $CF_2ClCOOH$ (chlorodifluoroacetic acid) [76-04-0] OAWAZQITIZDJRB-UHFFFAOYSA-N	2.5×10^{2}	10000	Burkholder et al. (2019)	L	
	2.5×10^{2}	10000	Burkholder et al. (2015)	L	
	2.5×10^{2}	10000	Sander et al. (2011)	L	
	2.4×10^{2}	10000	Bowden et al. (1998a)	M	
	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	4.4×10^{1}		Duchowicz et al. (2020)	Q	
	9.9×10^{1}		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^{-1}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{1}		Raventos-Duran et al. (2010)	Q	245
	2.4×10^{2}		Duchowicz et al. (2020)	?	185, 21
carbonic chloride fluoride $COFCl$ [353-49-1] OXVVNXMNLYYMOL-UHFFFAOYSA-N	9.9×10^{-2}		George et al. (1993)	X	627

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Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
trifluoroacetylchloride	2.0×10^{-2}		Mirabel et al. (1996)	M	
CF_3COCl	2.7×10^{-3}		De Bruyn et al. (1995a)	M	449
[354-32-5]	2.0×10^{-2}		George et al. (1994b)	M	630
PNQBEPDZQUOCNY-UHFFFAOYSA-N	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	9.3×10^{-3}		Duchowicz et al. (2020)	Q	299
	2.2×10^{-2}		Duchowicz et al. (2020)	?	185, 21
2,2-dichloro-1,1-difluoro-1-methoxyethane	2.9×10^{-3}	4100	Fogg and Sangster (2003)	L	
$C_3H_4Cl_2F_2O$	1.7×10^{-3}		Steward et al. (1973)	L	14
(methoxyflurane)	3.0×10^{-3}	4300	Allott et al. (1973)	L	
[76-38-0]	1.7×10^{-3}		Lerman et al. (1983)	M	14
RFKMCNOHBTXSMU-UHFFFAOYSA-N	2.9×10^{-3}	3600	Smith et al. (1981b)	M	773
	1.8×10^{-3}		Stoelting and Longshore (1972)	M	14
	2.9×10^{-2}		Keshavarz et al. (2022)	Q	
	1.7×10^{-2}		Duchowicz et al. (2020)	Q	
	4.1×10^{-3}		Hilal et al. (2008)	Q	
	1.8×10^{-2}		Modarresi et al. (2007)	Q	67
		4800	Kühne et al. (2005)	Q	
	2.7×10^{-3}		Duchowicz et al. (2020)	?	185, 21
	2.7×10^{-3}		HSDB (2015)	?	419
		4000	Kühne et al. (2005)	?	
	1.7×10^{-3}		Abraham and Weathersby (1994)	?	21
	2.7×10^{-3}		Abraham et al. (1990)	?	
2-(chlorodifluoromethoxy)-1,1,1-trifluoroethane $C_3H_2ClF_5O$ [33018-78-9] HPDPVPUXPBZBOJ-UHFFFAOYSA-N	1.7×10^{-5}		Ebert et al. (2023)	?	365
2-(chlorofluoromethoxy)-1,1,1,2-tetrafluoroethane $C_3H_2ClF_5O$ [56885-28-0] GGEBMRHBGQLKGJ-UHFFFAOYSA-N	2.2×10^{-4}		Ebert et al. (2023)	?	365
1-chloro-2,2,2-trifluoroethyl difluoromethyl ether	2.4×10^{-4}		Fogg and Sangster (2003)	L	
$C_3H_2ClF_5O$	2.4×10^{-4}		Steward et al. (1973)	L	14
(forane; isoflurane)	2.4×10^{-4}		Allott et al. (1973)	L	14
[26675-46-7]	2.4×10^{-4}		Lerman et al. (1983)	M	14
PIWKPBJCKXDKJR-UHFFFAOYSA-N	4.8×10^{-4}	5300	Smith et al. (1981b)	M	
	5.7×10^{-4}		Keshavarz et al. (2022)	Q	
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	184
	4.2×10^{-4}		Hilal et al. (2008)	Q	
	1.2×10^{-3}		Modarresi et al. (2007)	Q	67
		4400	Kühne et al. (2005)	Q	
	3.8×10^{-4}		Goss (2005)	Q	

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.4×10^{-4}		Duchowicz et al. (2020)	?	185, 21
	3.4×10^{-4}		HSDB (2015)	?	419
		4500	Kühne et al. (2005)	?	
	2.4×10^{-4}		Abraham and Weathersby (1994)	?	21
	3.4×10^{-4}		Abraham et al. (1990)	?	
2-chloro-1,1,2-trifluoroethyl difluoromethyl ether	3.0×10^{-4}		Fogg and Sangster (2003)	L	
$C_3H_2ClF_5O$	3.0×10^{-4}		Allott et al. (1973)	L	14
(enflurane)	2.7×10^{-4}		Guitart et al. (1989)	M	14
[13838-16-9]	2.9×10^{-4}		Lerman et al. (1983)	M	14
JPGQOUSTVILISH-UHFFFAOYSA-N	1.3×10^{-3}		HSDB (2015)	V	
	3.0×10^{-4}		Steward et al. (1973)	C	14
	6.9×10^{-4}		Hilal et al. (2008)	Q	
	3.1×10^{-4}		Abraham and Weathersby (1994)	?	21
3-[2-chloro-4-(trifluoromethyl)phenoxy]benzoic acid	6.4×10^{2}		Zhang et al. (2010)	Q	287, 288
$C_{14}H_8ClF_3O_3$	3.3×10^{2}		Zhang et al. (2010)	Q	287, 289
[63734-62-3]	2.1×10^{5}		Zhang et al. (2010)	Q	287, 290
ONKRUAQFUNKYAX-UHFFFAOYSA-N	2.9×10^{3}		Zhang et al. (2010)	Q	287, 291
3-(2-chloro-4-(trifluoromethyl)phenoxy)phenyl acetate	1.1		Zhang et al. (2010)	Q	287, 288
$C_{15}H_{10}ClF_3O_3$	2.4×10^{1}		Zhang et al. (2010)	Q	287, 289
[50594-77-9]	2.9×10^{1}		Zhang et al. (2010)	Q	287, 290
KNFRYRRZMRETJX-UHFFFAOYSA-N	3.6		Zhang et al. (2010)	Q	287, 291
transfluthrin $C_{15}H_{12}Cl_2F_4O_2$ [118712-89-3] DDVNRFNDOPPVQJ-HQJQHLMTSA-N	2.2×10^{-1}		Ebert et al. (2023)	?	318
tefluthrin	6.2×10^{-3}		HSDB (2015)	V	
$C_{17}H_{14}O_2ClF_7$	5.0×10^{-3}		Maniere et al. (2011)	?	12, 165
[79538-32-2]					
ZFHGXWPMULPQSE-GPCIZFCYSA-N					
clobetasol $C_{22}H_{28}ClFO_4$ [25122-41-2] FCSHDIVRCWTZOX-DVTGEIKXSA-N	6.2×10^{4}		HSDB (2015)	Q	99
flufenprox $C_{24}H_{22}ClF_3O_3$ [107713-58-6] RURQAJURNPMSSK-UHFFFAOYSA-N	2.1×10^{1}		Ebert et al. (2023)	?	318

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
EINECS 273-236-7	1.5×10^{14}		Zhang et al. (2010)	Q	287, 288
$C_{28}H_{33}Cl_3F_6O_{11}$	6.9×10^{18}		Zhang et al. (2010)	Q	287, 289
[68954-01-8]	2.3×10^{12}		Zhang et al. (2010)	Q	287, 290
KVXVLCBFSKMBAR-UHFFFAOYSA-N	1.6×10^{15}		Zhang et al. (2010)	Q	287, 291
3,5-dichloro-2,4,6-trifluoropyridine	1.6		Zhang et al. (2010)	Q	287, 288
$C_5Cl_2F_3N$	7.7×10^{-4}		Zhang et al. (2010)	Q	287, 289
[1737-93-5]	1.6×10^{-3}		Zhang et al. (2010)	Q	287, 290
PKSORSNCSXBXOT-UHFFFAOYSA-N	2.7×10^{-2}		Zhang et al. (2010)	Q	287, 291
chlorodifluoronitrooxymethane $CClF_2OONO_2$ [70490-95-8] HWHZTSGXJYKIPK-UHFFFAOYSA-N	2.9×10^{-2}	5900	Kanakidou et al. (1995)	E	774
1-chloro-2-nitro-4-(trifluoromethyl)-benzene	7.2×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_7H_3ClF_3NO_2$	1.2×10^{-1}		Zhang et al. (2010)	Q	287, 289
[121-17-5]	1.1×10^{-1}		Zhang et al. (2010)	Q	287, 290
TZGFQIXRVUHDLE-UHFFFAOYSA-N	1.0×10^{-2}		Zhang et al. (2010)	Q	287, 291
2-chloro-1,3-dinitro-5-(trifluoromethyl)-benzene	1.8×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_7H_2ClF_3N_2O_4$	2.8		Zhang et al. (2010)	Q	287, 289
[393-75-9]	1.7×10^{-1}		Zhang et al. (2010)	Q	287, 290
HFHAVERNVFNSHL-UHFFFAOYSA-N	9.0×10^{-1}		Zhang et al. (2010)	Q	287, 291
fluroxypyr	5.7×10^{5}		HSDB (2015)	V	
$C_7H_5Cl_2FN_2O_3$	5.9×10^{9}		Maniere et al. (2011)	?	12, 165
[69377-81-7] MEFQWPUMEMWTJP-UHFFFAOYSA-N					
fluoroimide $C_{10}H_4Cl_2FNO_2$ [41205-21-4] IPENDKRRWFURRE-UHFFFAOYSA-N	7.7×10^{-1}		Ebert et al. (2023)	?	318
norflurazon	2.9×10^{4}		Duchowicz et al. (2020)	V	186
$C_{12}H_9ClF_3N_3O$	2.9×10^{4}		HSDB (2015)	V	
[27314-13-2]	5.5×10^{3}		Duchowicz et al. (2020)	Q	
NVGOPFQZYCNLDU-UHFFFAOYSA-N					
fluchloralin	6.6×10^{-1}		HSDB (2015)	V	
$C_{12}H_{13}ClF_3N_3O_4$	7.4×10^{-1}		Mackay et al. (2006d)	V	
[33245-39-5] MNFMIVVPXOGUMX-UHFFFAOYSA-N					
flurochloridone	2.6×10^{2}		Duchowicz et al. (2020)	V	186
$C_{12}H_{10}Cl_2F_3NO$	8.2×10^{-1}		Duchowicz et al. (2020)	Q	
[61213-25-0]	4.2×10^{2}		Maniere et al. (2011)	?	165
OQZCSNDVOWYALR-UHFFFAOYSA-N					

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
flupyradifurone $C_{12}H_{11}ClF_2N_2O_2$ [951659-40-8] QOIYTRGFOFZNKF-UHFFFAOYSA-N	6.5×10^{6}		Ebert et al. (2023)	?	318
fluxofenim $C_{12}H_{11}NO_3ClF_3$ [88485-37-4] UKSLKNUCVPZQCQ-GZTJUZNOSA-N	2.6 5.8×10^{2}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
fluazinam $C_{13}H_4Cl_2F_6N_4O_4$ [79622-59-6] UZCGKGPEKUCDTF-UHFFFAOYSA-N	3.9×10^{-2} 3.9×10^{-2}		HSDB (2015) Maniere et al. (2011)	V ?	 12, 165
5-(2-chloro-4-(trifluoromethyl)phenoxy)-2-nitrophenol $C_{13}H_7ClF_3NO_4$ [42874-63-5] WYTRKEWETULQOA-UHFFFAOYSA-N	9.9 1.1×10^{3} 2.3×10^{6} 2.3×10^{1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
florpyrauxifen $C_{13}H_8Cl_2F_2N_2O_3$ [943832-81-3] XFZUQTKDBCOXPP-UHFFFAOYSA-N	3.2×10^{7}		Ebert et al. (2023)	?	318
tetraconazole $C_{13}H_{11}Cl_2F_4N_3O$ [112281-77-3] LQDARGUHUSPFNL-UHFFFAOYSA-N	2.3×10^{3} 2.8×10^{3}		HSDB (2015) Maniere et al. (2011)	V ?	 241, 165
fluopicolide $C_{14}H_8Cl_3F_3N_2O$ [239110-15-7] GBOYJIHYACSLGN-UHFFFAOYSA-N	9.0×10^{3} 2.4×10^{4}		HSDB (2015) Maniere et al. (2011)	V ?	 241, 165
diflubenzuron $C_{14}H_9ClF_2N_2O_2$ (difluron) [35367-38-5] QQQYTWIFVNKMRW-UHFFFAOYSA-N	2.1×10^{3} 2.1×10^{3} 2.1×10^{3} 2.1×10^{1} 7.2×10^{3} 3.3×10^{1} 1.7×10^{3}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Barcelo and Hennion (1997) Duchowicz et al. (2020) Goodarzi et al. (2010) Maniere et al. (2011)	V V V X Q Q ?	186 567 568 165
efavirenz $C_{14}H_9ClF_3NO_2$ [154598-52-4] XPOQHMRABVBWPR-ZDUSSCGKSA-N	1.4×10^{3}		HSDB (2015)	Q	99

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
halauxifen-methyl	8.1×10^5		Maniere et al. (2011)	?	241, 570, 165
$C_{14}H_{11}Cl_2FN_2O_3$	8.2×10^5		Maniere et al. (2011)	?	241, 493, 165
[943831-98-9]	8.3×10^5		Maniere et al. (2011)	?	241, 573, 165
KDHKOPYYWOHESS-UHFFFAOYSA-N	9.0×10^5		Maniere et al. (2011)	?	241, 165
fluroxypyr-butometyl $C_{14}H_{19}Cl_2FN_2O_4$ [154486-27-8] ZKFARSBUEBZZJT-UHFFFAOYSA-N	2.4×10^3		Ebert et al. (2023)	?	318
teflubenzuron	6.2×10^4		Duchowicz et al. (2020)	V	186
$C_{14}H_6N_2O_2Cl_2F_4$	2.5×10^4		Duchowicz et al. (2020)	Q	
[83121-18-0]					
CJDWRQLODFKPEL-UHFFFAOYSA-N					
fluroxypyr-meptyl $C_{15}H_{21}Cl_2FN_2O_3$ (attain A) [81406-37-3] OLZQTUCTGLHFTQ-UHFFFAOYSA-N	3.7×10^1		Maniere et al. (2011)	?	12, 165
quinoxyfen $C_{15}H_8Cl_2FNO$ [124495-18-7] WRPIRSINYZBGPK-UHFFFAOYSA-N	1.0×10^3		HSDB (2015)	Q	99
5-(2-chloro-4-(trifluoromethyl)phenoxy)-2-nitrophenyl acetate	2.7×10^2		Zhang et al. (2010)	Q	287, 288
$C_{15}H_9ClF_3NO_5$	1.5×10^3		Zhang et al. (2010)	Q	287, 289
[50594-44-0]	3.7×10^4		Zhang et al. (2010)	Q	287, 290
PSWSPFSDVZVVDC-UHFFFAOYSA-N	3.1×10^2		Zhang et al. (2010)	Q	287, 291
triflumuron $C_{15}H_{10}ClF_3N_2O_3$ [64628-44-0] XAIPTRIXGHTTNT-UHFFFAOYSA-N	1.1×10^3		Ebert et al. (2023)	?	318
oxyfluorfen	1.2×10^1		Duchowicz et al. (2020)	V	186
$C_{15}H_{11}ClF_3NO_4$	1.2×10^1		HSDB (2015)	V	
[42874-03-3]	8.3×10^1		Duchowicz et al. (2020)	Q	
OQMBBFQZGJFLBU-UHFFFAOYSA-N	4.2×10^1		Maniere et al. (2011)	?	165
pyraflufen-ethyl	1.2×10^4		MacBean (2012b)	X	350
$C_{15}H_{13}Cl_2F_3N_2O_4$	4.5×10^4		Maniere et al. (2011)	?	12, 165
[129630-19-9]					
APTZNLHMIGJTEW-UHFFFAOYSA-N					

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cis-furconazole $C_{15}H_{14}Cl_2F_3N_3O_2$ [112839-32-4] ULCWZQJLFZEXCS-KGLIPLIRSA-N	3.7×10^{3}		Ebert et al. (2023)	?	318
carfentrazone ethyl $C_{15}H_{14}Cl_2F_3N_3O_3$ [128639-02-1] MLKCGVHIFJBRCD-UHFFFAOYSA-N	3.3×10^{3} 3.3×10^{3} 1.7×10^{4} 6.4×10^{3}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Maniere et al. (2011)	V V Q ?	186 12, 165
triflumizole $C_{15}H_{15}ClF_3N_3O$ [68694-11-1] HSMVPDGQOIQYSR-UHFFFAOYSA-N	1.9×10^{5} 2.5×10^{7} 3.7×10^{1}		Duchowicz et al. (2020) Mackay et al. (2006d) Duchowicz et al. (2020)	V V Q	186
diflumetorim $C_{15}H_{16}N_3OClF_2$ [130339-07-0] NEKULYKCZPJMMJ-UHFFFAOYSA-N	3.1×10^{2} 2.8×10^{3}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
3-(2,4-dichlorophenyl)-6-fluoro-2-(1H-1,2,4-triazol-1-yl)-quinazolin-4(3H)-one $C_{16}H_8Cl_2FN_5O$ (fluquinconazole) [136426-54-5] IJJVMEJXYNJXOJ-UHFFFAOYSA-N	5.6×10^{8} 1.4×10^{5} 4.8×10^{5}		Hilal et al. (2008) Modarresi et al. (2007) Maniere et al. (2011)	Q Q ?	 67 241, 165
hexaflumuron $C_{16}H_8Cl_2F_6N_2O_3$ [86479-06-3] RGNPBRKPHBKNKX-UHFFFAOYSA-N	9.9×10^{-1} 9.9×10^{-1} 4.3×10^{4}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
fluopyram $C_{16}H_{11}ClF_6N_2O$ [658066-35-4] KVDJTXBXMWJJEF-UHFFFAOYSA-N	3.4×10^{4}		Maniere et al. (2011)	?	241, 165
haloxyfop-p-methyl $C_{16}H_{13}ClF_3NO_4$ [72619-32-0] MFSWTRQUCLNFOM-SECBINFHSA-N	8.3×10^{2}		Maniere et al. (2011)	?	241, 165
flumetralin $C_{16}H_{12}ClF_4N_3O_4$ [62924-70-3] PWNAWOCHVWERAR-UHFFFAOYSA-N	5.2 4.0×10^{3}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186

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haloxyfop-methyl $C_{16}H_{13}ClF_3NO_4$ [69806-40-2] MFSWTRQUCLNFOM-UHFFFAOYSA-N	3.1×10^{1} 3.1×10^{2}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
pydiflumetofen $C_{16}H_{16}Cl_3F_2N_3O_2$ [1228284-64-7] DGOAXBPOVUPPEB-UHFFFAOYSA-N	6.6×10^{3}		Ebert et al. (2023)	?	318
nuarimol $C_{17}H_{12}ClFN_2O$ [63284-71-9] SAPGTCDSBGMXCD-UHFFFAOYSA-N	1.5×10^{7}		MacBean (2012a)	?	
clodinafop-propargyl $C_{17}H_{13}ClFNO_4$ [105512-06-9] JBDHZKLJNAIJNC-LLVKDONJSA-N	3.6×10^{3} 3.5×10^{3} 2.4×10^{3} 3.6×10^{3}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Maniere et al. (2011)	V V Q ?	186 241, 165
flamprop-methyl $C_{17}H_{15}ClFNO_3$ [52756-25-9] RBNIGDFIUWJJEV-UHFFFAOYSA-N	2.2×10^{3}		MacBean (2012a)	?	
pyridalyl $C_{18}H_{14}Cl_4F_3NO_3$ [179101-81-6] UBSUICNYBBPFHD-UHFFFAOYSA-N	4.9×10^{6}		HSDB (2015)	V	
mefentrifluconazole $C_{18}H_{15}ClF_3N_3O_2$ [1417782-03-6] JERZEQUMJNCPRJ-UHFFFAOYSA-N	6.2×10^{2}		Maniere et al. (2011)	?	12, 165
bixafen $C_{18}H_{12}N_3OCl_2F_3$ [581809-46-3] LDLMOOXUCMHBMZ-UHFFFAOYSA-N	2.6×10^{4}		Maniere et al. (2011)	?	241, 165
benzovindiflupyr $C_{18}H_{15}Cl_2F_2N_3O$ [1072957-71-1] CCCGEKHKTPTUHJ-UHFFFAOYSA-N	7.7×10^{5}		Maniere et al. (2011)	?	241, 165
lactofen $C_{19}H_{15}ClF_3NO_7$ [77501-63-4] CONWAEURSVPLRM-UHFFFAOYSA-N	2.1×10^{1} 2.3×10^{1} 4.0×10^{4}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (...continued)

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flupoxam $C_{19}H_{14}N_4O_2ClF_5$ [119126-15-7] AOQMRUTZEYVDIL-UHFFFAOYSA-N	1.1×10^2 2.7×10^7		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
flamprop-m-isopropyl $C_{19}H_{19}NO_3ClF$ [63782-90-1] IKVXBIIHQGXQRQ-CYBMUJFWSA-N	3.9×10^2 2.3×10^1		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
haloxyfop-ethoxyethyl $C_{19}H_{19}ClF_3NO_5$ [87237-48-7] MIJLZGZLQLAQCM-UHFFFAOYSA-N	3.8×10^4		Ebert et al. (2023)	?	318
chlorfluazuron $C_{20}H_9Cl_3F_5N_3O_3$ [71422-67-8] UISUNVFOGSJSKD-UHFFFAOYSA-N	8.2×10^6 1.1×10^6 3.9×10^8 2.1×10^6 5.5×10^6		Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Duchowicz et al. (2020)	Q Q Q Q ?	 67 185, 21
fluazuron $C_{20}H_{10}N_3O_3Cl_2F_5$ [86811-58-7] YOWNVPAUWYHLQX-UHFFFAOYSA-N	$>2.3\times10^{10}$		MacBean (2012a)	?	
flufenoxuron $C_{21}H_{11}ClF_6N_2O_3$ [101463-69-8] RYLHNOVXKPXDIP-UHFFFAOYSA-N	3.8×10^6		HSDB (2015)	Q	99
fluoxastrobin $C_{21}H_{16}N_4O_5ClF$ [361377-29-9] UFEODZBUAFNAEU-NLRVBDNBSA-N	9.0×10^6 1.0×10^7		HSDB (2015) Maniere et al. (2011)	V ?	 12, 165
haloperidol $C_{21}H_{23}ClFNO_2$ [52-86-8] LNEPOXFFQSENCJ-UHFFFAOYSA-N	4.3×10^8		HSDB (2015)	Q	99
indoxacarb $C_{22}H_{17}ClF_3N_3O_7$ [173584-44-6] VBCVPMMZEGZULK-NRFANRHFSA-N	1.5×10^4 $>1.7\times10^4$		HSDB (2015) Maniere et al. (2011)	V ?	 165
cyfluthrin $C_{22}H_{18}Cl_2FNO_3$ [68359-37-5] QQODLKZGRKWIFG-UHFFFAOYSA-N	3.4×10^2 1.1×10^1 1.7		HSDB (2015) Maniere et al. (2011) Maniere et al. (2011)	V ? ?	 12, 165 12, 165

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
cyfluthrin I $C_{22}H_{18}Cl_2FNO_3$ [86560-92-1] QQODLKZGRKWIFG-QSFXBCCZSA-N	2.2		Ebert et al. (2023)	?	318
β-cyfluthrin (cis) $C_{22}H_{18}Cl_2FNO_3$ [86560-93-2] QQODLKZGRKWIFG-XFQXTVEOSA-N	1.4×10^{2}		Ebert et al. (2023)	?	365
cyfluthrin II $C_{22}H_{18}Cl_2FNO_3$ [86560-94-3] QQODLKZGRKWIFG-BPAFIMBUSA-N	1.1×10^{2}		Ebert et al. (2023)	?	365
β-cyfluthrin (trans) $C_{22}H_{18}Cl_2FNO_3$ [86560-95-4] QQODLKZGRKWIFG-QKYXUNIQSA-N	3.6×10^{1}		Ebert et al. (2023)	?	365
metamifop $C_{23}H_{18}N_2O_4ClF$ [256412-89-2] ADDQHLREJDZPMT-CQSZACIVSA-N	1.6×10^{1}		MacBean (2012a)	?	12
pyriminostrobin $C_{23}H_{18}Cl_2F_3N_3O_4$ [1257598-43-8] YYXSCUSVVALMNW-FOWTUZBSSA-N	8.3×10^{3}		Ebert et al. (2023)	?	318
cyhalothrin $C_{23}H_{19}NO_3ClF_3$ [68085-85-8] ZXQYGBMAQZUVMI-BWHPXCRDSA-N	7.0×10^{-1}		HSDB (2015)	Q	99
bifenthrin $C_{23}H_{22}ClF_3O_2$ [82657-04-3] OMFRMAHOUUJSGP-UNOMPAQXSA-N	9.9 9.9 9.9 2.7×10^{-1} 4.7		Duchowicz et al. (2020) HSDB (2015) Hilal et al. (2008) Duchowicz et al. (2020) Hilal et al. (2008)	V V C Q Q	186
λ-cyhalothrin $C_{23}H_{19}ClF_3NO_3$ [91465-08-6] DFVKOWFGNASVPK-QQDHXZELSA-N	5.0×10^{1}		Maniere et al. (2011)	?	12, 165
γ-cyhalothrin $C_{23}H_{19}ClF_3NO_3$ [76703-62-3] ZXQYGBMAQZUVMI-GCMPRSNUSA-N	4.5×10^{1}		Maniere et al. (2011)	?	241, 165

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Table A6.9: Chlorofluorocarbons (C, H, O, N, F, Cl) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
flucycloxuron $C_{25}H_{20}ClF_2N_3O_3$ [94050-52-9] PCKNFPQPGUWFHO-UQRQXUALSA-N	3.8×10^{1}		MacBean (2012a)	?	
τ-fluvalinate $C_{26}H_{22}ClF_3N_2O_3$ [102851-06-9] INISTDXBRIBGOC-XMMISQBUSA-N	8.3×10^{3}		Maniere et al. (2011)	?	165
fluvalinate $C_{26}H_{22}ClF_3N_2O_3$ [69409-94-5] INISTDXBRIBGOC-UHFFFAOYSA-N	6.6×10^{2}		HSDB (2015)	Q	99

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A7 Organic species with bromine (Br)

A7.1 Bromocarbons (C, H, O, N, Br)

Table A7.1: Bromocarbons (C, H, O, N, Br)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bromomethane	1.5×10^{-3}	3300	Burkholder et al. (2019)	L	775
CH_3Br	1.5×10^{-3}	3000	Burkholder et al. (2019)	L	70
(methyl bromide)	1.7×10^{-3}	3100	Burkholder et al. (2015)	L	
[74-83-9]	1.5×10^{-3}	3000	Burkholder et al. (2015)	L	70
GZUXJHMPEANEGY-UHFFFAOYSA-N	1.5×10^{-3}	3800	Brockbank (2013)	L	1
	1.7×10^{-3}	3100	Sander et al. (2011)	L	
	1.7×10^{-3}	3100	Sander et al. (2006)	L	
	1.7×10^{-3}	3100	Staudinger and Roberts (2001)	L	
	1.6×10^{-3}	3100	Wilhelm et al. (1977)	L	
	1.3×10^{-3}	2800	Hiatt (2013)	M	
	2.0×10^{-3}		Thomas et al. (2006)	M	154, 703
	1.8×10^{-3}	2500	De Bruyn and Saltzman (1997)	M	776
	1.4×10^{-3}		Gan and Yates (1996)	M	294
	1.7×10^{-3}	3400	Elliott and Rowland (1993)	M	
	1.5×10^{-3}	2600	Swain and Thornton (1962)	M	
	1.6×10^{-3}	3200	Glew and Moelwyn-Hughes (1953)	M	777
	1.6×10^{-3}		Mackay et al. (2006b)	V	
	1.6×10^{-3}		Lide and Frederikse (1995)	V	
	1.6×10^{-3}		Mackay et al. (1993)	V	
	1.9×10^{-3}		Mackay and Shiu (1981)	V	12
	1.5×10^{-3}		Hine and Mookerjee (1975)	V	
	1.5×10^{-3}		Yaws (2003)	X	237
	4.4×10^{-5}	350	Goldstein (1982)	X	298
	1.8×10^{-4}		Keshavarz et al. (2022)	Q	
	3.5×10^{-3}		Duchowicz et al. (2020)	Q	184
	5.5×10^{-4}		Wang et al. (2017)	Q	80, 238
	3.8×10^{-3}		Wang et al. (2017)	Q	80, 239
	2.3×10^{-3}		Wang et al. (2017)	Q	80, 240
	3.7×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.7×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.3×10^{-3}		Modarresi et al. (2007)	Q	67
		3400	Kühne et al. (2005)	Q	
	1.9×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.8×10^{-3}		Yao et al. (2002)	Q	229
	1.2×10^{-3}		English and Carroll (2001)	Q	230, 231
	9.9×10^{-5}		Katritzky et al. (1998)	Q	
	1.5×10^{-3}		Suzuki et al. (1992)	Q	232
	3.1×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	7.9×10^{-4}		Irmann (1965)	Q	
	1.3×10^{-3}		Duchowicz et al. (2020)	?	185, 21

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.8×10^{-3}		Thomas et al. (2006)	?	154, 704
		3200	Kühne et al. (2005)	?	
	1.5×10^{-3}		Yaws (1999)	?	21
	1.7×10^{-3}		Yates and Gan (1998)	?	
	1.4×10^{-3}		Yaws and Yang (1992)	?	21
	1.6×10^{-3}		Abraham et al. (1990)	?	
dibromomethane	1.2×10^{-2}	4300	Burkholder et al. (2019)	L	1
CH_2Br_2	9.0×10^{-3}	4600	Burkholder et al. (2019)	L	70
[74-95-3]	9.0×10^{-3}	4600	Burkholder et al. (2015)	L	70
FJBFPHVGVWTDIP-UHFFFAOYSA-N	1.2×10^{-2}	4300	Brockbank (2013)	L	1, 778
	3.1×10^{-2}		Mackay and Shiu (1981)	L	
	1.2×10^{-2}	5000	Hiatt (2013)	M	
	8.9×10^{-3}	4400	Ooki and Yokouchi (2011)	M	70
	1.4×10^{-2}		Dohnal and Hovorka (1999)	M	12
	1.5×10^{-2}		Hovorka and Dohnal (1997)	M	12
	1.2×10^{-2}	4900	Kondoh and Nakajima (1997)	M	
	9.7×10^{-3}	3800	Moore et al. (1995)	M	779, 70
	1.1×10^{-2}	4000	Wright et al. (1992)	M	780
	1.1×10^{-2}	4100	Tse et al. (1992)	M	
	1.1×10^{-2}	4400	Rex (1906)	M	
	1.1×10^{-2}		Mackay et al. (2006b)	V	
	1.3×10^{-2}	4200	Fogg and Sangster (2003)	V	
	7.1×10^{-3}		Mackay et al. (1993)	V	
	1.1×10^{-2}		Hine and Mookerjee (1975)	V	
	1.1×10^{-2}		Yaws (2003)	X	237
	3.2×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-1}		Gharagheizi et al. (2010)	Q	246
	3.8×10^{-2}		Hilal et al. (2008)	Q	
	1.7×10^{-3}		Modarresi et al. (2007)	Q	67
		4500	Kühne et al. (2005)	Q	
	1.2×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	8.2×10^{-3}		Yao et al. (2002)	Q	229, 267
	2.7×10^{-3}		Katritzky et al. (1998)	Q	
	9.5×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.2×10^{-2}		Mackay et al. (2006b)	?	
		4300	Kühne et al. (2005)	?	
	1.1×10^{-2}		Yaws (1999)	?	21
	1.2×10^{-2}		Mackay et al. (1993)	?	
	1.1×10^{-2}		Abraham et al. (1990)	?	

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Table A7.1: Bromocarbons (C, H, O, N, Br) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tribromomethane	1.7×10^{-2}	5200	Burkholder et al. (2019)	L	
$CHBr_3$	1.1×10^{-2}	6200	Burkholder et al. (2019)	L	70
(bromoform)	1.7×10^{-2}	5200	Burkholder et al. (2015)	L	
[75-25-2]	1.1×10^{-2}	6200	Burkholder et al. (2015)	L	70
DIKBFYAXUHHXCS-UHFFFAOYSA-N	1.8×10^{-2}	4800	Brockbank (2013)	L	1
	1.7×10^{-2}	5200	Sander et al. (2011)	L	
	1.7×10^{-2}	5200	Sander et al. (2006)	L	
	1.7×10^{-2}	5200	Staudinger and Roberts (2001)	L	
	1.7×10^{-2}	5200	Staudinger and Roberts (1996)	L	
	1.6×10^{-2}		Mackay and Shiu (1981)	L	
	2.2×10^{-2}	6300	Hiatt (2013)	M	
	9.9×10^{-3}	6200	Ooki and Yokouchi (2011)	M	70
	2.0×10^{-2}		Ruiz-Bevia and Fernandez-Torres (2010)	M	
	9.6×10^{-3}		Zhang et al. (2002)	M	14
	2.3×10^{-2}		Hovorka and Dohnal (1997)	M	12
	1.4×10^{-2}	4500	Kondoh and Nakajima (1997)	M	
	1.5×10^{-2}	4300	Moore et al. (1995)	M	781, 70
	8.5×10^{-3}	1500	Khalfaoui and Newsham (1994a)	M	
	2.4×10^{-2}	4100	Wright et al. (1992)	M	782
	1.9×10^{-2}	5000	Tse et al. (1992)	M	
	1.8×10^{-2}	4700	Munz and Roberts (1987)	M	
	1.6×10^{-2}	5700	Nicholson et al. (1984)	M	
	1.9×10^{-2}		Warner et al. (1980)	M	
	1.7×10^{-2}		Mackay et al. (2006b)	V	
	1.8×10^{-2}	5300	Fogg and Sangster (2003)	V	
	1.7×10^{-2}		Mackay et al. (1993)	V	
	1.7×10^{-2}		Warner et al. (1980)	V	
	1.5×10^{-2}		Hine and Mookerjee (1975)	V	
	1.8×10^{-2}	2700	Goldstein (1982)	X	298
	1.7×10^{-2}		Ryan et al. (1988)	C	
	1.7×10^{-2}		Nicholson et al. (1984)	C	
	1.9×10^{-2}		Shen (1982)	C	
	8.8×10^{-3}		Keshavarz et al. (2022)	Q	
	1.0×10^{-2}		Duchowicz et al. (2020)	Q	
	7.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	7.3×10^{-3}		Hilal et al. (2008)	Q	
	9.8×10^{-4}		Modarresi et al. (2007)	Q	67
		5600	Kühne et al. (2005)	Q	
	1.8×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.3×10^{-2}		Yao et al. (2002)	Q	229
	1.4×10^{-2}		Katritzky et al. (1998)	Q	
	2.4×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
	1.8×10^{-2}		Duchowicz et al. (2020)	?	185, 21

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.1×10^{-2}		Mackay et al. (2006b)	?	
		5000	Kühne et al. (2005)	?	
	1.7×10^{-2}		Yaws (1999)	?	21
	2.1×10^{-2}		Mackay et al. (1993)	?	
	1.5×10^{-2}		Abraham et al. (1990)	?	
tetrabromomethane	2.0×10^{-2}		Duchowicz et al. (2020)	V	186
CBr_4	2.0×10^{-2}		HSDB (2015)	V	
[558-13-4]	1.2×10^{-2}		Fogg and Sangster (2003)	V	783, 38
HJUGFYREWKUQJT-UHFFFAOYSA-N	2.0×10^{-2}		Hilal et al. (2008)	C	
	9.8×10^{-4}		Duchowicz et al. (2020)	Q	
	2.1×10^{-3}		Hilal et al. (2008)	Q	
	2.2×10^{-4}		Modarresi et al. (2007)	Q	67
bromoethane	1.3×10^{-3}	3900	Burkholder et al. (2019)	L	
C_2H_5Br	1.3×10^{-3}	3900	Brockbank (2013)	L	1
[74-96-4]	1.3×10^{-3}		Li et al. (1993)	M	
RDHPKYGYEGBMSE-UHFFFAOYSA-N	1.3×10^{-3}	3900	Rex (1906)	M	
	1.3×10^{-3}		Duchowicz et al. (2020)	V	186
			Mackay et al. (2006b)	V	683
	8.1×10^{-4}		Mackay et al. (1993)	V	
	1.4×10^{-3}		Abraham (1984)	V	
	1.3×10^{-3}		Hine and Mookerjee (1975)	V	
	1.3×10^{-3}		Yaws (2003)	X	237
	9.2×10^{-5}		Ryan et al. (1988)	C	
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	3.2×10^{-3}		Gharagheizi et al. (2012)	Q	
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
	3.4×10^{-3}		Hilal et al. (2008)	Q	
	1.2×10^{-3}		Modarresi et al. (2007)	Q	67
		3700	Kühne et al. (2005)	Q	
	1.4×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	7.7×10^{-4}		Yao et al. (2002)	Q	229
	1.1×10^{-3}		English and Carroll (2001)	Q	230, 231
	2.3×10^{-4}		Katritzky et al. (1998)	Q	
	1.1×10^{-3}		Suzuki et al. (1992)	Q	232
	1.6×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
		3800	Kühne et al. (2005)	?	
	1.3×10^{-3}		Yaws (1999)	?	21
	1.3×10^{-3}		Yaws and Yang (1992)	?	21
	1.4×10^{-3}		Abraham et al. (1990)	?	

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
1,1-dibromoethane $C_2H_4Br_2$ [557-91-5] APQIUTYORBAGEZ-UHFFFAOYSA-N	7.6×10^{-3}		HSDB (2015)	Q	99
1,2-dibromoethane	1.4×10^{-2}	4300	Burkholder et al. (2019)	L	
$C_2H_4Br_2$	1.5×10^{-2}	3900	Burkholder et al. (2015)	L	
(ethylene dibromide)	1.4×10^{-2}	4200	Brockbank (2013)	L	1
[106-93-4]	1.7×10^{-2}	5500	Hiatt (2013)	M	
PAAZPARNPHGIKF-UHFFFAOYSA-N	1.9×10^{-2}		Dohnal and Hovorka (1999)	M	12
	1.3×10^{-2}		Welke et al. (1998)	M	
	1.9×10^{-2}		Hovorka and Dohnal (1997)	M	12
	1.8×10^{-2}	5500	Kondoh and Nakajima (1997)	M	
	1.1×10^{-2}	3000	Khalfaoui and Newsham (1994a)	M	33
	1.5×10^{-2}	3900	Ashworth et al. (1988)	M	278
	1.5×10^{-2}		Mackay et al. (2006b)	V	
	2.1×10^{-3}		Mackay et al. (1993)	V	
	1.4×10^{-2}		Hine and Mookerjee (1975)	V	
	1.2×10^{-2}		Yaws (2003)	X	237
	1.1×10^{-2}	1900	Goldstein (1982)	X	298
	1.5×10^{-2}		HSDB (2015)	C	
	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	3.3×10^{-3}		Duchowicz et al. (2020)	Q	184
	6.2×10^{-3}		Wang et al. (2017)	Q	80, 238
	4.6×10^{-2}		Wang et al. (2017)	Q	80, 239
	4.4×10^{-2}		Wang et al. (2017)	Q	80, 240
	2.8×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
	3.9×10^{-2}		Hilal et al. (2008)	Q	
	6.5×10^{-3}		Modarresi et al. (2007)	Q	67
		4800	Kühne et al. (2005)	Q	
	1.6×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	4.1×10^{-3}		Katritzky et al. (1998)	Q	
	7.5×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.2×10^{-3}		Rumble (2021)	?	784, 785
	1.5×10^{-2}		Duchowicz et al. (2020)	?	185, 21
	1.5×10^{-2}		Mackay et al. (2006b)	?	
		4200	Kühne et al. (2005)	?	
	1.3×10^{-2}		Yaws (1999)	?	21
	1.5×10^{-2}		Mackay et al. (1993)	?	
	1.4×10^{-2}		Yaws and Yang (1992)	?	21
	2.1×10^{-2}		Abraham et al. (1990)	?	
	1.6×10^{-2}		Mackay and Yeun (1983)	?	
	1.8×10^{-2}		Chiou et al. (1980)	?	79

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-dibromoethane-d4 $C_2D_4Br_2$ (ethylene dibromide-d4) [22581-63-1] PAAZPARNPHGIKF-LNLMKGTHSA-N	1.6×10^{-2}	4800	Hiatt (2013)	M	
1,1,2-tribromoethane $C_2H_3Br_3$ [78-74-0] QUMDOMSJJIFTCA-UHFFFAOYSA-N	2.4×10^{-2}		Ebert et al. (2023)	?	316
1,1,2,2-tetrabromoethane	1.4×10^{-2}	1300	Burkholder et al. (2019)	L	
$C_2H_2Br_4$	1.4×10^{-2}	1300	Brockbank (2013)	L	1
[79-27-6]	1.0×10^{-2}	840	Khalfaoui and Newsham (1994a)	M	
QXSZNDIIPUOQMB-UHFFFAOYSA-N	7.4×10^{-1}		Duchowicz et al. (2020)	V	186
	7.6×10^{-1}		HSDB (2015)	V	
	7.3×10^{-1}		Yaws (2003)	X	237
	1.4×10^{-2}		Duchowicz et al. (2020)	Q	
	5.7×10^{-1}		Zhang et al. (2010)	Q	287, 288
	2.9×10^{-1}		Zhang et al. (2010)	Q	287, 289
	4.3×10^{-1}		Zhang et al. (2010)	Q	287, 290
	1.5×10^{-1}		Zhang et al. (2010)	Q	287, 291
	7.2×10^{-1}		Gharagheizi et al. (2010)	Q	246
	2.4×10^{-1}		Hilal et al. (2008)	Q	
	7.0×10^{-1}		Yaffe et al. (2003)	Q	248, 249
	2.3×10^{-1}		Katritzky et al. (1998)	Q	
	7.3×10^{-1}		Yaws (1999)	?	21
1-bromopropane	1.1×10^{-3}	4600	Brockbank (2013)	L	1
C_3H_7Br	1.1×10^{-3}		Li et al. (1993)	M	
[106-94-5]	1.1×10^{-3}	4500	Rex (1906)	M	
CYNYIHKIEHGYOZ-UHFFFAOYSA-N	1.4×10^{-3}		HSDB (2015)	V	
	2.6×10^{-4}		Mackay et al. (2006b)	V	
	2.6×10^{-4}		Mackay et al. (1993)	V	
	1.0×10^{-3}		Abraham (1984)	V	
	1.0×10^{-3}		Hine and Mookerjee (1975)	V	
	1.3×10^{-3}		Yaws (2003)	X	237, 12
	1.5×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.8×10^{-3}		Hilal et al. (2008)	Q	
	1.2×10^{-3}		Modarresi et al. (2007)	Q	67
	1.4×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	3.9×10^{-4}		Yao et al. (2002)	Q	229
	8.4×10^{-4}		English and Carroll (2001)	Q	230, 274
	3.4×10^{-4}		Katritzky et al. (1998)	Q	
	3.5×10^{-4}		Russell et al. (1992)	Q	279

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Table A7.1: Bromocarbons (C, H, O, N, Br) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	8.4×10^{-4}		Suzuki et al. (1992)	Q	232
	1.3×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.1×10^{-3}		Yaws (1999)	?	21, 12
	1.4×10^{-3}		Yaws and Yang (1992)	?	21, 12
	1.0×10^{-3}		Abraham et al. (1990)	?	
2-bromopropane	9.0×10^{-4}	3900	Brockbank (2013)	L	1
C_3H_7Br	8.4×10^{-4}		Li et al. (1993)	M	
[75-26-3]	9.0×10^{-4}	4500	Rex (1906)	M	
NAMYKGVDVNBCFQ-UHFFFAOYSA-N	9.0×10^{-4}		Duchowicz et al. (2020)	V	186
	9.0×10^{-4}		HSDB (2015)	V	
	7.9×10^{-4}		Mackay et al. (2006b)	V	
	7.9×10^{-4}		Mackay et al. (1993)	V	
	9.0×10^{-4}		Hine and Mookerjee (1975)	V	
	1.0×10^{-3}		Yaws (2003)	X	237, 12
	5.4×10^{-4}		Duchowicz et al. (2020)	Q	
	3.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	9.4×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.5×10^{-3}		Hilal et al. (2008)	Q	
	7.5×10^{-4}		Modarresi et al. (2007)	Q	67
	9.2×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	3.4×10^{-4}		Yao et al. (2002)	Q	229, 267
	6.7×10^{-4}		English and Carroll (2001)	Q	230, 231
	3.3×10^{-4}		Katritzky et al. (1998)	Q	
	7.3×10^{-4}		Suzuki et al. (1992)	Q	232
	9.2×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	8.1×10^{-4}		Yaws (1999)	?	21, 12
	1.0×10^{-3}		Yaws and Yang (1992)	?	21, 12
	9.0×10^{-4}		Abraham et al. (1990)	?	
1,2-dibromopropane	5.3×10^{-3}		Albanese et al. (1987)	M	
$C_3H_6Br_2$	6.8×10^{-3}		Duchowicz et al. (2020)	V	186
[78-75-1]	6.8×10^{-3}		HSDB (2015)	V	
XFNJYAKDBJUJAJ-UHFFFAOYSA-N	6.8×10^{-3}		Mackay et al. (2006b)	V	
	1.1×10^{-2}		Hine and Mookerjee (1975)	V	
	6.3×10^{-3}		Yaws (2003)	X	237
	1.5×10^{-3}		Duchowicz et al. (2020)	Q	
	3.5×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.6×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.9×10^{-2}		Hilal et al. (2008)	Q	
	2.8×10^{-3}		Modarresi et al. (2007)	Q	67
	6.9×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	5.2×10^{-3}		Katritzky et al. (1998)	Q	
	4.4×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	6.6×10^{-3}		Yaws and Yang (1992)	?	21

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3-dibromopropane	1.1×10^{-3}		Mackay et al. (1993)	V	
$C_3H_6Br_2$	1.1×10^{-2}		Hine and Mookerjee (1975)	V	
[109-64-8]	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
VEFLKXRACNJHOV-UHFFFAOYSA-N	3.0×10^{-3}		Duchowicz et al. (2020)	Q	299
	7.2×10^{-2}		Hilal et al. (2008)	Q	
	5.0×10^{-3}		Modarresi et al. (2007)	Q	67
	1.2×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	5.6×10^{-3}		Katritzky et al. (1998)	Q	
	6.0×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.1×10^{-2}		Duchowicz et al. (2020)	?	185, 21
1-bromobutane	7.4×10^{-4}		Brockbank (2013)	L	
C_4H_9Br	4.6×10^{-4}		Hoff et al. (1993)	M	
[109-65-9]	8.2×10^{-4}		Li et al. (1993)	M	
MPPPKRYCTPRNTB-UHFFFAOYSA-N	1.1×10^{-3}		Duchowicz et al. (2020)	V	186
	1.1×10^{-3}		HSDB (2015)	V	
	8.0×10^{-4}		Abraham (1984)	V	
	8.0×10^{-4}		Hine and Mookerjee (1975)	V	
	8.0×10^{-4}		Yaws (2003)	X	237
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	9.6×10^{-4}		Ghasragheizi et al. (2012)	Q	
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	7.5×10^{-4}		Ghasragheizi et al. (2010)	Q	246
	2.2×10^{-3}		Hilal et al. (2008)	Q	
	8.7×10^{-4}		Modarresi et al. (2007)	Q	67
	1.1×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	2.7×10^{-4}		Yao et al. (2002)	Q	229
	6.2×10^{-4}		English and Carroll (2001)	Q	230, 231
	4.1×10^{-4}		Katritzky et al. (1998)	Q	
	5.8×10^{-4}		Russell et al. (1992)	Q	279
	6.5×10^{-4}		Suzuki et al. (1992)	Q	232
	1.0×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	8.3×10^{-4}		Haynes (2014)	?	786
	8.1×10^{-4}		Yaws (1999)	?	21
	8.1×10^{-4}		Yaws and Yang (1992)	?	21
	7.9×10^{-4}		Abraham et al. (1990)	?	
2-bromobutane	8.8×10^{-4}		Brockbank (2013)	L	
C_4H_9Br	7.7×10^{-4}		Li et al. (1993)	M	
[78-76-2]	6.2×10^{-4}		HSDB (2015)	Q	99
UPSXAPQYNGXVBF-UHFFFAOYSA-N	1.4×10^{-3}		Hilal et al. (2008)	Q	

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-bromo-2-methylpropane	4.2×10^{-4}		Hine and Mookerjee (1975)	V	
C_4H_9Br	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
[78-77-3]	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	244
HLVFKOKELQSXIQ-UHFFFAOYSA-N	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	2.0×10^{-3}		Hilal et al. (2008)	Q	
	7.7×10^{-4}		Modarresi et al. (2007)	Q	67
	4.2×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	4.0×10^{-4}		English and Carroll (2001)	Q	230, 231
	8.6×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	5.8×10^{-4}		Suzuki et al. (1992)	Q	232
	4.2×10^{-4}		Abraham et al. (1990)	?	
2-bromo-2-methylpropane	2.4×10^{-4}		Duchowicz et al. (2020)	V	186
C_4H_9Br	2.4×10^{-4}		HSDB (2015)	V	
[507-19-7]	2.0×10^{-4}		Duchowicz et al. (2020)	Q	
RKSOPLXZQNSWAS-UHFFFAOYSA-N	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	5.2×10^{-4}		Hilal et al. (2008)	Q	
	5.1×10^{-4}		Modarresi et al. (2007)	Q	67
	4.5×10^{-4}		English and Carroll (2001)	Q	230, 231
	4.2×10^{-4}		Katritzky et al. (1998)	Q	
	5.2×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	3.1×10^{-4}		Yaws and Yang (1992)	?	21, 28
	9.7×10^{-5}		Abraham et al. (1990)	?	
1-bromo-3-methylbutane	4.9×10^{-4}		Mackay et al. (1993)	V	
$C_5H_{11}Br$	2.9×10^{-4}		Hine and Mookerjee (1975)	V	
[107-82-4]	5.9×10^{-4}		Keshavarz et al. (2022)	Q	
YXZFFTJAHVMMLF-UHFFFAOYSA-N	4.5×10^{-4}		Duchowicz et al. (2020)	Q	184
	1.8×10^{-3}		Hilal et al. (2008)	Q	
	7.8×10^{-4}		Modarresi et al. (2007)	Q	67
	4.7×10^{-4}		Katritzky et al. (1998)	Q	
	7.0×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	4.5×10^{-4}		Suzuki et al. (1992)	Q	232
	2.9×10^{-4}		Duchowicz et al. (2020)	?	185, 21
1,4-dibromobutane	1.7×10^{-2}		Albanese et al. (1987)	M	
$C_4H_8Br_2$	7.3×10^{-2}		Hilal et al. (2008)	Q	
[110-52-1]	4.3×10^{-3}		Modarresi et al. (2007)	Q	67
ULTHEAFYOOPTTB-UHFFFAOYSA-N					
1-bromopentane	5.0×10^{-4}		Duchowicz et al. (2020)	V	186
$C_5H_{11}Br$	4.7×10^{-4}		Abraham (1984)	V	
[110-53-2]	5.6×10^{-4}		Yaws (2003)	X	237
YZWKKMVJZFACSU-UHFFFAOYSA-N	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	6.1×10^{-4}		Gharagheizi et al. (2012)	Q	
	5.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.8×10^{-3}		Hilal et al. (2008)	Q	

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.5×10^{-4}		Modarresi et al. (2007)	Q	67
	5.1×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	4.6×10^{-4}		English and Carroll (2001)	Q	230, 231
	5.1×10^{-4}		Katritzky et al. (1998)	Q	
	8.0×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	5.6×10^{-4}		Yaws (1999)	?	21
	5.0×10^{-4}		Yaws and Yang (1992)	?	21
	4.7×10^{-4}		Abraham et al. (1990)	?	
1-bromo-2-methylbutane $C_5H_{11}Br$ [10422-35-2] XKVLZBNEPALHIO-UHFFFAOYSA-N	8.8×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
1-bromohexane $C_6H_{13}Br$ [111-25-1] MNDIARAMWBIKFW-UHFFFAOYSA-N	3.0×10^{-4}		Duchowicz et al. (2020)	V	186
	3.0×10^{-4}		Abraham (1984)	V	
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	3.1×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.5×10^{-3}		Hilal et al. (2008)	Q	
	5.2×10^{-4}		Modarresi et al. (2007)	Q	67
	2.2×10^{-4}		Yaffe et al. (2003)	Q	248, 272
	3.4×10^{-4}		English and Carroll (2001)	Q	230, 231
	5.3×10^{-4}		Katritzky et al. (1998)	Q	
	6.2×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	3.0×10^{-4}		Abraham et al. (1990)	?	
1-bromo-3-methylpentane $C_6H_{13}Br$ [51116-73-5] MDCCBJLCTOTLKM-UHFFFAOYSA-N	2.3×10^{-4}		English and Carroll (2001)	Q	230, 231
	5.8×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
bromocyclohexane $C_6H_{11}Br$ [108-85-0] AQNQQHJNRPDOQV-UHFFFAOYSA-N	7.0×10^{-3}		Hilal et al. (2008)	Q	
1-bromoheptane $C_7H_{15}Br$ [629-04-9] LSXKDWGTSHCFPP-UHFFFAOYSA-N	2.2×10^{-4}		Brockbank (2013)	L	
	2.2×10^{-4}		Duchowicz et al. (2020)	V	186
	2.3×10^{-4}		Abraham (1984)	V	
	2.2×10^{-4}		Yaws (2003)	X	237
	1.1×10^{-3}		Duchowicz et al. (2020)	Q	
	3.5×10^{-4}		Gharagheizi et al. (2012)	Q	
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	2.3×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.2×10^{-3}		Hilal et al. (2008)	Q	
	4.7×10^{-4}		Modarresi et al. (2007)	Q	67

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	6.5×10^{-5}		Yao et al. (2002)	Q	229
	2.6×10^{-4}		English and Carroll (2001)	Q	230, 274
	5.6×10^{-4}		Katritzky et al. (1998)	Q	
	5.0×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	2.2×10^{-4}		Yaws (1999)	?	21
	2.3×10^{-4}		Abraham et al. (1990)	?	
1-bromooctane $C_8H_{17}Br$ [111-83-1] VMKOFRJSULQZRM-UHFFFAOYSA-N	1.7×10^{-4}		Duchowicz et al. (2020)	V	186
	2.4×10^{-4}	4600	Sarraute et al. (2004)	V	
	1.7×10^{-4}		Abraham (1984)	V	
	1.1×10^{-3}		Duchowicz et al. (2020)	Q	
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	9.7×10^{-4}		Hilal et al. (2008)	Q	
	4.0×10^{-4}		Modarresi et al. (2007)	Q	67
	1.7×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	1.9×10^{-4}		English and Carroll (2001)	Q	230, 231
	5.6×10^{-4}		Katritzky et al. (1998)	Q	
	3.9×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	1.7×10^{-4}		Abraham et al. (1990)	?	
1,8-dibromooctane $C_8H_{16}Br_2$ [4549-32-0] DKEGCUDAFWNSSO-UHFFFAOYSA-N	1.3×10^{-2}	6900	Sarraute et al. (2006)	M	787
1,2-dibromo-4-(1,2-dibromoethyl)cyclohexane $C_8H_{12}Br_4$ [3322-93-8] PQRRSJBLKOPVJV-UHFFFAOYSA-N	1.7×10^{2}		HSDB (2015)	Q	99
	2.4×10^{-1}		Zhang et al. (2010)	Q	287, 288
	2.9		Zhang et al. (2010)	Q	287, 289
	1.0×10^{1}		Zhang et al. (2010)	Q	287, 290
	2.5×10^{-1}		Zhang et al. (2010)	Q	287, 291
1-bromononane $C_9H_{19}Br$ [693-58-3] AYMUQTNXKPEMLM-UHFFFAOYSA-N	7.9×10^{-4}		Hilal et al. (2008)	Q	
1-bromodecane $C_{10}H_{21}Br$ [112-29-8] MYMSJFSOOQERIO-UHFFFAOYSA-N	1.7×10^{-4}		Ebert et al. (2023)	?	316

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexabromocyclododecane	2.1×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{12}H_{18}Br_6$	2.1×10^{-1}		HSDB (2015)	V	
[3194-55-6]	1.6×10^{-2}		HSDB (2015)	V	
DEIGXXQKDWULML-UHFFFAOYSA-N	1.3×10^{-2}		Duchowicz et al. (2020)	Q	
	5.7		Zhang et al. (2010)	Q	287, 288
	1.7×10^{2}		Zhang et al. (2010)	Q	287, 289
	5.7×10^{3}		Zhang et al. (2010)	Q	287, 290
	6.5		Zhang et al. (2010)	Q	287, 291
vinyl bromide	7.0×10^{-4}		HSDB (2015)	Q	99
C_2H_3Br	8.0×10^{-4}		Zhang et al. (2010)	Q	287, 288
[593-60-2]	7.7×10^{-4}		Zhang et al. (2010)	Q	287, 289
INLLPKCGLOXCIV-UHFFFAOYSA-N	4.8×10^{-4}		Zhang et al. (2010)	Q	287, 290
	8.2×10^{-4}		Zhang et al. (2010)	Q	287, 291
1,2-dibromoethene	1.2×10^{-2}		Duchowicz et al. (2020)	V	186
$C_2H_2Br_2$	1.2×10^{-2}		HSDB (2015)	V	
[540-49-8]	4.8×10^{-3}		Duchowicz et al. (2020)	Q	
UWTUEMKLYAGTNQ-UHFFFAOYSA-N					
(*Z*)-1,2-dibromoethene	2.4×10^{-3}		Yaffe et al. (2003)	Q	248, 249
$C_2H_2Br_2$					
(*cis*-1,2-dibromoethene)					
[590-11-4]					
UWTUEMKLYAGTNQ-UPHRSURJSA-N					
3-bromo-1-propene	1.7×10^{-3}		Yaws (2003)	X	237
C_3H_5Br	9.0×10^{-4}		HSDB (2015)	Q	99
(allyl bromide)	3.9×10^{-3}		Gharagheizi et al. (2012)	Q	
[106-95-6]	1.6×10^{-3}		Gharagheizi et al. (2010)	Q	246
BHELZAPQIKSEDF-UHFFFAOYSA-N	8.6×10^{-3}		Hilal et al. (2008)	Q	
	2.6×10^{-3}		Modarresi et al. (2007)	Q	67
	1.0×10^{-3}		Yao et al. (2002)	Q	229
	1.7×10^{-3}		Yaws (1999)	?	21
	1.7×10^{-3}		Yaws and Yang (1992)	?	21
	1.7×10^{-3}		Abraham et al. (1990)	?	
3-bromo-1-propyne	8.8×10^{-3}	4000	Yates and Gan (1998)	M	1
C_3H_3Br	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
(propargyl bromide)	8.4×10^{-3}		Duchowicz et al. (2020)	Q	
[106-96-7]		3200	Kühne et al. (2005)	Q	
YORCIIVHUBAYBQ-UHFFFAOYSA-N	8.7×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4200	Kühne et al. (2005)	?	
			Fogg and Sangster (2003)	W	788
1-bromocyclohexene	2.0×10^{-3}		Hilal et al. (2008)	Q	
C_6H_9Br					
[2044-08-8]					
QBUMXSSCYUMVAW-UHFFFAOYSA-N					

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
1-bromo-4-methylcyclohexene $C_7H_{11}Br$ [31053-84-6] LIUFYLLBQSSKQS-UHFFFAOYSA-N	1.4×10^{-3}		Hilal et al. (2008)	Q	
bromobenzene C_6H_5Br [108-86-1] QARVLSVVCXYDNA-UHFFFAOYSA-N	4.3×10^{-3}	4500	Brockbank (2013)	L	1
	5.0×10^{-3}	4200	Fogg and Sangster (2003)	L	
	4.8×10^{-3}		Mackay and Shiu (1981)	L	
	6.0×10^{-3}	4300	Hiatt (2013)	M	
	3.9×10^{-3}	2900	Lau et al. (2010)	M	11
	5.0×10^{-3}		de Wolf and Lieder (1998)	M	87
	4.0×10^{-3}		Shiu and Mackay (1997)	M	
	6.1×10^{-3}		Hovorka and Dohnal (1997)	M	12
	4.9×10^{-3}	4200	Kondoh and Nakajima (1997)	M	
	5.3×10^{-3}	5300	Hansen et al. (1993)	M	281
	4.4×10^{-3}		Li and Carr (1993)	M	
	4.0×10^{-3}		Mackay and Shiu (1981)	M	
	4.7×10^{-3}		Shiu and Mackay (1997)	V	
	4.7×10^{-3}		Mackay et al. (1993)	V	
	5.0×10^{-3}		Hwang et al. (1992)	V	
	4.7×10^{-3}		Hine and Mookerjee (1975)	V	
	4.6×10^{-3}		Yaws (2003)	X	237
	4.7×10^{-3}		HSDB (2015)	C	
	4.0×10^{-3}		Schüürmann (2000)	C	21
	7.4×10^{-3}		Keshavarz et al. (2022)	Q	
	7.9×10^{-3}		Duchowicz et al. (2020)	Q	184
	3.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	4.2×10^{-3}		Gharagheizi et al. (2010)	Q	246
	5.2×10^{-3}		Hilal et al. (2008)	Q	
	7.7×10^{-3}		Modarresi et al. (2007)	Q	67
		4800	Kühne et al. (2005)	Q	
	4.1×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	4.2×10^{-3}		Yao et al. (2002)	Q	229
	5.4×10^{-3}		English and Carroll (2001)	Q	230, 231
	2.9×10^{-3}		Katritzky et al. (1998)	Q	
	5.1×10^{-3}		Suzuki et al. (1992)	Q	232
	7.3×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	4.0×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4300	Kühne et al. (2005)	?	
	4.6×10^{-3}		Yaws (1999)	?	21
	4.7×10^{-3}		Yaws and Yang (1992)	?	21
	4.7×10^{-3}		Abraham et al. (1990)	?	

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bromobenzene-d5 C_6D_5Br [4165-57-5] QARVLSVVCXYDNA-RALIUCGRSA-N	6.5×10^{-3}	4200	Hiatt (2013)	M	
1,2-dibromobenzene $C_6H_4Br_2$ [583-53-9] WQONPSCCEXUXTQ-UHFFFAOYSA-N	9.5×10^{-3}		Schüürmann (2000)	V	
1,3-dibromobenzene	1.2×10^{-2}		Brockbank (2013)	L	
$C_6H_4Br_2$	8.0×10^{-3}		Duchowicz et al. (2020)	V	186
[108-36-1]	5.0×10^{-3}		Mackay and Shiu (1981)	V	555
JSRLURSZEMLAFO-UHFFFAOYSA-N	1.2×10^{-2}		Yaws (2003)	X	237
	7.7×10^{-3}		Duchowicz et al. (2020)	Q	
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-2}		Gharagheizi et al. (2010)	Q	246
	9.0×10^{-3}		Hilal et al. (2008)	Q	
	6.4×10^{-3}		Modarresi et al. (2007)	Q	67
	7.0×10^{-3}		Yao et al. (2002)	Q	229
	4.2×10^{-2}		Katritzky et al. (1998)	Q	
	1.2×10^{-2}		Yaws (1999)	?	21
1,4-dibromobenzene	9.4×10^{-3}		Kuramochi et al. (2004)	M	
$C_6H_4Br_2$	1.1×10^{-2}		Duchowicz et al. (2020)	V	186
[106-37-6]	1.1×10^{-2}		HSDB (2015)	V	
SWJPEBQEEAHIGZ-UHFFFAOYSA-N	4.3×10^{-3}		Schüürmann (2000)	V	
	4.8×10^{-3}		Mackay and Shiu (1981)	V	555
	2.0×10^{-2}		Hine and Mookerjee (1975)	V	
	1.1×10^{-2}		Kuramochi et al. (2004)	C	
	7.1×10^{-3}		Duchowicz et al. (2020)	Q	
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	1.0×10^{-2}		Modarresi et al. (2007)	Q	67
		5600	Kühne et al. (2005)	Q	
	4.5×10^{-3}		English and Carroll (2001)	Q	230, 274
	4.1×10^{-2}		Katritzky et al. (1998)	Q	
	2.4×10^{-2}		Nirmalakhandan and Speece (1988)	Q	
		6900	Kühne et al. (2005)	?	
1,2,4-tribromobenzene	3.1×10^{-2}		Kuramochi et al. (2004)	M	
$C_6H_3Br_3$	2.9×10^{-2}		Kuramochi et al. (2004)	C	
[615-54-3]	1.8×10^{-2}		Hilal et al. (2008)	Q	
FWAJPSIPOULHHH-UHFFFAOYSA-N					

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,3,5-tribromobenzene	1.3×10^{-2}		Duchowicz et al. (2020)	V	186
$C_6H_3Br_3$	5.8×10^{-3}		Duchowicz et al. (2020)	Q	
[626-39-1]	2.9×10^{-2}		Zhang et al. (2010)	Q	287, 288
YWDUZLFWHVQCHY-UHFFFAOYSA-N	4.0×10^{-2}		Zhang et al. (2010)	Q	287, 289
	2.5×10^{-2}		Zhang et al. (2010)	Q	287, 290
	2.6×10^{-2}		Zhang et al. (2010)	Q	287, 291
	5.1×10^{-1}		Katritzky et al. (1998)	Q	
1,2,4,5-tetrabromobenzene	2.7×10^{-3}		Kuramochi et al. (2004)	M	
$C_6H_2Br_4$	2.0×10^{-2}		Hilal et al. (2008)	Q	
[636-28-2]					
QCKHVNQHBOGZER-UHFFFAOYSA-N					
hexabromobenzene	9.3×10^{-2}		Kuramochi et al. (2004)	M	
C_6Br_6	4.1×10^{-1}		Kuramochi et al. (2014)	V	
[87-82-1]	7.1		Tittlemier et al. (2002)	V	
CAYGQBVSOZLICD-UHFFFAOYSA-N	3.5×10^{-1}		HSDB (2015)	Q	99
	4.0×10^{-1}		Xiao et al. (2012)	Q	
	4.6×10^{-1}		Zhang et al. (2010)	Q	287, 288
	4.6×10^{-1}		Zhang et al. (2010)	Q	287, 289
	6.0×10^{-2}		Zhang et al. (2010)	Q	287, 290
	6.7×10^{-1}		Zhang et al. (2010)	Q	287, 291
	1.2×10^{-2}		Hilal et al. (2008)	Q	
(bromomethyl)-benzene	1.4×10^{-3}		HSDB (2015)	Q	99
C_7H_7Br	5.4×10^{-2}		Hilal et al. (2008)	Q	
(benzyl bromide)	2.2×10^{-2}		Abraham et al. (1990)	?	
[100-39-0]					
AGEZXYOZHKGVCM-UHFFFAOYSA-N					
p-bromobenzyl bromide	3.6×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_7H_6Br_2$	2.7×10^{-1}		Zhang et al. (2010)	Q	287, 289
[589-15-1]	2.0×10^{-1}		Zhang et al. (2010)	Q	287, 290
YLRBJYMANQKEAW-UHFFFAOYSA-N	2.4×10^{-2}		Zhang et al. (2010)	Q	287, 291
1-bromo-2-methylbenzene	4.1×10^{-3}		HSDB (2015)	Q	99
$BrC_6H_4CH_3$	5.3×10^{-3}		Hilal et al. (2008)	Q	
(*o*-bromotoluene)					
[95-46-5]					
QSSXJPIWXQTSIX-UHFFFAOYSA-N					
1-bromo-3-methylbenzene	1.5×10^{-3}		Duchowicz et al. (2020)	V	186
$BrC_6H_4CH_3$	1.5×10^{-3}		HSDB (2015)	V	
(*m*-bromotoluene)	4.0×10^{-3}		Duchowicz et al. (2020)	Q	
[591-17-3]	5.2×10^{-3}		Hilal et al. (2008)	Q	
WJIFKOVZNJTSGO-UHFFFAOYSA-N	4.8×10^{-3}		Modarresi et al. (2007)	Q	67
	1.5×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	7.9×10^{-3}		Katritzky et al. (1998)	Q	

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Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-bromo-4-methylbenzene	3.6×10^{-3}	4800	Brockbank (2013)	L	1
$BrC_6H_4CH_3$	3.4×10^{-3}	4600	Brockbank et al. (2013)	M	
(p-bromotoluene)	4.2×10^{-3}		Hine and Mookerjee (1975)	V	
[106-38-7]	5.3×10^{-2}		Keshavarz et al. (2022)	Q	
ZBTMRBYMKUEVEU-UHFFFAOYSA-N	4.0×10^{-3}		Duchowicz et al. (2020)	Q	299
	4.2×10^{-3}		Li et al. (2014)	Q	241
	5.6×10^{-3}		Hilal et al. (2008)	Q	
	5.5×10^{-3}		Modarresi et al. (2007)	Q	67
	4.5×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	3.4×10^{-3}		English and Carroll (2001)	Q	230, 231
	8.0×10^{-3}		Katritzky et al. (1998)	Q	
	5.2×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	3.6×10^{-3}		Suzuki et al. (1992)	Q	232
	5.2×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	4.2×10^{-3}		Duchowicz et al. (2020)	?	185, 21
	4.2×10^{-3}		Abraham et al. (1990)	?	
3,5-dibromotoluene	1.7×10^{-2}	4800	Hiatt (2013)	M	
$C_7H_6Br_2$					
[1611-92-3]					
DPKKOVGCHDUSAI-UHFFFAOYSA-N					
pentabromotoluene	4.0×10^{-1}		Xiao et al. (2012)	Q	
$C_7H_3Br_5$					
[87-83-2]					
OZHJEQVYCBTHJT-UHFFFAOYSA-N					
1-bromo-2-ethylbenzene	3.0×10^{-3}		Hine and Mookerjee (1975)	V	
C_8H_9Br	4.3×10^{-3}		Hilal et al. (2008)	Q	
[1973-22-4]	2.8×10^{-3}		English and Carroll (2001)	Q	230, 231
HVRUGFJYCAFAAN-UHFFFAOYSA-N	2.9×10^{-3}		Suzuki et al. (1992)	Q	232
	4.5×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
1-bromo-4-ethylbenzene	3.1×10^{-3}		Zhang et al. (2010)	Q	287, 288
C_8H_9Br	6.1×10^{-3}		Zhang et al. (2010)	Q	287, 289
[1585-07-5]	4.2×10^{-3}		Zhang et al. (2010)	Q	287, 290
URFPRAHGGBYNPW-UHFFFAOYSA-N	5.2×10^{-3}		Zhang et al. (2010)	Q	287, 291
1-(bromomethyl)-2-methylbenzene	1.3×10^{-2}		HSDB (2015)	Q	99
C_8H_9Br					
(o-xylyl bromide)					
[89-92-9]					
WGVYCXYGPNNUQA-UHFFFAOYSA-N					
1-(bromomethyl)-3-methylbenzene	1.3×10^{-2}		HSDB (2015)	Q	99
C_8H_9Br					
(m-xylyl bromide)					
[620-13-3]					
FWLWTILKTABGKQ-UHFFFAOYSA-N					

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-(bromomethyl)-4-methylbenzene C_8H_9Br (p-xylyl bromide) [104-81-4] WZRKSPFYXUXINF-UHFFFAOYSA-N	1.3×10^{-2}		HSDB (2015)	Q	99
(2-bromoethyl)-benzene C_8H_9Br [103-63-9] WMPPDTMATNBGJN-UHFFFAOYSA-N	6.5×10^{-3}		Duchowicz et al. (2020)	V	186
	6.5×10^{-3}		HSDB (2015)	V	
	7.9×10^{-3}		Duchowicz et al. (2020)	Q	
	2.2×10^{-2}		Modarresi et al. (2007)	Q	67
	6.9×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.3×10^{-2}		Katritzky et al. (1998)	Q	
2-bromostyrene C_8H_7Br [125904-11-2] SSZOCHFYWWVSAI-UHFFFAOYSA-N	9.0×10^{-3}		Zhang et al. (2010)	Q	287, 288
	9.5×10^{-3}		Zhang et al. (2010)	Q	287, 289
	7.3×10^{-3}		Zhang et al. (2010)	Q	287, 290
	1.5×10^{-2}		Zhang et al. (2010)	Q	287, 291
(2-bromoethenyl)benzene C_8H_7Br [103-64-0] YMOONIIMQBGTDU-VOTSOKGWSA-N	1.8×10^{-2}		HSDB (2015)	Q	99
2,3,4,5,6-pentabromoethylbenzene $C_8H_5Br_5$ [85-22-3] FIAXCDIQXHJNIX-UHFFFAOYSA-N	1.2×10^{-1}		Zhang et al. (2010)	Q	287, 288
	3.6×10^{-1}		Zhang et al. (2010)	Q	287, 289
	3.3×10^{-2}		Zhang et al. (2010)	Q	287, 290
	9.7×10^{-2}		Zhang et al. (2010)	Q	287, 291
1-bromo-2-(2-propyl)-benzene $BrC_6H_4C_3H_7$ (o-bromocumene) [7073-94-1] LECYCYNAEJDSIL-UHFFFAOYSA-N	1.7×10^{-3}		Hine and Mookerjee (1975)	V	
	2.5×10^{-3}		Hilal et al. (2008)	Q	
	2.0×10^{-3}		Suzuki et al. (1992)	Q	232
	3.1×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
1-bromonaphthalene $C_{10}H_7Br$ [90-11-9] DLKQHBOKULLWDQ-UHFFFAOYSA-N	3.5×10^{-2}		Duchowicz et al. (2020)	V	186
	5.0×10^{-2}		Yaws (2003)	X	237, 294
	3.0×10^{-2}		Duchowicz et al. (2020)	Q	
	5.0×10^{-2}		Gharagheizi et al. (2010)	Q	246
	8.2×10^{-2}		Hilal et al. (2008)	Q	
	3.7×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.8×10^{-2}		Katritzky et al. (1998)	Q	
	3.5×10^{-2}		Yaws (1999)	?	21, 294
2-bromonaphthalene $C_{10}H_7Br$ [580-13-2] APSMUYYLXZULMS-UHFFFAOYSA-N	4.3×10^{-2}		Ebert et al. (2023)	?	318

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,4-dibromonaphthalene $C_{10}H_6Br_2$ [83-53-4] IBGUDZMIAZLJNY-UHFFFAOYSA-N	5.8×10^{-2}		Ebert et al. (2023)	?	316
decabromobiphenyl $C_{12}Br_{10}$ [13654-09-6] AQPHBYQUCKHJLT-UHFFFAOYSA-N	2.3×10^{2} 2.4×10^{2} 3.0×10^{2} 2.3×10^{2} 5.0×10^{2}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	99 287, 288 287, 289 287, 290 287, 291
4-bromo-1,1'-biphenyl $C_{12}H_9Br$ [92-66-0] PKJBWOWQJHHAHG-UHFFFAOYSA-N	6.0×10^{-2} 6.9×10^{-2} 1.7×10^{-1} 3.5×10^{-1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
octabromobiphenyl $C_{12}H_2Br_8$ [27858-07-7] NDRKXFLZSRHAJE-UHFFFAOYSA-N	4.1×10^{3}		HSDB (2015)	V	
2,2',4,4',5,5'-hexabromobiphenyl $C_{12}H_4Br_6$ [59080-40-9] HMBBJSKXDBUNNT-UHFFFAOYSA-N	2.3		HSDB (2015)	V	
1,2-bis(pentabromophenyl) ethane $C_{14}H_4Br_{10}$ [84852-53-9] BZQKBFHEWDPQHD-UHFFFAOYSA-N	1.5×10^{2} 8.8×10^{2} 8.6×10^{1} 1.7×10^{2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
1,3,6,8-tetrabromopyrene $C_{16}H_6Br_4$ [128-63-2] ZKBKRTZIYOKNRG-UHFFFAOYSA-N	4.7×10^{1} 4.4×10^{1} 6.2×10^{-1} 6.5×10^{1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
6-bromobenzo[a]pyrene $C_{20}H_{11}Br$ [21248-00-0] MJSYSGSEEADMTK-UHFFFAOYSA-N	1.2×10^{2}		HSDB (2015)	Q	99
bromomethanol CH_2BrOH [50398-29-3] OEDMOCYNWLHUDP-UHFFFAOYSA-N	4.1 3.2×10^{1} 2.5×10^{2} 2.0×10^{1}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) Krysztofiak et al. (2012)	Q Q Q Q	80, 238 80, 239 80, 240
dibromomethanol $CHBr_2OH$ [166600-78-8] WICMSCLXMMZMFF-UHFFFAOYSA-N	1.7×10^{2}		Krysztofiak et al. (2012)	Q	

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tribromomethanol CBr_3OH [5405-30-1] ACRXLLXANWELLX-UHFFFAOYSA-N	1.5×10^{3}		Krysztofiak et al. (2012)	Q	
formyl bromide	4.5×10^{-1}		Wang et al. (2017)	Q	80, 238
$CHBrO$	3.2×10^{-2}		Wang et al. (2017)	Q	80, 239
[7726-11-6]	3.7×10^{-3}		Wang et al. (2017)	Q	80, 240
AIFARXRIYKCEEV-UHFFFAOYSA-N	7.3×10^{-1}		Krysztofiak et al. (2012)	Q	
carbonyl bromide CBr_2O [593-95-3] MOIPGXQKZSZOQX-UHFFFAOYSA-N	2.1×10^{-1}		Krysztofiak et al. (2012)	Q	
bromomethyl peroxide	3.7×10^{1}		Wang et al. (2017)	Q	80, 238
CH_2BrO_2H	1.3×10^{2}		Wang et al. (2017)	Q	80, 239
WXVCUAGYVVWQBP-UHFFFAOYSA-N	3.0×10^{1}		Wang et al. (2017)	Q	80, 240
	2.5×10^{1}		Krysztofiak et al. (2012)	Q	
dibromomethyl peroxide $CHBr_2O_2H$ JBKQCSQVMCXDPZ-UHFFFAOYSA-N	2.2×10^{2}		Krysztofiak et al. (2012)	Q	
tribromomethyl peroxide CBr_3O_2H WJYKCADCZNTKBI-UHFFFAOYSA-N	1.9×10^{3}		Krysztofiak et al. (2012)	Q	
bromoethanoic acid	1.5×10^{3}	9300	Burkholder et al. (2019)	L	
$CH_2BrCOOH$	1.5×10^{3}	9300	Burkholder et al. (2015)	L	
(bromoacetic acid)	1.5×10^{3}	9300	Sander et al. (2011)	L	
[79-08-3]	1.5×10^{3}	9300	Bowden et al. (1998a)	M	
KDPAWGWELVVRCH-UHFFFAOYSA-N	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	1.5×10^{2}		Duchowicz et al. (2020)	Q	184
	4.2×10^{2}		Wang et al. (2017)	Q	80, 238
	5.6×10^{3}		Wang et al. (2017)	Q	80, 239
	5.5×10^{2}		Wang et al. (2017)	Q	80, 240
	2.0×10^{3}		Raventos-Duran et al. (2010)	Q	242, 243
	2.5×10^{3}		Raventos-Duran et al. (2010)	Q	244
	1.6×10^{2}		Raventos-Duran et al. (2010)	Q	245
		8800	Kühne et al. (2005)	Q	
	1.5×10^{3}		Duchowicz et al. (2020)	?	185, 21
		9300	Kühne et al. (2005)	?	
dibromoethanoic acid	2.3×10^{3}	8900	Burkholder et al. (2019)	L	
$CHBr_2COOH$	2.3×10^{3}	8900	Burkholder et al. (2015)	L	
(dibromoacetic acid)	2.3×10^{3}	8900	Sander et al. (2011)	L	
[631-64-1]	2.2×10^{3}	8900	Bowden et al. (1998a)	M	
SIEILFNCEFEENQ-UHFFFAOYSA-N	5.6×10^{2}		Keshavarz et al. (2022)	Q	
	4.9×10^{2}		Duchowicz et al. (2020)	Q	184
	3.9×10^{3}		Raventos-Duran et al. (2010)	Q	242, 243

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	6.2×10^2		Raventos-Duran et al. (2010)	Q	244
	1.2×10^3		Raventos-Duran et al. (2010)	Q	245
		9900	Kühne et al. (2005)	Q	
	2.2×10^3		Duchowicz et al. (2020)	?	185, 21
		9000	Kühne et al. (2005)	?	
tribromoethanoic acid	3.0×10^3	9000	Burkholder et al. (2019)	L	
CBr_3COOH	3.0×10^3	9000	Burkholder et al. (2015)	L	
(tribromoacetic acid)	3.0×10^3	9000	Sander et al. (2011)	L	
[75-96-7]	2.9×10^3	9000	Bowden et al. (1998a)	M	
QIONYIKHPASLHO-UHFFFAOYSA-N	5.6×10^2		Keshavarz et al. (2022)	Q	
	3.5×10^2		Duchowicz et al. (2020)	Q	
	2.0×10^3		Raventos-Duran et al. (2010)	Q	271, 243
	9.9		Raventos-Duran et al. (2010)	Q	244
	1.2×10^4		Raventos-Duran et al. (2010)	Q	245
	3.0×10^3		Duchowicz et al. (2020)	?	185, 21
MCM:BRETO3H	4.5×10^2		Wang et al. (2017)	Q	80, 238
$C_2H_3O_3Br$	1.4×10^2		Wang et al. (2017)	Q	80, 239
RGXORGOPJDPEIK-UHFFFAOYSA-N	9.8×10^{-1}		Wang et al. (2017)	Q	80, 240
MCM:DIBRETO2H	5.4×10^2		Wang et al. (2017)	Q	80, 238
$C_2H_4O_2Br_2$	2.2×10^2		Wang et al. (2017)	Q	80, 239
ZXSZEFURCAPOPD-UHFFFAOYSA-N	9.6×10^1		Wang et al. (2017)	Q	80, 240
MCM:DIBRETOH	1.1×10^2		Wang et al. (2017)	Q	80, 238
$C_2H_4OBr_2$	1.1×10^2		Wang et al. (2017)	Q	80, 239
IYJYRKYSUOTLAE-UHFFFAOYSA-N	1.7×10^3		Wang et al. (2017)	Q	80, 240
MCM:BRETAL	4.1×10^{-1}		Wang et al. (2017)	Q	80, 238
C_2H_3OBr	6.0		Wang et al. (2017)	Q	80, 239
NMPVEAUIHMEAQP-UHFFFAOYSA-N	2.5×10^{-1}		Wang et al. (2017)	Q	80, 240
3-bromopropanol C_3H_7BrO [627-18-9] RQFUZUMFPRMVDX-UHFFFAOYSA-N	8.2		Modarresi et al. (2007)	Q	67
2,3-dibromopropanol	1.6×10^2		HSDB (2015)	Q	99
$C_3H_6Br_2O$	1.6×10^2		Zhang et al. (2010)	Q	287, 288
[96-13-9]	1.1×10^2		Zhang et al. (2010)	Q	287, 289
QWVCIORZLNBIIC-UHFFFAOYSA-N	1.2×10^1		Zhang et al. (2010)	Q	287, 290
	1.4×10^1		Zhang et al. (2010)	Q	287, 291
bromoacetone C_3H_5BrO [598-31-2] VQFAIAKCILWQPZ-UHFFFAOYSA-N	1.7		HSDB (2015)	Q	99

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(bromomethyl)oxirane C_3H_5BrO (epibromohydrin) [3132-64-7] GKIPXFAANLTWBM-UHFFFAOYSA-N	4.1		HSDB (2015)	Q	99
2,3-dibromobutane-1,4-diol $C_4H_8Br_2O_2$ [90801-18-6] OXYNQEOLHRWEPE-QWWZWVQMSA-N	3.2×10^3 1.0×10^5 1.5×10^6 4.7×10^4		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
bromoacetic acid, ethyl ester $C_4H_7BrO_2$ [105-36-2] PQJJJMRNHATNKG-UHFFFAOYSA-N	3.7×10^{-1}		HSDB (2015)	Q	99
brometone $C_4H_7Br_3O$ (1,1,1-tribromo-2-methyl-2-propanol) [76-08-4] JUGRTVJQTFZHOM-UHFFFAOYSA-N	1.0×10^3		HSDB (2015)	Q	99
2,2-bis(bromomethyl)-1,3-propanediol $C_5H_{10}Br_2O_2$ [3296-90-0] CHUGKEQJSLOLHL-UHFFFAOYSA-N	2.4×10^3		HSDB (2015)	Q	99
trisbromoneopentyl alcohol $C_5H_9Br_3O$ [36483-57-5] HQWKMYFWGMCJSW-UHFFFAOYSA-N	7.7×10^2 7.5 1.1×10^1 1.0		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
2-bromophenol HOC_6H_4Br [95-56-7] VADKRMSMGWJZCF-UHFFFAOYSA-N	4.5×10^1 4.2		HSDB (2015) Hilal et al. (2008)	Q Q	99
3-bromophenol HOC_6H_4Br [591-20-8] MNOJRWOWILAHAV-UHFFFAOYSA-N	4.5×10^1 2.3×10^1		HSDB (2015) Hilal et al. (2008)	Q Q	99
4-bromophenol HOC_6H_4Br [106-41-2] GZFGOTFRPZRKDS-UHFFFAOYSA-N	6.7×10^1 6.8×10^1 4.3 1.5×10^2 6.5×10^1 2.0×10^1 2.5×10^1	 8200 	Abraham et al. (1994a) Parsons et al. (1971) Keshavarz et al. (2022) Duchowicz et al. (2020) Li et al. (2014) Raventos-Duran et al. (2010) Raventos-Duran et al. (2010)	R T Q Q Q Q Q	 417 241 242, 243 244

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	4.9×10^{1}		Raventos-Duran et al. (2010)	Q	245
	1.6×10^{1}		Hilal et al. (2008)	Q	
	2.3×10^{1}		Modarresi et al. (2007)	Q	67
	6.5×10^{1}		Yaffe et al. (2003)	Q	248, 249
	3.5×10^{1}		English and Carroll (2001)	Q	230, 231
	1.3×10^{2}		Katritzky et al. (1998)	Q	
	3.0×10^{2}		Nirmalakhandan et al. (1997)	Q	
	3.3×10^{1}		Nirmalakhandan and Speece (1988)	Q	
	6.5×10^{1}		Duchowicz et al. (2020)	?	185, 21
	6.9×10^{1}		Abraham et al. (1990)	?	
2,4-dibromophenol $C_6H_4Br_2O$ [615-58-7] FAXWFCTVSHEODL-UHFFFAOYSA-N	1.1×10^{2}		HSDB (2015)	Q	99
2,6-dibromophenol $C_6H_4Br_2O$ [608-33-3] SSIZLKDLDKIHEV-UHFFFAOYSA-N	1.1×10^{2}		HSDB (2015)	Q	99
2,4,6-tribromophenol $C_6H_3Br_3O$ [118-79-6] BSWWXRFVMJHFBN-UHFFFAOYSA-N	2.1×10^{2}		HSDB (2015)	Q	99
	2.8×10^{2}		Zhang et al. (2010)	Q	287, 288
	1.5×10^{-1}		Zhang et al. (2010)	Q	287, 289
	6.2		Zhang et al. (2010)	Q	287, 290
	7.7		Zhang et al. (2010)	Q	287, 291
2,3,4,6-tetrabromophenol $C_6H_2Br_4O$ [14400-94-3] CXPJZISGVIVNEL-UHFFFAOYSA-N	7.0×10^{2}		HSDB (2015)	Q	99
pentabromophenol C_6HBr_5O [608-71-9] SVHOVVJFOWGYJO-UHFFFAOYSA-N	1.8×10^{3}		HSDB (2015)	Q	99
	1.8×10^{3}		Zhang et al. (2010)	Q	287, 288
	1.2		Zhang et al. (2010)	Q	287, 289
	2.2×10^{1}		Zhang et al. (2010)	Q	287, 290
	1.3×10^{2}		Zhang et al. (2010)	Q	287, 291
1-bromo-2-methoxybenzene C_7H_7BrO (2-bromoanisole) [578-57-4] HTDQSWDEWGSAMN-UHFFFAOYSA-N	2.9×10^{-2}		Pfeifer et al. (2001)	M	731
1-bromo-3-methoxybenzene C_7H_7BrO (3-bromoanisole) [2398-37-0] PLDWAJLZAAHOGG-UHFFFAOYSA-N	7.2×10^{-3}		Pfeifer et al. (2001)	M	731

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
1-bromo-4-methoxybenzene C_7H_7BrO (4-bromoanisole) [104-92-7] QJPJQTDYNZXKQF-UHFFFAOYSA-N	1.1×10^{-2}		Pfeifer et al. (2001)	M	731
1,5-dibromo-2-methoxybenzene $C_7H_6Br_2O$ (2,4-dibromoanisole) [21702-84-1] XGXUGXPKRBQINS-UHFFFAOYSA-N	8.1×10^{-2}		Pfeifer et al. (2001)	M	731
1,3-dibromo-2-methoxybenzene $C_7H_6Br_2O$ (2,6-dibromoanisole) [38603-09-7] BMZVDHQOAJUZJL-UHFFFAOYSA-N	3.7×10^{-2}		Pfeifer et al. (2001)	M	731
1,2,3-tribromo-4-methoxybenzene $C_7H_5Br_3O$ (2,3,4-tribromoanisole) [95970-13-1] NKWYZAWFQZLPSU-UHFFFAOYSA-N	9.9×10^{-3}		Ebert et al. (2023)	?	789
1,3,4-tribromo-2-methoxybenzene $C_7H_5Br_3O$ (2,3,6-tribromoanisole) [95970-19-7] XZYCSFIRWAPGJV-UHFFFAOYSA-N	5.2×10^{-3}	2800	Diaz et al. (2005)	M	790
1,3,5-tribromo-2-methoxybenzene $C_7H_5Br_3O$ (2,4,6-tribromoanisole) [607-99-8] YXTRCOAFNXQTKL-UHFFFAOYSA-N	1.9×10^{-2} 1.3×10^{-2} 3.1×10^{-2}	6400	Diaz et al. (2005) Pfeifer et al. (2001) HSDB (2015)	M M Q	 731 99
pentabromomethoxybenzene $C_7H_3Br_5O$ (pentabromoanisole) [1825-26-9] VEFNQGLEDJPUJF-UHFFFAOYSA-N	1.0		Pfeifer et al. (2001)	M	731
1,3,5-tribromo-2-methoxy-4-methylbenzene $C_8H_7Br_3O$ [41424-36-6] NMPPAMFEYWGNCI-UHFFFAOYSA-N	4.4×10^{-1} 2.0×10^{-1} 3.2×10^{-1} 1.9×10^{-1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,5,6,7-tetrabromo-1,3-isobenzofurandione	6.1×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_8Br_4O_3$	4.4×10^{5}		Zhang et al. (2010)	Q	287, 289
[632-79-1]	2.4×10^{2}		Zhang et al. (2010)	Q	287, 290
QHWKHLYUUZGSCW-UHFFFAOYSA-N	8.0×10^{2}		Zhang et al. (2010)	Q	287, 291
allyl 2,4,6-tribromophenyl ether	3.8×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_9H_7Br_3O$	1.3×10^{-1}		Zhang et al. (2010)	Q	287, 289
[3278-89-5]	2.0×10^{-1}		Zhang et al. (2010)	Q	287, 290
RZLLIOPGUFOWOD-UHFFFAOYSA-N	6.2×10^{-1}		Zhang et al. (2010)	Q	287, 291
2,4-dibromo-6-methylphenyl glycidyl ether	8.2×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_{10}H_{10}Br_2O_2$	7.0		Zhang et al. (2010)	Q	287, 289
[75150-13-9]	5.2×10^{1}		Zhang et al. (2010)	Q	287, 290
XQTJZNGNEJLXTR-UHFFFAOYSA-N	5.4		Zhang et al. (2010)	Q	287, 291
2-(2,4,6-tribromophenoxy)ethyl acrylate	2.9×10^{2}		Zhang et al. (2010)	Q	287, 288
$C_{11}H_9Br_3O_3$	1.6×10^{1}		Zhang et al. (2010)	Q	287, 289
[7347-19-5]	4.3×10^{3}		Zhang et al. (2010)	Q	287, 290
AMBJXYFIMKHOQE-UHFFFAOYSA-N	1.3×10^{2}		Zhang et al. (2010)	Q	287, 291
2,3,7,8-tetrabromodibenzo-*p*-dioxin $C_{12}H_4Br_4O_2$ [50585-41-6] JZLQUWSWOJPCAK-UHFFFAOYSA-N	3.0		Ebert et al. (2023)	?	318
octabromodibenzo-*p*-dioxin $C_{12}Br_8O_2$ [2170-45-8] XAHTWKGGNHXJRP-UHFFFAOYSA-N	5.1×10^{1}		Ebert et al. (2023)	?	318
4,4'-methylenebis(2,6-dibromophenol)	7.5×10^{7}		Zhang et al. (2010)	Q	287, 288
$C_{13}H_8Br_4O_2$	9.0×10^{1}		Zhang et al. (2010)	Q	287, 289
[21825-03-6]	1.3×10^{4}		Zhang et al. (2010)	Q	287, 290
WPZJSWWEEJJSIZ-UHFFFAOYSA-N	3.4×10^{3}		Zhang et al. (2010)	Q	287, 291
1,1'-[1,2-ethanediylbis(oxy)]bis pentabromobenzene	5.3×10^{4}		Zhang et al. (2010)	Q	287, 288
$C_{14}H_4Br_{10}O_2$	8.6×10^{2}		Zhang et al. (2010)	Q	287, 289
[61262-53-1]	2.2×10^{2}		Zhang et al. (2010)	Q	287, 290
JJEPQBZQAGCZTH-UHFFFAOYSA-N	1.1×10^{3}		Zhang et al. (2010)	Q	287, 291
4,4'-dibromobenzil	8.0×10^{3}		Zhang et al. (2010)	Q	287, 288
$C_{14}H_8Br_2O_2$	2.6×10^{3}		Zhang et al. (2010)	Q	287, 289
[35578-47-3]	1.9×10^{2}		Zhang et al. (2010)	Q	287, 290
NYCBYBDDECLFPE-UHFFFAOYSA-N	1.3×10^{5}		Zhang et al. (2010)	Q	287, 291

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2-bis(2,4,6-tribromophenoxy)ethane	1.8×10^{1}		Kuramochi et al. (2014)	V	
$C_{14}H_8Br_6O_2$	2.3×10^{1}		HSDB (2015)	Q	99
(BTBPE)	6.4×10^{1}		Xiao et al. (2012)	Q	
[37853-59-1]	1.3×10^{3}		Zhang et al. (2010)	Q	287, 288
YATIGPZCMOYEGE-UHFFFAOYSA-N	7.3×10^{1}		Zhang et al. (2010)	Q	287, 289
	1.1×10^{3}		Zhang et al. (2010)	Q	287, 290
	1.0×10^{3}		Zhang et al. (2010)	Q	287, 291
2-ethylhexyl-2,3,4,5-tetrabromobenzoate	1.6		Xiao et al. (2012)	Q	
$C_{15}H_{18}Br_4O_2$					
(EHTeBB)					
[183658-27-7]					
HVDXCGSGEQKWGB-UHFFFAOYSA-N					
tribromobisphenol A	1.1×10^{2}		HSDB (2015)	Q	447
$C_{15}H_{13}Br_3O_2$					
[6386-73-8]					
WYBOEVJIVYIEJL-UHFFFAOYSA-N					
4,4'-(1-methylethylidene)bis(2,6-dibromophenol)	2.4×10^{2}		HSDB (2015)	V	
$C_{15}H_{12}Br_4O_2$	4.2×10^{7}		Zhang et al. (2010)	Q	287, 288
[79-94-7]	3.9×10^{1}		Zhang et al. (2010)	Q	287, 289
VEORPZCZECFIRK-UHFFFAOYSA-N	8.0×10^{4}		Zhang et al. (2010)	Q	287, 290
	1.6×10^{3}		Zhang et al. (2010)	Q	287, 291
4-[2-[2,6-bis(bromanyl)-4-oxidanyl-phenyl]propan-2-yl]-3,5-bis(bromanyl)phenol	4.2×10^{7}		Zhang et al. (2010)	Q	287, 288
$C_{15}H_{12}Br_4O_2$	2.0×10^{7}		Zhang et al. (2010)	Q	287, 289
[94334-64-2]	2.2×10^{7}		Zhang et al. (2010)	Q	287, 290
KIZJVNGSIWXYTL-UHFFFAOYSA-N	1.7×10^{8}		Zhang et al. (2010)	Q	287, 291
2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl 3,4,5,6-tetrabromophthalate	3.6×10^{10}		Zhang et al. (2010)	Q	287, 288
$C_{15}H_{16}Br_4O_7$	1.5×10^{11}		Zhang et al. (2010)	Q	287, 289
[20566-35-2]	3.1×10^{13}		Zhang et al. (2010)	Q	287, 290
OQHHASWHOGRCRC-UHFFFAOYSA-N	5.7×10^{10}		Zhang et al. (2010)	Q	287, 291
bromopropylate	2.1×10^{1}		Duchowicz et al. (2020)	V	186
$C_{17}H_{16}Br_2O_3$	2.1×10^{1}		HSDB (2015)	V	
[18181-80-1]	4.2×10^{2}		Duchowicz et al. (2020)	Q	
FOANIXZHAMJWOI-UHFFFAOYSA-N					

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,2,4,5-tetrabromo-3,6-bis(pentabromophenoxy)benzene	1.5×10^{6}		Zhang et al. (2010)	Q	287, 288
$C_{18}O_2Br_{14}$	4.1×10^{5}		Zhang et al. (2010)	Q	287, 289
[58965-66-5]	2.1×10^{6}		Zhang et al. (2010)	Q	287, 290
YMIUHIAWWDYGGU-UHFFFAOYSA-N	6.7×10^{5}		Zhang et al. (2010)	Q	287, 291
2,2-bis(3,5-dibromo-4-(2-hydroxyethoxy)phenyl)propane	5.6×10^{7}		Zhang et al. (2010)	Q	287, 288
$C_{19}H_{20}Br_4O_4$	1.5×10^{8}		Zhang et al. (2010)	Q	287, 289
[4162-45-2]	6.1×10^{9}		Zhang et al. (2010)	Q	287, 290
RVHUMFJSCJBNGS-UHFFFAOYSA-N	2.5×10^{8}		Zhang et al. (2010)	Q	287, 291
metrafenone $C_{19}H_{21}BrO_5$ [220899-03-6] AMSPWOYQQAWRRM-UHFFFAOYSA-N	7.6		Maniere et al. (2011)	?	12, 165
solvent red 43	4.4×10^{12}		Zhang et al. (2010)	Q	287, 288
$C_{20}H_8Br_4O_5$	1.5×10^{8}		Zhang et al. (2010)	Q	287, 289
[15086-94-9]	2.7×10^{10}		Zhang et al. (2010)	Q	287, 290
DBZJJPROPLPMSN-UHFFFAOYSA-N	2.9×10^{8}		Zhang et al. (2010)	Q	287, 291
2,2-bis[4-(2,3-dibromopropoxy)-3,5-dibromophenyl]-propane	2.4×10^{5}		Zhang et al. (2010)	Q	287, 288
$C_{21}H_{20}Br_8O_2$	4.0×10^{4}		Zhang et al. (2010)	Q	287, 289
[21850-44-2]	1.7×10^{5}		Zhang et al. (2010)	Q	287, 290
LXIZRZRTWSDLKK-UHFFFAOYSA-N	8.6×10^{4}		Zhang et al. (2010)	Q	287, 291
2,2-bis(4-allyloxy-3,5-dibromophenyl)propane	7.7×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_{21}H_{20}Br_4O_2$	1.3×10^{1}		Zhang et al. (2010)	Q	287, 289
[25327-89-3]	1.7×10^{2}		Zhang et al. (2010)	Q	287, 290
PWXTUWQHMIFLKL-UHFFFAOYSA-N	1.9×10^{2}		Zhang et al. (2010)	Q	287, 291
AC1MJ2TG	1.3×10^{8}		Zhang et al. (2010)	Q	287, 288
$C_{21}H_{24}Br_4O_4$	4.7×10^{6}		Zhang et al. (2010)	Q	287, 289
[33294-14-3]	9.2×10^{6}		Zhang et al. (2010)	Q	287, 290
UTMWVHZWNKBNKF-UHFFFAOYSA-N	1.2×10^{6}		Zhang et al. (2010)	Q	287, 291
tetrabromophenolphthalein, ethyl ester	1.0×10^{11}		Zhang et al. (2010)	Q	287, 288
$C_{22}H_{14}Br_4O_4$	1.2×10^{7}		Zhang et al. (2010)	Q	287, 289
[1176-74-5]	3.1×10^{10}		Zhang et al. (2010)	Q	287, 290
SQFXATUXPUCFFO-UHFFFAOYSA-N	3.5×10^{8}		Zhang et al. (2010)	Q	287, 291
4,10-dibromodibenzo[def,mno]chrysene-6,12-dione	5.8×10^{6}		Zhang et al. (2010)	Q	287, 288
$C_{22}H_8Br_2O_2$	2.7×10^{5}		Zhang et al. (2010)	Q	287, 289
[4378-61-4]	4.1×10^{6}		Zhang et al. (2010)	Q	287, 290
HTENFZMEHKCNMD-UHFFFAOYSA-N	1.1×10^{8}		Zhang et al. (2010)	Q	287, 291

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Table A7.1: Bromocarbons (C, H, O, N, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bis(2-ethylhexyl)-3,4,5,6-tetrabromophthalate $C_{24}H_{34}Br_4O_4$ (TBPH) [26040-51-7] UUEDINPOVKWVAZ-UHFFFAOYSA-N	4.0×10^2		Xiao et al. (2012)	Q	
bromadiolone $C_{30}H_{23}BrO_4$ [28772-56-7] OWNRRUFOJXFKCU-UHFFFAOYSA-N	1.1×10^6 1.1×10^6		HSDB (2015) Maniere et al. (2011)	V ?	 241, 165
brodifacoum $C_{31}H_{23}BrO_3$ [56073-10-0] VEUZZDOCACZPRY-UHFFFAOYSA-N	4.6×10^2		Rubbiani (2013)	?	

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A7.2 Polybrominated diphenyl ethers (PBDEs)

Table A7.2: Polybrominated diphenyl ethers (PBDEs)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-bromodiphenyl ether $C_{12}H_9BrO$ (PBDE-1) [36563-47-0] RRWFUWRLNIZICP-UHFFFAOYSA-N	2.3×10^{-2}	7400	Long et al. (2017)	Q	287
3-bromodiphenyl ether $C_{12}H_9BrO$ (PBDE-2) [6876-00-2] AHDAKFFMKLQPTD-UHFFFAOYSA-N	2.3×10^{-2}	7400	Long et al. (2017)	Q	287
4-bromodiphenyl ether $C_{12}H_9BrO$ (PBDE-3) [101-55-3] JDUYPUMQALQRCN-UHFFFAOYSA-N	5.0×10^{-2} 4.3×10^{-2} 5.8×10^{-2} 9.6×10^{-2} 1.4×10^{-2} 8.2×10^{-2}	 5500 7400 	Lau et al. (2006) Lau et al. (2006) Charles and Destaillats (2005) Mackay et al. (1993) Long et al. (2017) HSDB (2015)	M M M V Q Q	719 720 287 99
2,2'-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-4) [51452-87-0] JMSKYMHFNWGUJG-UHFFFAOYSA-N	9.5×10^{-2}	7400	Long et al. (2017)	Q	287
2,3-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-5) [446254-14-4] JTYRXXKXOULVAP-UHFFFAOYSA-N	5.1×10^{-2}	7400	Long et al. (2017)	Q	287
2,3'-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-6) [147217-72-9] GODQTPRKFHOLPH-UHFFFAOYSA-N	9.4×10^{-2}	7400	Long et al. (2017)	Q	287
2,4-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-7) [171977-44-9] JMCIHKKTRDLVCO-UHFFFAOYSA-N	6.9×10^{-2}	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4'-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-8) [147217-71-8] RJQLQJZMLISKRJ-UHFFFAOYSA-N	5.8×10^{-2}	7400	Long et al. (2017)	Q	287
2,5-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-9) [337513-66-3] URDWJMUOJJSXAE-UHFFFAOYSA-N	8.0×10^{-2}	7400	Long et al. (2017)	Q	287
2,6-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-10) [51930-04-2] MUVDKHMQIZJFTC-UHFFFAOYSA-N	8.3×10^{-2}	7400	Long et al. (2017)	Q	287
3,3'-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-11) [6903-63-5] ALSVFJIXSNRBLE-UHFFFAOYSA-N	7.8×10^{-2}	7400	Long et al. (2017)	Q	287
3,4-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-12) [189084-59-1] SUUJFDKVPDCZQZ-UHFFFAOYSA-N	3.3×10^{-2}	7400	Long et al. (2017)	Q	287
3,4'-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-13) [83694-71-7] BGPOVBPKODCMMN-UHFFFAOYSA-N	5.5×10^{-2}	7400	Long et al. (2017)	Q	287
3,5-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-14) [46438-88-4] FOXBZJLXVUHYQZ-UHFFFAOYSA-N	9.9×10^{-2}	7400	Long et al. (2017)	Q	287
4,4'-dibromodiphenyl ether $C_{12}H_8Br_2O$ (PBDE-15) [2050-47-7] YAWIAFUBXXPJMQ-UHFFFAOYSA-N	8.3×10^{-2}		Lau et al. (2006)	M	719
	7.1×10^{-2}		Lau et al. (2006)	M	720
	7.3×10^{-2}	4500	Charles and Destaillats (2005)	M	
	4.8×10^{-2}		Tittlemier et al. (2002)	V	
	2.4×10^{-1}		Wania and Dugani (2003)	R	
	3.9×10^{-2}	7400	Long et al. (2017)	Q	287
	9.0×10^{-2}		Hilal et al. (2008)	Q	

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-16) [147217-74-1] VRNGWCVCSHJUEJ-UHFFFAOYSA-N	2.2×10^{-1}	7400	Long et al. (2017)	Q	287
2,2',4-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-17) [147217-75-2] VYBFILXLBMWOLI-UHFFFAOYSA-N	2.3×10^{-1}	7400	Long et al. (2017)	Q	287
2,2',5-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-18) [407606-55-7] FAZLXBWRNJAGSV-UHFFFAOYSA-N	2.4×10^{-1}	7400	Long et al. (2017)	Q	287
2,2',6-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-19) [147217-73-0] YDFQHBRKURQGAH-UHFFFAOYSA-N	3.6×10^{-1}	7400	Long et al. (2017)	Q	287
2,3,3'-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-20) [147217-76-3] RQJUBSPXDSGLRB-UHFFFAOYSA-N	1.8×10^{-1}	7400	Long et al. (2017)	Q	287
2,3,4-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-21) [337513-67-4] RXWRVYYPLRPDOS-UHFFFAOYSA-N	1.0×10^{-1}	7400	Long et al. (2017)	Q	287
2,3,4'-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-22) [446254-15-5] WZHNIFQVNBINLF-UHFFFAOYSA-N	1.2×10^{-1}	7400	Long et al. (2017)	Q	287
2,3,5-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-23) [446254-16-6] XQHLKDAUZRXBGC-UHFFFAOYSA-N	2.3×10^{-1}	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,6-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-24) [218304-36-0] GFLRHBRMAZDOIG-UHFFFAOYSA-N	1.8×10^{-1}	7400	Long et al. (2017)	Q	287
2,3',4-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-25) [147217-77-4] AURKEOPYVUYTLO-UHFFFAOYSA-N	2.3×10^{-1}	7400	Long et al. (2017)	Q	287
2,3',5-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-26) [337513-75-4] VUOBKVBAFJQQDB-UHFFFAOYSA-N	2.5×10^{-1}	7400	Long et al. (2017)	Q	287
2,3',6-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-27) [337513-53-8] JUPZALSVNWJHII-UHFFFAOYSA-N	3.4×10^{-1}	7400	Long et al. (2017)	Q	287
2,4,4'-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-28) [41318-75-6] UPNBETHEXPIWQX-UHFFFAOYSA-N	1.6×10^{-1} 1.1×10^{-1} 7.7×10^{-2} 1.8×10^{-1} 1.2×10^{-1} 2.0×10^{-1} 5.2×10^{-1} 1.8×10^{-1} 1.4×10^{-1}	8100 7400 12000 7400 	Long et al. (2017) Lau et al. (2006) Lau et al. (2006) Cetin and Odabasi (2005) Charles and Destaillats (2005) Tittlemier et al. (2002) Wania and Dugani (2003) Long et al. (2017) Hilal et al. (2008)	M M M M M V R Q Q	287 719 720 33 287
2,4,5-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-29) [337513-56-1] LTMKAFUXYKEDLR-UHFFFAOYSA-N	1.6×10^{-1}	7400	Long et al. (2017)	Q	287
2,4,6-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-30) [155999-95-4] TVZAPPGLBLTACB-UHFFFAOYSA-N	3.4×10^{-1}	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,4',5-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-31) [65075-08-3] PURZBWMLFRWRMG-UHFFFAOYSA-N	1.9×10^{-1}	7400	Long et al. (2017)	Q	287
2,4',6-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-32) [189084-60-4] TYDVYKIQSZGUMV-UHFFFAOYSA-N	1.6×10^{-1}	7400	Long et al. (2017)	Q	287
2,3',4'-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-33) [49690-94-0] BUQBQEYUVAKJQK-UHFFFAOYSA-N	1.3×10^{-1}	7400	Long et al. (2017)	Q	287
2,3',5'-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-34) [446254-17-7] XMNXHCHZIPYCNA-UHFFFAOYSA-N	4.2×10^{-1}	7400	Long et al. (2017)	Q	287
3,3',4-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-35) [147217-80-9] CDVYKQPKJYPWRO-UHFFFAOYSA-N	1.2×10^{-1}	7400	Long et al. (2017)	Q	287
3,3',5-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-36) [147217-79-6] XUKPJLVONRTECE-UHFFFAOYSA-N	2.8×10^{-1}	7400	Long et al. (2017)	Q	287
3,4,4'-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-37) [147217-81-0] YALAYFVVZFORPV-UHFFFAOYSA-N	9.0×10^{-2}	7400	Long et al. (2017)	Q	287
3,4,5-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-38) [337513-54-9] DPGVQKLGQZZLMI-UHFFFAOYSA-N	9.9×10^{-2}	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,4',5-tribromodiphenyl ether $C_{12}H_7Br_3O$ (PBDE-39) [407606-57-9] UFFNOPDHJNQYKD-UHFFFAOYSA-N	2.0×10^{-1}	7400	Long et al. (2017)	Q	287
2,2',3,3'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-40) [337513-77-6] SXSUUFZWSVMTRL-UHFFFAOYSA-N	4.8×10^{-1}	7400	Long et al. (2017)	Q	287
2,2',3,4-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-41) [337513-68-5] UAEBSKBXZAIRMX-UHFFFAOYSA-N	3.2×10^{-1}	7400	Long et al. (2017)	Q	287
2,2',3,4'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-42) [446254-18-8] HQDQKPAHIDGGMH-UHFFFAOYSA-N	5.2×10^{-1}	7400	Long et al. (2017)	Q	287
2,2',3,5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-43) [446254-19-9] LKMQHSYDVDIECC-UHFFFAOYSA-N	6.6×10^{-1}	7400	Long et al. (2017)	Q	287
2,2',3,5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-44) [446254-20-2] VBGBGTYMDIVKNK-UHFFFAOYSA-N	5.7×10^{-1}	7400	Long et al. (2017)	Q	287
2,2',3,6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-45) [446254-21-3] VTFWUBIOZQCMQS-UHFFFAOYSA-N	7.3×10^{-1}	7400	Long et al. (2017)	Q	287
2,2',3,6'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-46) [446254-22-4] GBUUKJRFSKCMTB-UHFFFAOYSA-N	1.1	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',4,4'-tetrabromodiphenyl ether	9.1×10^{-1}	7400	Long et al. (2017)	M	287
$C_{12}H_6Br_4O$	1.6×10^{-1}		Lau et al. (2006)	M	719
(PBDE-47)	1.7×10^{-1}		Lau et al. (2006)	M	720
[5436-43-1]	8.7×10^{-1}	7300	Cetin and Odabasi (2005)	M	
XYBSIYMGXVUVGY-UHFFFAOYSA-N	1.7×10^{-1}	620	Charles and Destaillats (2005)	M	42
	9.3×10^{-1}		Kuramochi et al. (2014)	V	
	6.7×10^{-1}		Tittlemier et al. (2002)	V	
	9.0×10^{-1}		Wania and Dugani (2003)	R	
	8.5×10^{-1}	7400	Long et al. (2017)	Q	287
	2.2×10^{-1}		Hilal et al. (2008)	Q	
2,2',4,5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-48) [337513-55-0] FJGDNHOVDFREMP-UHFFFAOYSA-N	4.8×10^{-1}	7400	Long et al. (2017)	Q	287
2,2',4,5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-49) [243982-82-3] QWVDUBDYUPHNHY-UHFFFAOYSA-N	8.6×10^{-1}	7400	Long et al. (2017)	Q	287
2,2',4,6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-50) [446254-23-5] FXUAKFRJBKFDSY-UHFFFAOYSA-N	1.1	7400	Long et al. (2017)	Q	287
2,2',4,6'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-51) [189084-57-9] WKBBBTLDLKYGBI-UHFFFAOYSA-N	1.3	7400	Long et al. (2017)	Q	287
2,2',5,5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-52) [446254-24-6] CDTHXJORUCZHMD-UHFFFAOYSA-N	8.9×10^{-1}	7400	Long et al. (2017)	Q	287
2,2',5,6'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-53) [446254-25-7] SDVQGIMOFXMKHR-UHFFFAOYSA-N	1.4	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',6,6'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-54) [446254-26-8] WCDCHQGVTZHVSO-UHFFFAOYSA-N	1.7	7400	Long et al. (2017)	Q	287
2,3,3',4-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-55) [446254-27-9] VIHUMJGEWQPWOT-UHFFFAOYSA-N	3.0×10^{-1}	7400	Long et al. (2017)	Q	287
2,3,3',4'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-56) [446254-28-0] NFOIVCGFYJIYIB-UHFFFAOYSA-N	2.8×10^{-1}	7400	Long et al. (2017)	Q	287
2,3,3',5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-57) [337513-82-3] CSIFWDKYUJLQEB-UHFFFAOYSA-N	6.2×10^{-1}	7400	Long et al. (2017)	Q	287
2,3,3',5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-58) [446254-29-1] SWOYBZHGPZIRHS-UHFFFAOYSA-N	1.3	7400	Long et al. (2017)	Q	287
2,3,3',6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-59) [446254-30-4] DMAMJZQQOWYEHT-UHFFFAOYSA-N	6.5×10^{-1}	7400	Long et al. (2017)	Q	287
2,3,4,4'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-60) [446254-31-5] ARERIMFZYPFJAV-UHFFFAOYSA-N	2.3×10^{-1}	7400	Long et al. (2017)	Q	287
2,3,4,5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-61) [446254-32-6] NDRSXNBQWAOQPP-UHFFFAOYSA-N	3.2×10^{-1}	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,4,6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-62) [446254-33-7] YIQYWYZZLOZVRM-UHFFFAOYSA-N	5.5×10^{-1}	7400	Long et al. (2017)	Q	287
2,3,4',5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-63) [446254-34-8] HNICYXFGCWPYGC-UHFFFAOYSA-N	5.0×10^{-1}	7400	Long et al. (2017)	Q	287
2,3,4',6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-64) [446254-35-9] LDCXVFJUWKKBNY-UHFFFAOYSA-N	3.3×10^{-1}	7400	Long et al. (2017)	Q	287
2,3,5,6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-65) [446254-36-0] HPEUYVBOPJQVPN-UHFFFAOYSA-N	4.8×10^{-1}	7400	Long et al. (2017)	Q	287
2,3',4,4'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-66) [189084-61-5] DHUMTYRHKMCVAG-UHFFFAOYSA-N	2.0 4.7×10^{-1}	 7400	Tittlemier et al. (2002) Long et al. (2017)	V Q	 287
2,3',4,5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-67) [446254-37-1] OARGWSONVLGXQA-UHFFFAOYSA-N	4.7×10^{-1}	7400	Long et al. (2017)	Q	287
2,3',4,5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-68) [446254-38-2] UFWGRLCUOLLWAO-UHFFFAOYSA-N	1.6	7400	Long et al. (2017)	Q	287
2,3',4,6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-69) [327185-09-1] NHZNRCYNZJADTG-UHFFFAOYSA-N	9.8×10^{-1}	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3',4',5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-70) [446254-39-3] GHQMTYWQVJZWAR-UHFFFAOYSA-N	5.2×10^{-1}	7400	Long et al. (2017)	Q	287
2,3',4',6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-71) [189084-62-6] COPAGYRSCJVION-UHFFFAOYSA-N	5.2×10^{-1}	7400	Long et al. (2017)	Q	287
2,3',5,5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-72) [446254-40-6] GBBNZKQTOOZGIS-UHFFFAOYSA-N	9.6×10^{-1}	7400	Long et al. (2017)	Q	287
2,3',5',6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-73) [446254-41-7] WQFLVWXBCRJAQN-UHFFFAOYSA-N	1.7	7400	Long et al. (2017)	Q	287
2,4,4',5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-74) [446254-42-8] LXCFDVVDUVPAGR-UHFFFAOYSA-N	3.9×10^{-1}	7400	Long et al. (2017)	Q	287
2,4,4',6-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-75) [189084-63-7] BWCNKMFFUGBFGB-UHFFFAOYSA-N	6.3×10^{-1}	7400	Long et al. (2017)	Q	287
2,3',4',5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-76) [446254-43-9] NCSWBJSFVPJPPK-UHFFFAOYSA-N	4.7×10^{-1}	7400	Long et al. (2017)	Q	287
3,3',4,4'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-77) [93703-48-1] RYGLOWMCGZHYRQ-UHFFFAOYSA-N	8.3×10^{-1} 2.3×10^{-1}	 7400	Tittlemier et al. (2002) Long et al. (2017)	V Q	 287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3',4,5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-78) [446254-45-1] HWOBLTZZSVXBOJ-UHFFFAOYSA-N	2.9×10^{-1}	7400	Long et al. (2017)	Q	287
3,3',4,5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-79) [446254-48-4] LELQGHJEUVRPEV-UHFFFAOYSA-N	4.7×10^{-1}	7400	Long et al. (2017)	Q	287
3,3',5,5'-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-80) [103173-66-6] HFIOZJQRZKNPKJ-UHFFFAOYSA-N	1.1	7400	Long et al. (2017)	Q	287
3,4,4',5-tetrabromodiphenyl ether $C_{12}H_6Br_4O$ (PBDE-81) [446254-50-8] ULFOIXCXIWHJDS-UHFFFAOYSA-N	2.4×10^{-1}	7400	Long et al. (2017)	Q	287
2,2',3,3',4-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-82) [327185-11-5] RQMSPGJESCCPQX-UHFFFAOYSA-N	7.1×10^{-1}	7400	Long et al. (2017)	Q	287
2,2',3,3',5-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-83) [446254-51-9] XAHYSNUYJLNDBX-UHFFFAOYSA-N	1.4	7400	Long et al. (2017)	Q	287
2,2',3,3',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-84) [446254-52-0] PPIZNRAVQHNLJM-UHFFFAOYSA-N	1.8	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,4'-pentabromodiphenyl ether	9.1		Tittlemier et al. (2002)	V	
$C_{12}H_5Br_5O$ (PBDE-85) [182346-21-0] DMLQSUZPTTUUDP-UHFFFAOYSA-N	1.3	7400	Long et al. (2017)	Q	287
2,2',3,4,5-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-86) [446254-53-1] YMVWYUWOUOQCQP-UHFFFAOYSA-N	9.2×10^{-1}	7400	Long et al. (2017)	Q	287
2,2',3,4,5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-87) [446254-54-2] WKYQUGCIKNOXFW-UHFFFAOYSA-N	1.1×10^{2}	7400	Long et al. (2017)	Q	287
2,2',3,4,6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-88) [446254-55-3] OPZUHBCVIZNZFB-UHFFFAOYSA-N	1.2	7400	Long et al. (2017)	Q	287
2,2',3,4,6'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-89) [446254-56-4] XGFLJLJXVIMCNR-UHFFFAOYSA-N	1.8	7400	Long et al. (2017)	Q	287
2,2',3,4',5-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-90) [446254-57-5] BATFXMGTVIESIQ-UHFFFAOYSA-N	2.3	7400	Long et al. (2017)	Q	287
2,2',3,4',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-91) [446254-58-6] HWNJTZKDPNZUSO-UHFFFAOYSA-N	1.7	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,5,5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-92) [446254-59-7] QWSQOVAGRDRZLM-UHFFFAOYSA-N	1.9	7400	Long et al. (2017)	Q	287
2,2',3,5,6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-93) [446254-60-0] BRTPVPJQMWLDNO-UHFFFAOYSA-N	1.5	7400	Long et al. (2017)	Q	287
2,2',3,5,6'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-94) [446254-61-1] JOPASNJHCFYVHD-UHFFFAOYSA-N	3.8	7400	Long et al. (2017)	Q	287
2,2',3,5',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-95) [446254-62-2] BZDYRALIEYVMEP-UHFFFAOYSA-N	1.8	7400	Long et al. (2017)	Q	287
2,2',3,6,6'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-96) [446254-63-3] ZFCJNRDWGBZUED-UHFFFAOYSA-N	3.9	7400	Long et al. (2017)	Q	287
2,2',3,4',5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-97) [446254-64-4] MAGYDGJRSCULJL-UHFFFAOYSA-N	1.0	7400	Long et al. (2017)	Q	287
2,2',3,4',6'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-98) [38463-82-0] OCLWEJVGAUFXQU-UHFFFAOYSA-N	3.5	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',4,4',5-pentabromodiphenyl ether	1.5	8900	Long et al. (2017)	M	287
$C_{12}H_5Br_5O$	6.2×10^{-1}		Lau et al. (2006)	M	719
(PBDE-99)	3.3×10^{-1}		Lau et al. (2006)	M	720
[60348-60-9]	1.5	8800	Cetin and Odabasi (2005)	M	
WHPVYXDFIXRKLN-UHFFFAOYSA-N	2.7×10^{-1}	-6700	Charles and Destaillats (2005)	M	42
	2.1		Kuramochi et al. (2014)	V	
	4.3		Tittlemier et al. (2002)	V	
	1.9		Wania and Dugani (2003)	R	
	1.6	7400	Long et al. (2017)	Q	287
	8.4		Zhang et al. (2010)	Q	287, 288
	3.7		Zhang et al. (2010)	Q	287, 289
	1.2×10^{2}		Zhang et al. (2010)	Q	287, 290
	2.4×10^{1}		Zhang et al. (2010)	Q	287, 291
	4.3×10^{-1}		Hilal et al. (2008)	Q	
2,2',4,4',6-pentabromodiphenyl ether	3.6	7300	Long et al. (2017)	M	287
$C_{12}H_5Br_5O$	3.3×10^{-1}		Lau et al. (2006)	M	719
(PBDE-100)	3.2×10^{-1}		Lau et al. (2006)	M	720
[189084-64-8]	3.8	6800	Cetin and Odabasi (2005)	M	
NSKIRYMHNFTRLR-UHFFFAOYSA-N	1.9×10^{-1}	12	Charles and Destaillats (2005)	M	42
	1.4×10^{1}		Tittlemier et al. (2002)	V	
	2.6		Wania and Dugani (2003)	R	
	3.9	7400	Long et al. (2017)	Q	287
	3.7×10^{-1}		Hilal et al. (2008)	Q	
2,2',4,5,5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-101) [446254-65-5] QUZWDWNIWWAQDI-UHFFFAOYSA-N	1.4	7400	Long et al. (2017)	Q	287
2,2',4,5,6'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-102) [446254-66-6] JHFMCUVMAIQWRI-UHFFFAOYSA-N	2.8	7400	Long et al. (2017)	Q	287
2,2',4,5',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-103) [446254-67-7] RJEMKRNASVHYKR-UHFFFAOYSA-N	3.4	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',4,6,6'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-104) [446254-68-8] CRSCWEYUPUKHPI-UHFFFAOYSA-N	6.7	7400	Long et al. (2017)	Q	287
2,3,3',4,4'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-105) [373594-78-6] LBPWAGZGYNOKAM-UHFFFAOYSA-N	6.1×10^{-1}	7400	Long et al. (2017)	Q	287
2,3,3',4,5-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-106) [446254-69-9] KLQKWMYXEWUAFP-UHFFFAOYSA-N	8.5×10^{-1}	7400	Long et al. (2017)	Q	287
2,3,3',4',5-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-107) [446254-70-2] OMGVAMFMRSETEG-UHFFFAOYSA-N	1.9	7400	Long et al. (2017)	Q	287
2,3,3',4,5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-108) [446254-71-3] VBKPKHVLHGOKOJ-UHFFFAOYSA-N	2.0	7400	Long et al. (2017)	Q	287
2,3,3',4,6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-109) [446254-72-4] FXXXWTMLIQLDRP-UHFFFAOYSA-N	1.2	7400	Long et al. (2017)	Q	287
2,3,3',4',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-110) [446254-73-5] LESZGJVTZILBTK-UHFFFAOYSA-N	9.4×10^{-1}	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',5,5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-111) [446254-74-6] PCHDCOXHJBWEPW-UHFFFAOYSA-N	2.1	7400	Long et al. (2017)	Q	287
2,3,3',5,6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-112) [446254-75-7] MFBMNSFADPTAKZ-UHFFFAOYSA-N	1.7	7400	Long et al. (2017)	Q	287
2,3,3',5',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-113) [446254-76-8] OGZHLJXRGZFVLI-UHFFFAOYSA-N	3.1	7400	Long et al. (2017)	Q	287
2,3,4,4',5-pentabromodiphenyl ether	6.2×10^{-1}		Lau et al. (2006)	M	719
$C_{12}H_5Br_5O$	7.7×10^{-1}		Lau et al. (2006)	M	720
(PBDE-114)	8.8×10^{-1}	4000	Charles and Destaillats (2005)	M	42
[446254-77-9]	7.5×10^{-1}	7400	Long et al. (2017)	Q	287
SFNAUTSNWPPDSY-UHFFFAOYSA-N					
2,3,4,4',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-115) [446254-78-0] BKTLDVXDOVSTEV-UHFFFAOYSA-N	9.8×10^{-1}	7400	Long et al. (2017)	Q	287
2,3,4,5,6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-116) [189084-65-9] ACRQLFSHISNWRY-UHFFFAOYSA-N	6.1×10^{-1}	7400	Long et al. (2017)	Q	287
2,3,4',5,6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-117) [446254-79-1] SOJBOGWFDBDWEG-UHFFFAOYSA-N	8.6×10^{-1}	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3',4,4',5-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-118) [446254-80-4] VTMFEPLDDHZBGI-UHFFFAOYSA-N	9.2×10^{-1}	7400	Long et al. (2017)	Q	287
2,3',4,4',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-119) [189084-66-0] KXEOYBYEJCRPGB-UHFFFAOYSA-N	1.8	7400	Long et al. (2017)	Q	287
2,3',4,5,5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-120) [417727-71-0] AKSBEUHDCRZJAN-UHFFFAOYSA-N	1.7	7400	Long et al. (2017)	Q	287
2,3',4,5',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-121) [446254-81-5] GVGNVZBJVFDAAO-UHFFFAOYSA-N	5.9	7400	Long et al. (2017)	Q	287
2,3,3',4',5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-122) [446254-82-6] CDNHGSPFIUITTN-UHFFFAOYSA-N	7.2×10^{-1}	7400	Long et al. (2017)	Q	287
2,3',4,4',5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-123) [446254-83-7] SBKMUEQNZNDYFW-UHFFFAOYSA-N	1.2	7400	Long et al. (2017)	Q	287
2,3',4',5,5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-124) [446254-84-8] FGHJTAAHIFEHLT-UHFFFAOYSA-N	1.1	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3',4',5',6-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-125) [446254-85-9] SESXKFPOVUVGLR-UHFFFAOYSA-N	1.3	7400	Long et al. (2017)	Q	287
3,3',4,4',5-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-126) [366791-32-4] SJNIIWPIAVQNRK-UHFFFAOYSA-N	5.6×10^{-1}	7400	Long et al. (2017)	Q	287
3,3',4,5,5'-pentabromodiphenyl ether $C_{12}H_5Br_5O$ (PBDE-127) [446254-86-0] RATMRXKBPDCKCZ-UHFFFAOYSA-N	1.1	7400	Long et al. (2017)	Q	287
2,2',3,3',4,4'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-128) [182677-28-7] WFLVELCLEGVBIH-UHFFFAOYSA-N	2.1	7400	Long et al. (2017)	Q	287
2,2',3,3',4,5-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-129) [446254-87-1] PRNCVYAUCSGSOE-UHFFFAOYSA-N	1.9	7400	Long et al. (2017)	Q	287
2,2',3,3',4,5'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-130) [446254-88-2] YURCHLXPAGSJHU-UHFFFAOYSA-N	3.7	7400	Long et al. (2017)	Q	287
2,2',3,3',4,6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-131) [446254-89-3] MGKVPJFIGGBCBA-UHFFFAOYSA-N	1.0×10^{1}	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-132) [446254-90-6] FFEKBOKDYRZGRV-UHFFFAOYSA-N	4.0	7400	Long et al. (2017)	Q	287
2,2',3,3',5,5'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-133) [446254-91-7] XTBFPFHQPGZZJX-UHFFFAOYSA-N	6.3	7400	Long et al. (2017)	Q	287
2,2',3,3',5,6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-134) [446254-92-8] MIBDGPWSGDWIQR-UHFFFAOYSA-N	4.8	7400	Long et al. (2017)	Q	287
2,2',3,3',5,6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-135) [446254-93-9] AMGHASDTWACNCS-UHFFFAOYSA-N	8.6	7400	Long et al. (2017)	Q	287
2,2',3,3',6,6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-136) [446254-94-0] NTWGDSLWLUPCDW-UHFFFAOYSA-N	7.8	7400	Long et al. (2017)	Q	287
2,2',3,4,4',5-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-137) [446254-95-1] HSTYYNPYXZYIAG-UHFFFAOYSA-N	3.0	7400	Long et al. (2017)	Q	287
2,2',3,4,4',5'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-138) [182677-30-1] IZFQCEZFGCMHOM-UHFFFAOYSA-N	2.7	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,4',6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-140) [243982-83-4] FLRODCDHJZNIGA-UHFFFAOYSA-N	7.7	7400	Long et al. (2017)	Q	287
2,2',3,4,5,5'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-141) [446254-97-3] XTXIYMGRRUJOIT-UHFFFAOYSA-N	2.6	7400	Long et al. (2017)	Q	287
2,2',3,4,5,6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-142) [446254-98-4] LJDGJCNHVGGOFW-UHFFFAOYSA-N	1.4	7400	Long et al. (2017)	Q	287
2,2',3,4,5,6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-143) [446254-99-5] RQLZDUSZXOOBTM-UHFFFAOYSA-N	5.1	7400	Long et al. (2017)	Q	287
2,2',3,4,5',6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-144) [446255-00-1] ZMSJCQOCTPYCQP-UHFFFAOYSA-N	5.2	7400	Long et al. (2017)	Q	287
2,2',3,4,6,6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-145) [446255-01-2] BTKLHMBWCRVCLC-UHFFFAOYSA-N	1.0×10^{1}	7400	Long et al. (2017)	Q	287
2,2',3,4',5,5'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-146) [446255-02-3] HGXPYDNHBUCRTR-UHFFFAOYSA-N	5.3	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4',5,6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-147) [116995-33-6] OWBKWMDBTWHGHS-UHFFFAOYSA-N	5.1	7400	Long et al. (2017)	Q	287
2,2',3,4',5,6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-148) [446255-03-4] OJMHGSMSQZEBFH-UHFFFAOYSA-N	1.2×10^{1}	7400	Long et al. (2017)	Q	287
2,2',3,4',5',6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-149) [446255-04-5] UJOUSZKYGGTPFQ-UHFFFAOYSA-N	5.1	7400	Long et al. (2017)	Q	287
2,2',3,4',6,6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-150) [446255-05-6] SQNOZOVDXXSLSG-UHFFFAOYSA-N	1.7×10^{1}	7400	Long et al. (2017)	Q	287
2,2',3,5,5',6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-151) [446255-06-7] NGOQQUYCSISZMY-UHFFFAOYSA-N	4.4	7400	Long et al. (2017)	Q	287
2,2',3,5,6,6'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-152) [446255-07-8] BYBJJARTBKUIJD-UHFFFAOYSA-N	9.4	7400	Long et al. (2017)	Q	287
2,2',4,4',5,5'-hexabromodiphenyl ether	3.7	7200	Long et al. (2017)	M	287
$C_{12}H_4Br_6O$	3.5	7800	Cetin and Odabasi (2005)	M	
(PBDE-153)	6.1		Kuramochi et al. (2014)	V	
[68631-49-2]	1.5×10^{1}		Tittlemier et al. (2002)	V	
RZXIRSKYBISPGF-UHFFFAOYSA-N	2.9		Wania and Dugani (2003)	R	
	3.9	7400	Long et al. (2017)	Q	287
	8.4×10^{-1}		Hilal et al. (2008)	Q	

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
2,2',4,4',5,6'-hexabromodiphenyl ether	7.1	6800	Long et al. (2017)	M	287
$C_{12}H_4Br_6O$	7.3	6800	Cetin and Odabasi (2005)	M	
(PBDE-154)	4.2		Tittlemier et al. (2002)	V	
[207122-15-4]	1.1×10^{1}	7400	Long et al. (2017)	Q	287
VHNPZYZQKWIWOD-UHFFFAOYSA-N	7.2×10^{-1}		Hilal et al. (2008)	Q	
2,2',4,4',6,6'-hexabromodiphenyl ether	2.5×10^{1}	7400	Long et al. (2017)	Q	287
$C_{12}H_4Br_6O$					
(PBDE-155)					
[35854-94-5]					
HRSCBOSGEKXXSI-UHFFFAOYSA-N					
2,3,3',4,4',5-hexabromodiphenyl ether	1.5	7400	Long et al. (2017)	Q	287
$C_{12}H_4Br_6O$					
(PBDE-156)					
[405237-85-6]					
JSDPCMJWYRDQEV-UHFFFAOYSA-N					
2,3,3',4,4',5'-hexabromodiphenyl ether	1.9	7400	Long et al. (2017)	Q	287
$C_{12}H_4Br_6O$					
(PBDE-157)					
[446255-08-9]					
JUOAMVUIJQJZSZ-UHFFFAOYSA-N					
2,3,3',4,4',6-hexabromodiphenyl ether	2.7	7400	Long et al. (2017)	Q	287
$C_{12}H_4Br_6O$					
(PBDE-158)					
[446255-09-0]					
KRYHHTVQOOJNHQ-UHFFFAOYSA-N					
2,3,3',4,5,5'-hexabromodiphenyl ether	3.0	7400	Long et al. (2017)	Q	287
$C_{12}H_4Br_6O$					
(PBDE-159)					
[446255-10-3]					
IDYFFNCFLRCOPZ-UHFFFAOYSA-N					
2,3,3',4,5,6-hexabromodiphenyl ether	2.8	7400	Long et al. (2017)	Q	287
$C_{12}H_4Br_6O$					
(PBDE-160)					
[446255-11-4]					
OCVOYHGOXIIONK-UHFFFAOYSA-N					

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',4,5',6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-161) [446255-12-5] WEYWRBBPPKSRGU-UHFFFAOYSA-N	9.0	7400	Long et al. (2017)	Q	287
2,3,3',4',5,5'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-162) [446255-13-6] UKPNCLHMNJCGCJ-UHFFFAOYSA-N	2.7	7400	Long et al. (2017)	Q	287
2,3,3',4',5,6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-163) [446255-14-7] NUEAHMLXQFHEJN-UHFFFAOYSA-N	2.3	7400	Long et al. (2017)	Q	287
2,3,3',4',5',6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-164) [446255-15-8] UJVYVXIHTJOJBZ-UHFFFAOYSA-N	3.1	7400	Long et al. (2017)	Q	287
2,3,3',5,5',6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-165) [446255-16-9] KXERERDGMTWBGZ-UHFFFAOYSA-N	7.9	7400	Long et al. (2017)	Q	287
2,3,4,4',5,6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-166) [189084-58-0] KVYODBMKQYVNEK-UHFFFAOYSA-N	1.2	7400	Long et al. (2017)	Q	287
2,3',4,4',5,5'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-167) [446255-17-0] NMUPLZRHSXJCJQ-UHFFFAOYSA-N	3.1	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3',4,4',5',6-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-168) [53551-87-4] HWZAPXGFMVEGPW-UHFFFAOYSA-N	5.0	7400	Long et al. (2017)	Q	287
3,3',4,4',5,5'-hexabromodiphenyl ether $C_{12}H_4Br_6O$ (PBDE-169) [446255-18-1] JKFBMDHBJYKFKL-UHFFFAOYSA-N	1.2	7400	Long et al. (2017)	Q	287
2,2',3,3',4,4',5-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-170) [327185-13-7] DLPNCMQTNWLTHD-UHFFFAOYSA-N	4.9	7400	Long et al. (2017)	Q	287
2,2',3,3',4,4',6-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-171) [446255-19-2] FRMMMROUUPQUMZ-UHFFFAOYSA-N	1.2×10^1	7400	Long et al. (2017)	Q	287
2,2',3,3',4,5,5'-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-172) [407606-59-1] DSRRSKFMOJQETR-UHFFFAOYSA-N	1.6×10^1	7400	Long et al. (2017)	Q	287
2,2',3,3',4,5,6-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-173) [446255-20-5] NLBLNZDNOSSGPW-UHFFFAOYSA-N	6.7	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,5,6'-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-174) [446255-21-6] VUUWOHUOYUGBEO-UHFFFAOYSA-N	1.2×10^1	7400	Long et al. (2017)	Q	287
2,2',3,3',4,5',6-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-175) [6255-22-7] YATZWTXATDYQCK-UHFFFAOYSA-N	1.7×10^1	7400	Long et al. (2017)	Q	287
2,2',3,3',4,6,6'-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-176) [407606-61-5] SWUALKCOTZOSMY-UHFFFAOYSA-N	2.5×10^1	7400	Long et al. (2017)	Q	287
2,2',3,3',4,5',6'-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-177) [446255-23-8] ZHUHLPXIJIBQBJ-UHFFFAOYSA-N	9.9	7400	Long et al. (2017)	Q	287
2,2',3,3',5,5',6-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-178) [446255-24-9] UWUVZUPEEORCRG-UHFFFAOYSA-N	1.3×10^1	7400	Long et al. (2017)	Q	287
2,2',3,3',5,6,6'-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-179) [446255-25-0] COVXWWKOLMNRQE-UHFFFAOYSA-N	2.2×10^1	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,4',5,5'-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-180) [446255-26-1] STMBXVOJNOJRPZ-UHFFFAOYSA-N	7.3	7400	Long et al. (2017)	Q	287
2,2',3,4,4',5,6-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-181) [189084-67-1] GVNRIAPLVGNZPL-UHFFFAOYSA-N	8.9	7400	Long et al. (2017)	Q	287
2,2',3,4,4',5,6'-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-182) [442690-45-1] ZYHDTADADSNMLV-UHFFFAOYSA-N	1.9×10^{1}	7400	Long et al. (2017)	Q	287
2,2',3,4,4',5',6-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-183) [207122-16-5] ILPSCQCLBHQUEM-UHFFFAOYSA-N	1.4×10^{2}		Tittlemier et al. (2002)	V	
	1.3×10^{1}	7400	Long et al. (2017)	Q	287
2,2',3,4,4',6,6'-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-184) [117948-63-7] JHDCZVAQPRXHEL-UHFFFAOYSA-N	3.7×10^{1}	7400	Long et al. (2017)	Q	287
2,2',3,4,5,5',6-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-185) [405237-86-7] YRNMIFAQDSUFTR-UHFFFAOYSA-N	5.1	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,5,6,6'-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-186) [446255-27-2] WUFQDCMRKKDNSF-UHFFFAOYSA-N	1.4×10^{1}	7400	Long et al. (2017)	Q	287
2,2',3,4',5,5',6-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-187) [446255-28-3] RFZPXOBFDARWHV-UHFFFAOYSA-N	9.4	7400	Long et al. (2017)	Q	287
2,2',3,4',5,6,6'-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-188) [116995-32-5] YGYDHFDPVGAMTL-UHFFFAOYSA-N	3.5×10^{1}	7400	Long et al. (2017)	Q	287
2,3,3',4,4',5,5'-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-189) [259087-35-9] CQVLRTUESBMMJW-UHFFFAOYSA-N	4.4	7400	Long et al. (2017)	Q	287
2,3,3',4,4',5,6-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-190) [189084-68-2] OUEYHQIMJGHOQN-UHFFFAOYSA-N	4.0	7400	Long et al. (2017)	Q	287
2,3,3',4,4',5',6-heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-191) [446255-30-7] BNBFKFHSIPERIM-UHFFFAOYSA-N	8.4	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,3',4,5,5',6- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-192) [407578-53-4] ABLZOLAUBUSUHT-UHFFFAOYSA-N	1.3×10^1	7400	Long et al. (2017)	Q	287
2,3,3',4',5,5',6- heptabromodiphenyl ether $C_{12}H_3Br_7O$ (PBDE-193) [446255-34-1] AUFJSWANTKXCFZ-UHFFFAOYSA-N	7.3	7400	Long et al. (2017)	Q	287
2,2',3,3',4,4',5,5'- octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-194) [32536-52-0] ORYGKUIDIMIRNN-UHFFFAOYSA-N	1.3×10^1	7400	Long et al. (2017)	Q	287
2,2',3,3',4,4',5,6- octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-195) [446255-38-5] GPQLSLKPHQEEOP-UHFFFAOYSA-N	1.6×10^1	7400	Long et al. (2017)	Q	287
2,2',3,3',4,4',5,6'- octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-196) [446255-39-6] IEWFKOVTVJNWFF-UHFFFAOYSA-N	3.7×10^1	7400	Long et al. (2017)	Q	287
2,2',3,3',4,4',6,6'- octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-197) [117964-21-3] AAFUUKPTSPVXJH-UHFFFAOYSA-N	7.1×10^1	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,3',4,5,5',6-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-198) [446255-42-1] IBKRHVDFFHQOSC-UHFFFAOYSA-N	1.8×10^1	7400	Long et al. (2017)	Q	287
2,2',3,3',4,5,5',6'-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-199) [446255-43-2] JNSLJYRXDGBNBE-UHFFFAOYSA-N	3.3×10^1	7400	Long et al. (2017)	Q	287
2,2',3,3',4,5,6,6'-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-200) [446255-46-5] JWMXGEPFVCRXQR-UHFFFAOYSA-N	3.7×10^1	7400	Long et al. (2017)	Q	287
2,2',3,3',4,5',6,6'-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-201) [446255-50-1] HQWFMMKREWXIGN-UHFFFAOYSA-N	6.8×10^1	7400	Long et al. (2017)	Q	287
2,2',3,3',5,5',6,6'-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-202) [67797-09-5] AHNZLQAZTWRRDW-UHFFFAOYSA-N	5.7×10^1	7400	Long et al. (2017)	Q	287
2,2',3,4,4',5,5',6-octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-203) [337513-72-1] RTUZOQFRIPIWPS-UHFFFAOYSA-N	2.0×10^1	7400	Long et al. (2017)	Q	287

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2',3,4,4',5,6,6'- octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-204) [446255-54-5] YZABCBOJTHQTSX-UHFFFAOYSA-N	6.2×10^{1}	7400	Long et al. (2017)	Q	287
2,3,3',4,4',5,5',6- octabromodiphenyl ether $C_{12}H_2Br_8O$ (PBDE-205) [446255-56-7] CVMKCYDBEYHNBM-UHFFFAOYSA-N	1.8×10^{1}	7400	Long et al. (2017)	Q	287
2,2',3,3',4,4',5,5',6- nonabromodiphenyl ether $C_{12}HBr_9O$ (PBDE-206) [63387-28-0] CYRHBNRLQMLULE-UHFFFAOYSA-N	4.7×10^{1}	7400	Long et al. (2017)	Q	287
2,2',3,3',4,4',5,6,6'- nonabromodiphenyl ether $C_{12}HBr_9O$ (PBDE-207) [437701-79-6] IEEVDIAVLGLVOW-UHFFFAOYSA-N	1.2×10^{2}	7400	Long et al. (2017)	Q	287
2,2',3,3',4,5,5',6,6'- nonabromodiphenyl ether $C_{12}HBr_9O$ (PBDE-208) [437701-78-5] ASGZXYIDLFWXID-UHFFFAOYSA-N	1.1×10^{2}	7400	Long et al. (2017)	Q	287
decabromodiphenyl ether $C_{12}Br_{10}O$ (PBDE-209) [1163-19-5] WHHGLZMJPXIBIX-UHFFFAOYSA-N	1.8×10^{1} 1.8×10^{1} 2.7×10^{1} 8.2×10^{2} 8.2×10^{2} 4.1×10^{2} 1.3×10^{3} 6.7×10^{2}	7600 7900 7400	Long et al. (2017) Cetin and Odabasi (2005) Long et al. (2017) HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	M M Q Q Q Q Q Q	287 287 99 287, 288 287, 289 287, 290 287, 291

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dibromoacetonitrile C_2HBr_2N [3252-43-5] NDSBDLSWTGLNQA-UHFFFAOYSA-N	2.4×10^{1}		HSDB (2015)	Q	99
bromoacetonitrile C_2H_2BrN [590-17-0] REXUYBKPWIPONM-UHFFFAOYSA-N	2.8		HSDB (2015)	Q	447
2-bromopyridine C_5H_4BrN [109-04-6] IMRWILPUOVGIMU-UHFFFAOYSA-N	1.3 1.8×10^{-1}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
3-bromopyridine C_5H_4BrN [626-55-1] NYPYPOZNGOXYSU-UHFFFAOYSA-N	8.3×10^{-1}		Ebert et al. (2023)	?	316
1,2-dibromo-2,4-dicyanobutane $C_6H_6Br_2N_2$ [35691-65-7] DHVLDKHFGIVEIP-UHFFFAOYSA-N	1.2×10^{3}		HSDB (2015)	V	
4-bromobenzenamine C_6H_6BrN [106-40-1] WDFQBORIUYODSI-UHFFFAOYSA-N	1.1×10^{1}		HSDB (2015)	Q	447
2,4,6-tribromobenzenamine $C_6H_4Br_3N$ [147-82-0] GVPODVKBTHCGFU-UHFFFAOYSA-N	8.2×10^{1} 2.6 6.0×10^{-1} 1.2×10^{2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
N,N'-dimethyl-3,3',4,4',5,5'-hexabromo-2,2'-bipyrrole $C_{10}H_6Br_6N_2$ (DBP-Br6) [253798-63-9] BUKWTHPBLJVYMZ-UHFFFAOYSA-N	5.0×10^{2} 5.1×10^{1}		Tittlemier et al. (2004) Hilal et al. (2008)	V Q	
1,1'-ethylene 2,2'-dipyridylium dibromide $C_{12}H_{12}N_2Br$ (diquat dibromide) [85-00-7] JXEXEPZXXFNEHA-UHFFFAOYSA-M	7.0×10^{7}		HSDB (2015)	Q	99

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tralomethrin $C_{22}H_{19}NO_3Br_4$ [66841-25-6] YWSCPYYRJXKUDB-KAKFPZCNSA-N	2.5×10^4 2.5×10^4 1.2×10^3		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
bromomethyl peroxynitrate $CH_2BrO_2NO_2$ JTAFUKGUWIYDNI-UHFFFAOYSA-N	3.5×10^{-1}		Krysztofiak et al. (2012)	Q	
dibromomethyl peroxynitrate $CHBr_2O_2NO_2$ CRBGJNSRTFAVGH-UHFFFAOYSA-N	3.0		Krysztofiak et al. (2012)	Q	
tribromomethyl peroxynitrate $CBr_3O_2NO_2$ BVMOLEXBJGZUAI-UHFFFAOYSA-N	4.0		Krysztofiak et al. (2012)	Q	
MCM:BRETPAN $C_2H_2NO_5Br$ OOFSXJVGALRPLK-UHFFFAOYSA-N	2.0×10^1 8.7×10^1 3.3×10^{-3}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
2,2-dibromo-2-cyanoacetamide $C_3H_2Br_2N_2O$ (2,2-dibromo-3-nitrilopropionamide) [10222-01-2] UUIVKBHZENILKB-UHFFFAOYSA-N	5.2×10^2 5.2×10^2 8.5×10^3		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
bronopol $C_3H_6BrNO_4$ [52-51-7] LVDKZNITIUWNER-UHFFFAOYSA-N	7.6×10^5		HSDB (2015)	V	
2,6-dibromo-4-nitroaniline $C_6H_4Br_2N_2O_2$ [827-94-1] YMZIFDLWYUSZCC-UHFFFAOYSA-N	8.2×10^3 1.7×10^2 1.9×10^3 5.7×10^3		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
2-bromo-4,6-dinitroaniline $C_6H_4BrN_3O_4$ [1817-73-8] KWMDHCLJYMVBNS-UHFFFAOYSA-N	3.9×10^4 2.7×10^2 1.8×10^3 5.7×10^4		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
3-bromonitrobenzene $C_6H_4BrNO_2$ (m-bromonitrobenzene) [585-79-5] FWIROFMBWVMWLB-UHFFFAOYSA-N	5.3 5.4 1.8		Duchowicz et al. (2020) Schüürmann (2000) Duchowicz et al. (2020)	V V Q	186

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-bromonitrobenzene $C_6H_4BrNO_2$ (*p*-bromonitrobenzene) [586-78-7] ZDFBKZUDCQQKAC-UHFFFAOYSA-N	2.2×10^{-1}		Li et al. (2014)	Q	241
3,5-dibromo-4-hydroxy-benzonitrile	7.4×10^{2}		Mackay et al. (2006d)	V	
$C_7H_3Br_2NO$	1.0×10^{6}		Maniere et al. (2011)	?	241, 573, 165
(bromoxynil)	2.2×10^{3}		Maniere et al. (2011)	?	241, 577, 165
[1689-84-5]	1.1×10^{6}		Maniere et al. (2011)	?	241, 493, 165
UPMXNNIRAGDFEH-UHFFFAOYSA-N					
2,6-dibromo-3-methyl-4-nitroanisole	4.5×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_8H_7Br_2NO_3$	3.5×10^{1}		Zhang et al. (2010)	Q	287, 289
[62265-99-0]	4.7		Zhang et al. (2010)	Q	287, 290
RBAJFFLBHVZCDY-UHFFFAOYSA-N	9.7		Zhang et al. (2010)	Q	287, 291
bromacil	7.6×10^{4}		HSDB (2015)	V	
$C_9H_{13}BrN_2O_2$	7.8×10^{4}		Mackay et al. (2006d)	V	
[314-40-9]	5.3×10^{2}		Suntio et al. (1988)	V	12
CTSLUCNDVMMDHG-UHFFFAOYSA-N	5.2		Barcelo and Hennion (1997)	X	567
	2.1×10^{1}		Goodarzi et al. (2010)	Q	568
N'-(4-bromophenyl)-N-methoxy-N-methylurea	3.2×10^{3}		HSDB (2015)	V	
$C_9H_{11}BrN_2O$	3.2×10^{3}		Mackay et al. (2006d)	V	
(metobromuron)	3.2×10^{1}		Barcelo and Hennion (1997)	X	567
[3060-89-7]	8.5		Goodarzi et al. (2010)	Q	568
WLFDQEVORAMCIM-UHFFFAOYSA-N	8.8×10^{3}		Maniere et al. (2011)	?	12, 165
bromuron $C_9H_{11}BrN_2O$ [3408-97-7] GSNZNZUNAJCHDO-UHFFFAOYSA-N	2.0×10^{4}		MacBean (2012a)	?	
bromoxynil butyrate $C_{11}H_9Br_2NO_2$ [3861-41-4] PGMZYNZXIYOOHJ-UHFFFAOYSA-N	5.6×10^{1}		Maniere et al. (2011)	?	12, 165
tris(2,3-dibromopropyl)isocyanurate	8.2×10^{12}		Zhang et al. (2010)	Q	287, 288
$C_{12}H_{15}Br_6N_3O_3$	6.5×10^{7}		Zhang et al. (2010)	Q	287, 289
[52434-90-9]	2.7×10^{8}		Zhang et al. (2010)	Q	287, 290
NZUPFZNVGSWLQC-UHFFFAOYSA-N	1.2×10^{10}		Zhang et al. (2010)	Q	287, 291

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bromofenoxim	3.1×10^{-3}		Barcelo and Hennion (1997)	X	567
$C_{13}H_7Br_2N_3O_6$	8.1×10^{-4}		Goodarzi et al. (2010)	Q	568, 569
[13181-17-4]	1.3×10^{5}		MacBean (2012a)	?	12
VTQWKUZUPOTXEH-UHFFFAOYSA-N					
tribromsalan	9.7×10^{5}		Zhang et al. (2010)	Q	287, 288
$C_{13}H_8Br_3NO_2$	1.2×10^{6}		Zhang et al. (2010)	Q	287, 289
[87-10-5]	1.6×10^{6}		Zhang et al. (2010)	Q	287, 290
KVSKGMLNBAPGKH-UHFFFAOYSA-N	1.2×10^{6}		Zhang et al. (2010)	Q	287, 291
bromoxynil heptanoate	5.3		Maniere et al. (2011)	?	12, 165
$C_{14}H_{15}Br_2NO_2$					
[56634-95-8]					
BHZWBQPHPLFZSV-UHFFFAOYSA-N					
1-amino-2,4-dibromo-9,10-anthracenedione	5.5×10^{7}		HSDB (2015)	Q	99
$C_{14}H_7Br_2NO_2$					
(1-amino-2,4-dibromoanthraquinone)					
[81-49-2]					
ZINRVIQBCHAZMM-UHFFFAOYSA-N					
2,6-dibromo-4-cyanophenyl octanoate	3.1×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{15}H_{17}BrNO_2$	3.1×10^{-1}		HSDB (2015)	V	
[1689-99-2]	4.1×10^{1}		Duchowicz et al. (2020)	Q	
DQKWXTIYGWPGOO-UHFFFAOYSA-N	<5.3		Maniere et al. (2011)	?	12, 165
bromobutide	1.9×10^{2}		Ebert et al. (2023)	?	318
$C_{15}H_{22}BrNO$					
[74712-19-9]					
WZDDLAZXUYIVMU-UHFFFAOYSA-N					
(2*E*)-N,N'-bis(2,4,6-tribromophenyl)-2-butenediamide	9.0×10^{9}		Zhang et al. (2010)	Q	287, 288
$C_{16}H_8Br_6N_2O_2$	5.1×10^{8}		Zhang et al. (2010)	Q	287, 289
[92484-07-6]	6.2×10^{9}		Zhang et al. (2010)	Q	287, 290
IJUNKLAVMFKPCX-OWOJBTEDSA-N	7.2×10^{13}		Zhang et al. (2010)	Q	287, 291
SAYTEX BT 93	2.7×10^{15}		HSDB (2015)	Q	99
$C_{18}H_4Br_8N_2O_4$	2.7×10^{15}		Zhang et al. (2010)	Q	287, 288
[32588-76-4]	2.3×10^{11}		Zhang et al. (2010)	Q	287, 289
DYIZJUDNMOIZQO-UHFFFAOYSA-N	3.5×10^{9}		Zhang et al. (2010)	Q	287, 290
	2.3×10^{13}		Zhang et al. (2010)	Q	287, 291
SAYTEX BN 451	2.5×10^{15}		Zhang et al. (2010)	Q	287, 288
$C_{20}H_{20}Br_4N_2O_4$	1.4×10^{11}		Zhang et al. (2010)	Q	287, 289
[52907-07-0]	5.7×10^{11}		Zhang et al. (2010)	Q	287, 290
WOFYQUJNULCFLN-UHFFFAOYSA-N	1.6×10^{15}		Zhang et al. (2010)	Q	287, 291

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Table A7.2: Polybrominated diphenyl ethers (PBDEs) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
deltamethrin	2.0		Duchowicz et al. (2020)	V	186
$C_{22}H_{19}Br_2NO_3$	2.0		HSDB (2015)	V	
[52918-63-5]	4.0×10^{-1}		Mackay et al. (2006d)	V	
OWZREIFADZCYQD-NSHGMRRFSA-N	2.0		Siebers and Mattusch (1996)	V	12
	1.0×10^{3}		Duchowicz et al. (2020)	Q	
	3.2×10^{1}		Maniere et al. (2011)	?	165
2,2'-(methylenedi-4,1-phenylene)bis(4,5,6,7-tetrabromo-1H-isoindole-1,3(2H)-dione	5.3×10^{14}		Zhang et al. (2010)	Q	287, 288
$C_{29}H_{10}N_2O_4Br_8$	1.7×10^{14}		Zhang et al. (2010)	Q	287, 289
[32588-74-2]	9.5×10^{9}		Zhang et al. (2010)	Q	287, 290
RHFKNNBDKARGKL-UHFFFAOYSA-N	4.7×10^{15}		Zhang et al. (2010)	Q	287, 291

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A7.3 Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br)

Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bromotrifluoromethane	2.0×10^{-5}		Hine and Mookerjee (1975)	V	
CF_3Br	2.0×10^{-5}		Yaws (2003)	X	237
[75-63-8]	2.0×10^{-5}		Irmann (1965)	C	
RJCQBQGAPKAMLL-UHFFFAOYSA-N	6.4×10^{-6}		Keshavarz et al. (2022)	Q	
	5.3×10^{-5}		Duchowicz et al. (2020)	Q	299
	4.7×10^{-5}		Gharagheizi et al. (2012)	Q	
	1.8×10^{-5}		Gharagheizi et al. (2010)	Q	246
	3.2×10^{-5}		Hilal et al. (2008)	Q	
	1.1×10^{-5}		Modarresi et al. (2007)	Q	67
	2.7×10^{-5}		Nirmalakhandan and Speece (1988)	Q	
	5.6×10^{-6}		Irmann (1965)	Q	
	2.0×10^{-5}		Duchowicz et al. (2020)	?	185, 21
	2.1×10^{-5}		Yaws (1999)	?	21
dibromodifluoromethane	3.3×10^{-4}		HSDB (2015)	Q	99
CBr_2F_2					
[75-61-6]					
AZSZCFSOHXEJQE-UHFFFAOYSA-N					
1-bromo-1,2,2,2-tetrafluoroethane	1.7×10^{-4}	2700	Allott et al. (1973)	L	
C_2HBrF_4	1.2×10^{-4}		Edelist et al. (1964)	M	14
(teflurane)	1.4×10^{-4}		Keshavarz et al. (2022)	Q	
[124-72-1]	1.5×10^{-3}		Duchowicz et al. (2020)	Q	
RZXZIZDRFQFCTA-UHFFFAOYSA-N	2.1×10^{-4}		Hilal et al. (2008)	Q	
	6.7×10^{-5}		Modarresi et al. (2007)	Q	67
	1.7×10^{-4}		Duchowicz et al. (2020)	?	185, 21
	1.3×10^{-4}		Abraham and Weathersby (1994)	?	21
	1.7×10^{-4}		Abraham et al. (1990)	?	
1,2-dibromotetrafluoroethane	2.7×10^{-7}		Duchowicz et al. (2020)	V	186
$C_2Br_2F_4$	2.7×10^{-7}		HSDB (2015)	V	
[124-73-2]	2.4×10^{-4}		Duchowicz et al. (2020)	Q	
KVBKAPANDHPRDG-UHFFFAOYSA-N					
1-bromo-2-fluorobenzene	4.1×10^{-3}		Ebert et al. (2023)	?	316
C_6H_4BrF					
[1072-85-1]					
IPWBFGUBXWMIPR-UHFFFAOYSA-N					
1-bromo-3-fluorobenzene	2.9×10^{-3}		Ebert et al. (2023)	?	316
C_6H_4BrF					
[1073-06-9]					
QDFKKJYEIFBEFC-UHFFFAOYSA-N					

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Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-bromo-4-fluorobenzene C_6H_4BrF [460-00-4] AITNMTXHTIIIBB-UHFFFAOYSA-N	5.3×10^{-3}	4400	Hiatt (2013)	M	
bromopentafluorobenzene C_6BrF_5 [344-04-7] XEKTVXADUPBFOA-UHFFFAOYSA-N	2.1×10^{-3} 1.6×10^{-4} 1.4×10^{-4} 6.7×10^{-4}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
halfenprox $C_{24}H_{23}BrF_2O_3$ [111872-58-3] WIFXJBMOTMKRMM-UHFFFAOYSA-N	1.9×10^{1}		Ebert et al. (2023)	?	318
bromethalin $C_{14}H_7Br_3F_3N_3O_4$ [63333-35-7] USMZPYXTVKAYST-UHFFFAOYSA-N	2.5×10^{3}		HSDB (2015)	Q	99
brofluthrinate $C_{26}H_{22}BrF_2NO_4$ [160791-64-0] BUHNCQOJJZAOMJ-UHFFFAOYSA-N	1.6×10^{1}		Ebert et al. (2023)	?	316
bromochloromethane CH_2BrCl [74-97-5] JPOXNPPZZKNXOV-UHFFFAOYSA-N	6.6×10^{-3} 7.8×10^{-3} 6.8×10^{-3} 5.8×10^{-3} 5.8×10^{-3} 6.2×10^{-3} 1.1×10^{-2} 2.5×10^{-2} 5.7×10^{-3} 5.3×10^{-3} 6.2×10^{-3}	4700 4600	Hiatt (2013) Kondoh and Nakajima (1997) HSDB (2015) Mackay et al. (2006b) Mackay et al. (1993) Yaws (2003) Gharagheizi et al. (2012) Gharagheizi et al. (2010) Yao et al. (2002) Katritzky et al. (1998) Yaws (1999) Fogg and Sangster (2003)	M M V V V X Q Q Q Q ? W	 237 246 229 21 791
bromodichloromethane $CHCl_2Br$ [75-27-4] FMWLUWPQPKEARP-UHFFFAOYSA-N	4.0×10^{-3} 3.9×10^{-3} 4.0×10^{-3} 3.9×10^{-3} 4.0×10^{-3} 4.0×10^{-3} 4.8×10^{-3} 4.0×10^{-3} 4.0×10^{-3} 5.2×10^{-3} 5.8×10^{-3}	5200 4900 5200 4900 5200 5200 3700 5200 5200 4700	Burkholder et al. (2019) Burkholder et al. (2019) Burkholder et al. (2015) Burkholder et al. (2015) Sander et al. (2011) Sander et al. (2006) Fogg and Sangster (2003) Staudinger and Roberts (2001) Staudinger and Roberts (1996) Hiatt (2013) Ruiz-Bevia and Fernandez-Torres (2010)	L L L L L L L L L M M	 70 70

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Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.9×10^{-3}		Zhang et al. (2002)	M	14
	5.4×10^{-3}	4400	Kondoh and Nakajima (1997)	M	
	3.9×10^{-3}	4800	Moore et al. (1995)	M	792, 70
	4.8×10^{-3}	4200	Tse et al. (1992)	M	
	4.7×10^{-3}	5200	Nicholson et al. (1984)	M	
	3.5×10^{-3}	5200	Ervin et al. (1980)	M	
	4.7×10^{-3}		Warner et al. (1980)	M	
	4.1×10^{-3}		Mackay et al. (2006b)	V	
	4.1×10^{-3}		Mackay et al. (1993)	V	
	4.6×10^{-3}	1200	Goldstein (1982)	X	298
	7.7×10^{-3}		Hilal et al. (2008)	C	
	4.3×10^{-3}		Nicholson et al. (1984)	C	
	4.7×10^{-3}		Nicholson et al. (1984)	C	12
	4.7×10^{-3}		Shen (1982)	C	
	8.8×10^{-3}		Keshavarz et al. (2022)	Q	
	9.4×10^{-3}		Duchowicz et al. (2020)	Q	184
	3.1×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	3.9×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.9×10^{-3}		Hilal et al. (2008)	Q	
	2.4×10^{-3}		Modarresi et al. (2007)	Q	67
		4100	Kühne et al. (2005)	Q	
	4.8×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	3.2×10^{-3}		Katritzky et al. (1998)	Q	
	4.7×10^{-3}		Duchowicz et al. (2020)	?	185, 21
	6.2×10^{-3}		Mackay et al. (2006b)	?	
		3800	Kühne et al. (2005)	?	
	6.2×10^{-3}		Mackay et al. (1993)	?	
bromotrichloromethane $CBrCl_3$ [75-62-7] XNNQFQFUQLJSQT-UHFFFAOYSA-N	2.7×10^{-2}		HSDB (2015)	Q	99
dibromochloromethane $CHClBr_2$ [124-48-1] GATVIKZLVQHOMN-UHFFFAOYSA-N	8.6×10^{-3}	5500	Burkholder et al. (2019)	L	
	7.2×10^{-3}	5200	Burkholder et al. (2019)	L	70
	8.6×10^{-3}	5500	Burkholder et al. (2015)	L	
	7.2×10^{-3}	5200	Burkholder et al. (2015)	L	70
	8.6×10^{-3}	5500	Sander et al. (2011)	L	
	8.6×10^{-3}	5500	Sander et al. (2006)	L	
	8.7×10^{-3}	4400	Fogg and Sangster (2003)	L	
	8.6×10^{-3}	5500	Staudinger and Roberts (2001)	L	
	8.5×10^{-3}	5500	Staudinger and Roberts (1996)	L	
	1.1×10^{-2}	5300	Hiatt (2013)	M	
	1.1×10^{-2}		Ruiz-Bevia and Fernandez-Torres (2010)	M	
	4.6×10^{-3}		Zhang et al. (2002)	M	14
	9.8×10^{-3}	5100	Kondoh and Nakajima (1997)	M	

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Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	7.4×10^{-3}	4600	Moore et al. (1995)	M	793, 70
	9.3×10^{-3}	4600	Tse et al. (1992)	M	
	8.5×10^{-3}	6400	Ashworth et al. (1988)	M	278
	8.6×10^{-3}	5200	Nicholson et al. (1984)	M	
	8.5×10^{-3}	5000	Ervin et al. (1980)	M	
	1.3×10^{-2}		Warner et al. (1980)	M	
	1.2×10^{-2}		Mackay et al. (2006b)	V	
	1.2×10^{-2}		Goldstein (1982)	X	446
	1.2×10^{-2}	2500	Goldstein (1982)	X	298
	1.2×10^{-2}		Nicholson et al. (1984)	C	
	1.1×10^{-2}		Nicholson et al. (1984)	C	12
	1.3×10^{-2}		Shen (1982)	C	
	5.4×10^{-3}		Hilal et al. (2008)	Q	
	2.2×10^{-3}		Modarresi et al. (2007)	Q	67
		4800	Kühne et al. (2005)	Q	
	1.3×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.6×10^{-2}		Katritzky et al. (1998)	Q	
		4600	Kühne et al. (2005)	?	
	1.2×10^{-2}		Mackay et al. (1993)	?	
1-chloro-2-bromoethane C_2H_4BrCl [107-04-0] IBYHHJPAARCAIE-UHFFFAOYSA-N	1.1×10^{-2}		Hine and Mookerjee (1975)	V	
	1.1×10^{-2}		Sieg et al. (2008)	C	
	1.2×10^{-2}		Keshavarz et al. (2022)	Q	
	3.6×10^{-3}		Duchowicz et al. (2020)	Q	
	1.8×10^{-2}		Hilal et al. (2008)	Q	
	5.5×10^{-3}		Modarresi et al. (2007)	Q	67
	1.2×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.7×10^{-2}		Katritzky et al. (1998)	Q	
	3.7×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.1×10^{-2}		Duchowicz et al. (2020)	?	185, 21
1,2-dibromo-1,1-dichloroethane $C_2H_2Br_2Cl_2$ [75-81-0] FIYBYNHDEOSJPL-UHFFFAOYSA-N	6.2×10^{-2}		HSDB (2015)	Q	99
1-bromo-3-chloropropane C_3H_6BrCl [109-70-6] MFESCIUQSIBMSM-UHFFFAOYSA-N	3.9×10^{-2}		HSDB (2015)	Q	99
1,2-dibromo-3-chloropropane $C_3H_5Br_2Cl$ [96-12-8] WBEJYOJJBDISQU-UHFFFAOYSA-N	9.7×10^{-2}	7100	Hiatt (2013)	M	
	5.0×10^{-1}	10000	Kondoh and Nakajima (1997)	M	
	6.6×10^{-2}		HSDB (2015)	V	
	6.7×10^{-2}		Meylan and Howard (1991)	V	
	9.0×10^{-2}		Hilal et al. (2008)	Q	
	1.1×10^{-2}		Modarresi et al. (2007)	Q	67
	6.4×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	2.1×10^{-1}		Katritzky et al. (1998)	Q	

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Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{-2}		Meylan and Howard (1991)	Q	
	4.0×10^{-2}		MacBean (2012a)	?	
1,2,3,4,5-pentabromo-6-chlorocyclohexane	1.0×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_6H_6Br_5Cl$	1.1×10^{2}		Zhang et al. (2010)	Q	287, 289
[87-84-3]	1.8×10^{3}		Zhang et al. (2010)	Q	287, 290
UZOSVZSBPTTWIG-UHFFFAOYSA-N	1.2×10^{1}		Zhang et al. (2010)	Q	287, 291
1,2,3,4-tetrabromo-5,6-dichlorocyclohexane	3.4		Zhang et al. (2010)	Q	287, 288
$C_6H_6Br_4Cl_2$	6.2×10^{1}		Zhang et al. (2010)	Q	287, 289
GABFTOZBVQIDBB-UHFFFAOYSA-N	9.9×10^{2}		Zhang et al. (2010)	Q	287, 290
	6.2		Zhang et al. (2010)	Q	287, 291
1,2,3-tribromo-4,5,6-trichlorocyclohexane	1.1		Zhang et al. (2010)	Q	287, 288
$C_6H_6Br_3Cl_3$	3.6×10^{1}		Zhang et al. (2010)	Q	287, 289
ZDEQCIGFZLZXBZ-UHFFFAOYSA-N	4.1×10^{2}		Zhang et al. (2010)	Q	287, 290
	3.0		Zhang et al. (2010)	Q	287, 291
1-bromo-4-chlorobenzene	6.8×10^{-3}		Duchowicz et al. (2020)	V	186
C_6H_4BrCl	6.8×10^{-3}		Mackay and Shiu (1981)	V	
[106-39-8]	7.7×10^{-3}		Duchowicz et al. (2020)	Q	
NHDODQWIKUYWMW-UHFFFAOYSA-N	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	1.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	9.0×10^{-3}		Hilal et al. (2008)	Q	
	6.8×10^{-3}		Modarresi et al. (2007)	Q	67
	6.9×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	3.3×10^{-2}		Katritzky et al. (1998)	Q	
1,2,4-tribromo-3,5,6-trichlorobenzene $C_6Br_3Cl_3$ [13075-01-9] XAIKFWSNTFEXDC-UHFFFAOYSA-N	4.1×10^{-2}		HSDB (2015)	Q	99
1-(bromomethyl)-2-chlorobenzene C_7H_6BrCl [611-17-6] PURSZYWBIQIANP-UHFFFAOYSA-N	1.9×10^{-2}		HSDB (2015)	Q	447
2-bromo-4-chloro-1-methoxybenzene C_7H_6BrClO (2-bromo-4-chloroanisole) [60633-25-2] YJEMGEBDXDPBSP-UHFFFAOYSA-N	1.8×10^{-2}		Pfeifer et al. (2001)	M	731

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Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-bromo-6-chloro-1-methoxybenzene C_7H_6BrClO (2-bromo-6-chloroanisole) [174913-10-1] NWOYYECMNBWCNK-UHFFFAOYSA-N	1.4×10^{-2}		Pfeifer et al. (2001)	M	731
4-bromo-2-chloro-1-methoxybenzene C_7H_6BrClO (4-bromo-2-chloroanisole) [50638-47-6] FPIQNBOUYZLESW-UHFFFAOYSA-N	1.3×10^{-2}		Pfeifer et al. (2001)	M	731
2-bromo-3,5-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (2-bromo-3,5-dichloroanisole) [73931-43-8] LCHJNNXHVDDVAT-UHFFFAOYSA-N	1.1×10^{-2}		Pfeifer et al. (2001)	M	731
2-bromo-4,6-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (2-bromo-4,6-dichloroanisole) [60633-26-3] OEYKUHBCPJRXGZ-UHFFFAOYSA-N	8.2×10^{-3} 1.2×10^{-2}	3100	Diaz et al. (2005) Pfeifer et al. (2001)	M M	 731
4-bromo-2,3-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (4-bromo-2,3-dichloroanisole) [109803-52-3] BTRCDLZQISXWHZ-UHFFFAOYSA-N	1.1×10^{-2}		Pfeifer et al. (2001)	M	731
4-bromo-2,6-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (4-bromo-2,6-dichloroanisole) [19240-91-6] OAYSFAKCFYRCRU-UHFFFAOYSA-N	1.2×10^{-2} 1.2×10^{-2}	4900	Diaz et al. (2005) Pfeifer et al. (2001)	M M	 731
4-bromo-3,5-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (4-bromo-3,5-dichloroanisole) [174913-20-3] SVEZPKVUIXAEOX-UHFFFAOYSA-N	1.1×10^{-2}		Pfeifer et al. (2001)	M	731

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Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-bromo-2,4-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (3-bromo-2,4-dichloroanisole) [174913-16-7] OXINPOQPENRUHL-UHFFFAOYSA-N	1.2×10^{-2}		Ebert et al. (2023)	?	789
3-bromo-2,6-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (3-bromo-2,6-dichloroanisole) [174913-18-9] ANLVZYYGYBXMIX-UHFFFAOYSA-N	1.1×10^{-2}	2700	Diaz et al. (2005)	M	790
5-bromo-2,4-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (5-bromo-2,4-dichloroanisole) [174913-22-5] SJIIFORJBWPNPM-UHFFFAOYSA-N	1.1×10^{-2}		Pfeifer et al. (2001)	M	731
6-bromo-2,3-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (6-bromo-2,3-dichloroanisole) [174913-23-6] PNLDDSLZYVNPQW-UHFFFAOYSA-N	1.1×10^{-2}		Pfeifer et al. (2001)	M	731
6-bromo-2,5-dichloro-1-methoxybenzene $C_7H_5BrCl_2O$ (6-bromo-2,5-dichloroanisole) [174913-14-5] BVSOVPUWHJWGEP-UHFFFAOYSA-N	7.7×10^{-3}	3000	Diaz et al. (2005)	M	
2-bromo-3,4,5-trichloro-1-methoxybenzene $C_7H_4BrCl_3O$ (2-bromo-3,4,5-trichloroanisole) JIVCPRHFBFVZQL-UHFFFAOYSA-N	9.8×10^{-3}		Pfeifer et al. (2001)	M	731
3-bromo-2,4,6-trichloro-1-methoxybenzene $C_7H_4BrCl_3O$ (3-bromo-2,4,6-trichloroanisole) [174913-28-1] OIHHRLYOSUNYTC-UHFFFAOYSA-N	1.0×10^{-2}		Pfeifer et al. (2001)	M	731

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Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-bromo-2,5,6-trichloro-1-methoxybenzene $C_7H_4BrCl_3O$ (3-bromo-2,5,6-trichloroanisole) [78647-93-5] ZUXVGCIQOSXRJN-UHFFFAOYSA-N	1.0×10^{-2}		Pfeifer et al. (2001)	M	731
4-bromo-2,3,6-trichloro-1-methoxybenzene $C_7H_4BrCl_3O$ (4-bromo-2,3,6-trichloroanisole) [78647-87-7] VZRSUQWPXPUWCS-UHFFFAOYSA-N	1.0×10^{-2}		Pfeifer et al. (2001)	M	731
6-bromo-2,3,4-trichloro-1-methoxybenzene $C_7H_4BrCl_3O$ (6-bromo-2,3,4-trichloroanisole) GVCDCZPXMGMNTR-UHFFFAOYSA-N	1.1×10^{-2}		Pfeifer et al. (2001)	M	731
4-bromo-2,3,5,6-tetrachloro-1-methoxybenzene $C_7H_3BrCl_4O$ (4-bromo-2,3,5,6-tetrachloroanisole) [174913-33-8] YSVAURKXNCNUNS-UHFFFAOYSA-N	9.2×10^{-3}		Pfeifer et al. (2001)	M	731
2,4-dibromo-3-chloro-1-methoxybenzene $C_7H_5Br_2ClO$ (2,4-dibromo-3-chloroanisole) YXYRJAVLYYNRCE-UHFFFAOYSA-N	1.0×10^{-2}		Ebert et al. (2023)	?	789
2,4-dibromo-5-chloro-1-methoxybenzene $C_7H_5Br_2ClO$ (2,4-dibromo-5-chloroanisole) [174913-38-3] OTZRCEAVEJYZQS-UHFFFAOYSA-N	1.0×10^{-2}		Ebert et al. (2023)	?	789
2,6-dibromo-3-chloro-1-methoxybenzene $C_7H_5Br_2ClO$ (2,6-dibromo-3-chloroanisole) AHBGIHFKTBTQJP-UHFFFAOYSA-N	7.4×10^{-3}	770	Diaz et al. (2005)	M	790

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Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,6-dibromo-4-chloro-1-methoxybenzene $C_7H_5Br_2ClO$ (2,6-dibromo-4-chloroanisole) [174913-44-1] WHRDPXDGAMJNGH-UHFFFAOYSA-N	2.0×10^{-2}	6700	Diaz et al. (2005)	M	
	1.1×10^{-2}		Pfeifer et al. (2001)	M	731
2,4-dibromo-3,5-dichloro-1-methoxybenzene $C_7H_4Br_2Cl_2O$ (2,4-dibromo-3,5-dichloroanisole) [174913-52-1] YZMXEWDTXSTFIJ-UHFFFAOYSA-N	9.1×10^{-3}		Pfeifer et al. (2001)	M	731
2,4-dibromo-5,6-dichloro-1-methoxybenzene $C_7H_4Br_2Cl_2O$ (2,4-dibromo-5,6-dichloroanisole) MUUDTVDSRYEMBU-UHFFFAOYSA-N	9.8×10^{-3}		Pfeifer et al. (2001)	M	731
2,3-dibromo-5,6-dichloro-1-methoxybenzene $C_7H_4Br_2Cl_2O$ (2,3-dibromo-5,6-dichloroanisole) WDRCOFFEZVLCLX-UHFFFAOYSA-N	9.1×10^{-3}		Pfeifer et al. (2001)	M	731
2,6-dibromo-3,4,5-trichloro-1-methoxybenzene $C_7H_3Br_2Cl_3O$ (2,6-dibromo-3,4,5-trichloroanisole) RFUGYJHXLQAXOX-UHFFFAOYSA-N	8.6×10^{-3}		Pfeifer et al. (2001)	M	731
2,4,6-tribromo-3-chloro-1-methoxybenzene $C_7H_4Br_3ClO$ (2,4,6-tribromo-3-chloroanisole) [174913-78-1] FWKUBDOTUFVPBX-UHFFFAOYSA-N	9.1×10^{-3}		Pfeifer et al. (2001)	M	731
2,3-dibromo-7,8-dichlorodibenzo-*p*-dioxin $C_{12}H_4Br_2Cl_2O_2$ [50585-40-5] SBSJXPIUKNBZND-UHFFFAOYSA-N	3.2		Ebert et al. (2023)	?	318

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Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2',4',5',7'-tetrabromo-3,4,5,6-tetrachlorofluorescein $C_{20}H_4Br_4Cl_4O_5$ [13473-26-2] ZYIBVBKZZZDFOY-UHFFFAOYSA-N	1.5×10^{13} 1.9×10^{8} 8.0×10^{10} 2.2×10^{8}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
bromochloroacetonitrile $C_2HBrClN$ [83463-62-1] BMWPPNAUMLRKML-UHFFFAOYSA-N	8.2		HSDB (2015)	Q	99
N,N'-dimethyl-3,3',4-tribromo-4,5,5'-trichloro-2,2'-bipyrrole $C_{10}H_6Br_3Cl_3N_2$ (DBP-Br3Cl3a) [400766-93-0] JSQYFPHYSOZLPT-UHFFFAOYSA-N	7.1 9.5		Tittlemier et al. (2004) Hilal et al. (2008)	V Q	
N,N'-dimethyl- 3,4,4'-tribromo-3',5,5'-trichloro-2,2'-bipyrrole $C_{10}H_6Br_3Cl_3N_2$ (DBP-Br3Cl3b) [666856-68-4] GUWAXPTVCYBOMV-UHFFFAOYSA-N	3.3×10^{1} 9.5		Tittlemier et al. (2004) Hilal et al. (2008)	V Q	
N,N'-dimethyl-3,3',4,4'-tetrabromo-5,5'-dichloro-2,2'-bipyrrole $C_{10}H_6Br_4Cl_2N_2$ (DBP-Br4Cl2) [253798-64-0] FQGSQKFVAAJWFY-UHFFFAOYSA-N	2.8×10^{1} 1.8×10^{1}		Tittlemier et al. (2004) Hilal et al. (2008)	V Q	
N,N'-dimethyl-3,3',4,4',5-pentabromo-5'-chloro-2,2'-bipyrrole $C_{10}H_6Br_5ClN_2$ (DBP-Br5Cl) [400767-00-2] LIYSVIAQQQEQBT-UHFFFAOYSA-N	1.5×10^{2} 3.0×10^{1}		Tittlemier et al. (2004) Hilal et al. (2008)	V Q	
1-bromo-3-chloro-5,5-dimethylhydantoin $C_5H_6BrClN_2O_2$ [16079-88-2] PIEXCQIOSMOEOU-UHFFFAOYSA-N	1.2×10^{1}		HSDB (2015)	Q	99

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Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-(4-bromo-3-chlorophenyl)-1-methoxy-1-methylurea	2.2×10^3		HSDB (2015)	V	
$C_9H_{10}BrClN_2O_2$	3.2×10^3		Mackay et al. (2006d)	V	
(chlorbromuron)	2.5×10^3		MacBean (2012a)	?	
[13360-45-7]					
NLYNUTMZTCLNOO-UHFFFAOYSA-N					
N-(4-bromo-2,6-dichloro-3-methylphenyl)acetamide	6.7×10^3		Zhang et al. (2010)	Q	287, 288
$C_9H_8BrCl_2NO$	6.2×10^2		Zhang et al. (2010)	Q	287, 289
[68399-95-1]	2.1×10^4		Zhang et al. (2010)	Q	287, 290
MRPNWLPYJSSISQ-UHFFFAOYSA-N	6.5×10^3		Zhang et al. (2010)	Q	287, 291
halacrinate	2.4×10^2		MacBean (2012a)	?	
$C_{12}H_7NO_2BrCl$					
[34462-96-9]					
YDNLKBDXQCHOTH-UHFFFAOYSA-N					
bromuconazole	3.3×10^4		Duchowicz et al. (2020)	V	186
$C_{13}H_{12}BrCl_2N_3O$	1.2×10^5		HSDB (2015)	V	
[116255-48-2]	1.4×10^2		Duchowicz et al. (2020)	Q	
HJJVPARKXDDIQD-UHFFFAOYSA-N	1.1×10^5		Maniere et al. (2011)	?	12, 165
(±)-(2R^*,4S^*)-bromuconazole	6.4×10^4		Ebert et al. (2023)	?	365
$C_{13}H_{12}BrCl_2N_3O$					
[114544-80-8]					
(±)-(2R^*,4R^*)-bromuconazole	9.5×10^4		Ebert et al. (2023)	?	365
$C_{13}H_{12}BrCl_2N_3O$					
[114544-81-9]					
5,7-dibromo-2-(5-bromo-7-chloro-1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one	4.2×10^9		Zhang et al. (2010)	Q	287, 288
$C_{16}H_6Br_3ClN_2O_2$	3.3×10^{15}		Zhang et al. (2010)	Q	287, 289
[85702-64-3]	2.4×10^5		Zhang et al. (2010)	Q	287, 290
UOWUGDPSFZLTMZ-BUHFOSPRSA-N	8.8×10^9		Zhang et al. (2010)	Q	287, 291
chlorantraniliprole	7.0×10^{15}		HSDB (2015)	Q	99
$C_{18}H_{14}BrCl_2N_5O_2$	3.1×10^8		Maniere et al. (2011)	?	241, 165
[500008-45-7]					
IZCBNTYXTMZSDP-UHFFFAOYSA-N					
cyantraniliprole	5.9×10^{12}		Maniere et al. (2011)	?	241, 165
$C_{19}H_{14}BrClN_6O_2$					
[736994-63-1]					
DVBUIBGJRQBEDP-UHFFFAOYSA-N					

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Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tribromofluoromethane CBr_3F [353-54-8] IHZAEIHJPNTART-UHFFFAOYSA-N	1.5×10^{-3}		Fogg and Sangster (2003)	V	
bromochlorodifluoromethane $CBrClF_2$ [353-59-3] MEXUFEQDCXZEON-UHFFFAOYSA-N	6.1×10^{-5}		Yaws (2003)	X	237, 153
	1.0×10^{-4}		HSDB (2015)	Q	99
	2.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	6.4×10^{-5}		Gharagheizi et al. (2010)	Q	246
	8.6×10^{-5}		Hilal et al. (2008)	Q	
	6.0×10^{-5}		Yaws (1999)	?	21, 153
1-bromo-1-chloro-2,2,2-trifluoroethane $C_2HBrClF_3$ (halothane) [151-67-7] BCQZXOMGPXTTIC-UHFFFAOYSA-N	5.6×10^{-4}	4700	Fogg and Sangster (2003)	L	
	3.1×10^{-4}		Steward et al. (1973)	L	14
	5.3×10^{-4}	4200	Allott et al. (1973)	L	
	2.8×10^{-4}		Guitart et al. (1989)	M	14
	3.3×10^{-4}		Lerman et al. (1983)	M	14
	5.3×10^{-4}	5000	Smith et al. (1981b)	M	
	3.2×10^{-4}		Stoelting and Longshore (1972)	M	14
	3.4×10^{-4}		Saidman et al. (1966)	M	14
	4.9×10^{-4}		Yaws (2003)	X	237, 79
	4.2×10^{-4}		Keshavarz et al. (2022)	Q	
	2.7×10^{-3}		Duchowicz et al. (2020)	Q	184
	4.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
	8.8×10^{-4}		Hilal et al. (2008)	Q	
	1.7×10^{-4}		Modarresi et al. (2007)	Q	67
		4100	Kühne et al. (2005)	Q	
	1.0×10^{-3}		English and Carroll (2001)	Q	230, 231
	4.9×10^{-4}		Duchowicz et al. (2020)	?	185, 21
	4.9×10^{-4}		HSDB (2015)	?	419
		5000	Kühne et al. (2005)	?	
	4.7×10^{-4}		Yaws (1999)	?	21, 79
	3.4×10^{-4}		Abraham and Weathersby (1994)	?	21
	4.8×10^{-4}		Abraham et al. (1990)	?	
tralopyril $C_{12}H_5BrClF_3N_2$ [122454-29-9] XNFIRYXKTXAHAC-UHFFFAOYSA-N	4.5×10^{3}		Ebert et al. (2023)	?	316
chlorfenapyr $C_{15}H_{11}BrClF_3N_2O$ [122453-73-0] CWFOCCVIPCEQCK-UHFFFAOYSA-N	1.7×10^{3}		HSDB (2015)	Q	99

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Table A7.3: Bromine, chlorine and fluorine (C, H, N, O, F, Cl, Br) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
fluazolate $C_{15}H_{12}N_2O_2BrClF_4$ [174514-07-9] FKLQIONHGSFYJY-UHFFFAOYSA-N	1.3×10^{1}		MacBean (2012a)	?	

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A8 Organic species with iodine (I)

A8.1 Iodocarbons (C, H, O, Cl, I)

Table A8.1: Iodocarbons (C, H, O, Cl, I)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
iodomethane	2.0×10^{-3}	3200	Burkholder et al. (2019)	L	1
CH_3I	1.5×10^{-3}	3900	Burkholder et al. (2019)	L	70
(methyl iodide)	2.0×10^{-3}	3600	Burkholder et al. (2015)	L	
[74-88-4]	1.5×10^{-3}	3900	Burkholder et al. (2015)	L	70
INQOMBQAUSQDDS-UHFFFAOYSA-N	2.0×10^{-3}	3100	Brockbank (2013)	L	1
	2.0×10^{-3}	3600	Sander et al. (2011)	L	
	2.0×10^{-3}	3600	Sander et al. (2006)	L	
	2.0×10^{-3}	3600	Staudinger and Roberts (2001)	L	
	1.8×10^{-3}	3200	Hiatt (2013)	M	
	1.4×10^{-3}	3900	Ooki and Yokouchi (2011)	M	70
	1.9×10^{-3}		Gan and Yates (1996)	M	294
	1.4×10^{-3}	4100	Moore et al. (1995)	M	794, 70
	2.0×10^{-3}	3700	Elliott and Rowland (1993)	M	
	1.9×10^{-3}	3800	Hunter-Smith et al. (1983)	M	658
	2.0×10^{-3}	3100	Balls (1980)	M	
	1.8×10^{-3}	3000	Swain and Thornton (1962)	M	
	1.9×10^{-3}	3000	Glew and Moelwyn-Hughes (1953)	M	795
	1.9×10^{-3}	3700	Rex (1906)	M	
	1.8×10^{-3}		Mackay et al. (2006b)	V	
	1.9×10^{-3}	3600	Fogg and Sangster (2003)	V	
	1.8×10^{-3}		Mackay et al. (1993)	V	
	1.8×10^{-3}		Abraham (1984)	V	
	1.8×10^{-3}		Hine and Mookerjee (1975)	V	
	3.5×10^{-3}		Yaws (2003)	X	237
	1.7×10^{-3}		Liss and Slater (1974)	C	
	8.8×10^{-3}		Keshavarz et al. (2022)	Q	
	3.7×10^{-3}		Duchowicz et al. (2020)	Q	
	7.4×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.6×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	2.0×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	3.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.1×10^{-3}		Hilal et al. (2008)	Q	
	6.8×10^{-4}		Modarresi et al. (2007)	Q	67
		3800	Kühne et al. (2005)	Q	
	1.9×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	2.1×10^{-4}		English and Carroll (2001)	Q	230, 231
	8.8×10^{-4}		Katritzky et al. (1998)	Q	
	1.8×10^{-3}		Suzuki et al. (1992)	Q	232
	3.6×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
	1.9×10^{-3}		Duchowicz et al. (2020)	?	185, 21
	1.8×10^{-3}		Mackay et al. (2006b)	?	
		3700	Kühne et al. (2005)	?	

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Table A8.1: Iodocarbons (C, H, O, Cl, I) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.5×10^{-3}		Yaws (1999)	?	21
	1.8×10^{-3}		Mackay et al. (1993)	?	
	3.5×10^{-3}		Yaws and Yang (1992)	?	21
diiodomethane	2.3×10^{-2}	5300	Burkholder et al. (2019)	L	70
CH_2I_2	2.3×10^{-2}	5300	Burkholder et al. (2015)	L	70
[75-11-6]	2.4×10^{-2}	4700	Moore et al. (1995)	M	796, 70
NZZFYRREKKOMAT-UHFFFAOYSA-N	3.2×10^{-2}		Mackay et al. (1993)	V	
	9.9×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	6.2×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	245
	7.3×10^{-2}		Hilal et al. (2008)	Q	
	1.3×10^{-3}		Modarresi et al. (2007)	Q	67
	2.7×10^{-2}		Yao et al. (2002)	Q	229
	3.1×10^{-2}		Katritzky et al. (1998)	Q	
	2.9×10^{-2}		Yaws (1999)	?	21
	2.8×10^{-2}		Yaws and Yang (1992)	?	21
	2.8×10^{-2}		Abraham et al. (1990)	?	
triiodomethane	6.2×10^{-3}		Fogg and Sangster (2003)	V	
CHI_3	4.3×10^{-3}		Yaws (2003)	X	237
(iodoform)	3.2×10^{-6}		HSDB (2015)	Q	99
[75-47-8]	4.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
OKJPEAGHQZHRQV-UHFFFAOYSA-N	1.3×10^{-3}		Hilal et al. (2008)	Q	
	3.4×10^{-3}		Yaws and Yang (1992)	?	21
iodoethane	1.4×10^{-3}	4800	Burkholder et al. (2019)	L	70
C_2H_5I	1.4×10^{-3}	4800	Burkholder et al. (2015)	L	70
[75-03-6]	1.5×10^{-3}	3600	Brockbank (2013)	L	1
HVTICUPFWKNHNG-UHFFFAOYSA-N	1.5×10^{-3}	4200	Fogg and Sangster (2003)	L	797
	1.4×10^{-3}	4800	Ooki and Yokouchi (2011)	M	70
	1.4×10^{-3}		Li et al. (1993)	M	
	1.5×10^{-3}	4000	Rex (1906)	M	
	1.4×10^{-3}		Duchowicz et al. (2020)	V	186
	1.4×10^{-3}		Mackay et al. (2006b)	V	
	1.9×10^{-3}		Mackay et al. (1993)	V	
	1.4×10^{-3}		Abraham (1984)	V	
	1.4×10^{-3}		Hine and Mookerjee (1975)	V	
	1.7×10^{-3}		Yaws (2003)	X	237, 12
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	244
	1.2×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	1.7×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.9×10^{-3}		Hilal et al. (2008)	Q	
		4200	Kühne et al. (2005)	Q	
	1.1×10^{-3}		Yaffe et al. (2003)	Q	248, 272
	4.2×10^{-3}		Yao et al. (2002)	Q	229, 267
	2.2×10^{-4}		English and Carroll (2001)	Q	230, 231

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Table A8.1: Iodocarbons (C, H, O, Cl, I) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-3}		Katritzky et al. (1998)	Q	
	1.3×10^{-3}		Suzuki et al. (1992)	Q	232
	1.2×10^{-3}		Nirmalakhandan and Speece (1988)	Q	
		4100	Kühne et al. (2005)	?	
	1.4×10^{-3}		Yaws (1999)	?	21, 12
	1.1×10^{-3}		Abraham and Weathersby (1994)	?	21
	1.8×10^{-3}		Yaws and Yang (1992)	?	21, 12
	1.4×10^{-3}		Abraham et al. (1990)	?	
(*E*)-1,2-diiodoethene $C_2H_2I_2$ [590-27-2] CVOGMKGEVNGRSK-OWOJBTEDSA-N	3.5×10^{-3}		Duchowicz et al. (2020)	V	186
	5.9×10^{-3}		Duchowicz et al. (2020)	Q	
1-iodopropane C_3H_7I (propyl iodide) [107-08-4] PVWOIHVRPOBWPI-UHFFFAOYSA-N	1.1×10^{-3}	4500	Brockbank (2013)	L	1
	1.1×10^{-3}		Li et al. (1993)	M	
	1.0×10^{-3}	4600	Rex (1906)	M	
	1.1×10^{-3}		Duchowicz et al. (2020)	V	186
	1.1×10^{-3}		Mackay et al. (2006b)	V	
	1.1×10^{-3}		Mackay et al. (1993)	V	
	9.9×10^{-4}		Abraham (1984)	V	
	1.1×10^{-3}		Hine and Mookerjee (1975)	V	
	1.2×10^{-3}		Yaws (2003)	X	237, 79
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	2.9×10^{-3}		Gharagheizi et al. (2012)	Q	
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	271, 243
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.6×10^{-3}		Hilal et al. (2008)	Q	
	2.4×10^{-4}		Modarresi et al. (2007)	Q	67
		4500	Kühne et al. (2005)	Q	
	1.1×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.9×10^{-3}		Yao et al. (2002)	Q	229
	1.1×10^{-3}		English and Carroll (2001)	Q	230, 231
	1.1×10^{-3}		Katritzky et al. (1998)	Q	
	9.9×10^{-4}		Suzuki et al. (1992)	Q	232
	9.5×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
		4500	Kühne et al. (2005)	?	
	1.1×10^{-3}		Yaws (1999)	?	21, 79
	1.2×10^{-3}		Yaws and Yang (1992)	?	21, 79
	9.9×10^{-4}		Abraham et al. (1990)	?	

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Table A8.1: Iodocarbons (C, H, O, Cl, I) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-iodopropane	8.5×10^{-4}	4700	Brockbank (2013)	L	1
C_3H_7I	8.5×10^{-4}	4500	Rex (1906)	M	
(isopropyl iodide)	1.4×10^{-3}		Duchowicz et al. (2020)	V	186
[75-30-9]	8.8×10^{-4}		Hine and Mookerjee (1975)	V	
FMKOJHQHASLBPH-UHFFFAOYSA-N	1.1×10^{-3}		Yaws (2003)	X	237, 12
	5.7×10^{-4}		Duchowicz et al. (2020)	Q	
	6.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	9.9×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
	7.9×10^{-4}		Hilal et al. (2008)	Q	
	1.7×10^{-4}		Modarresi et al. (2007)	Q	67
		4500	Kühne et al. (2005)	Q	
	1.5×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.8×10^{-3}		Yao et al. (2002)	Q	229
	7.9×10^{-4}		English and Carroll (2001)	Q	230, 231
	9.7×10^{-4}		Katritzky et al. (1998)	Q	
	8.6×10^{-4}		Suzuki et al. (1992)	Q	232
	5.4×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
		4700	Kühne et al. (2005)	?	
	8.7×10^{-4}		Yaws (1999)	?	21, 12
	1.1×10^{-3}		Yaws and Yang (1992)	?	21, 12
1-iodobutane	6.9×10^{-4}		Brockbank (2013)	L	
C_4H_9I	5.9×10^{-4}		Duchowicz et al. (2020)	V	186
[542-69-8]	5.4×10^{-4}		Mackay et al. (2006b)	V	
KMGBZBJJOKUPIA-UHFFFAOYSA-N	5.4×10^{-4}		Mackay et al. (1993)	V	
	6.1×10^{-4}		Abraham (1984)	V	
	6.2×10^{-4}		Hine and Mookerjee (1975)	V	
	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	1.2×10^{-3}		Hilal et al. (2008)	Q	
	1.8×10^{-4}		Modarresi et al. (2007)	Q	67
	6.7×10^{-4}		Yaffe et al. (2003)	Q	248, 249
	7.9×10^{-4}		English and Carroll (2001)	Q	230, 231
	1.1×10^{-3}		Katritzky et al. (1998)	Q	
	7.5×10^{-4}		Suzuki et al. (1992)	Q	232
	7.5×10^{-4}		Nirmalakhandan and Speece (1988)	Q	
	6.1×10^{-4}		Abraham et al. (1990)	?	

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Table A8.1: Iodocarbons (C, H, O, Cl, I) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-iodobutane	5.0×10^{-4}		Duchowicz et al. (2020)	V	186
C_4H_9I	5.7×10^{-4}		Duchowicz et al. (2020)	Q	
[513-48-4]	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
IQRUSQUYPCHEKN-UHFFFAOYSA-N	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	7.0×10^{-4}		Hilal et al. (2008)	Q	
1-iodopentane	5.9×10^{-4}		Keshavarz et al. (2022)	Q	
$C_5H_{11}I$	1.2×10^{-3}		Duchowicz et al. (2020)	Q	184
[628-17-1]	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
BLXSFCHWMBESKV-UHFFFAOYSA-N	4.9×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	6.2×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	9.9×10^{-4}		Hilal et al. (2008)	Q	
	1.4×10^{-4}		Modarresi et al. (2007)	Q	67
	5.8×10^{-4}		English and Carroll (2001)	Q	230, 231
	5.7×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	5.1×10^{-4}		Duchowicz et al. (2020)	?	185, 21
	5.1×10^{-4}		Abraham et al. (1990)	?	
1-iodohexane	3.4×10^{-4}		Brockbank (2013)	L	
$C_6H_{13}I$	8.0×10^{-4}		Keshavarz et al. (2022)	Q	
[638-45-9]	1.2×10^{-3}		Duchowicz et al. (2020)	Q	
ANOOTOPTCJRUPK-UHFFFAOYSA-N	8.2×10^{-4}		Hilal et al. (2008)	Q	
	1.2×10^{-4}		Modarresi et al. (2007)	Q	67
	4.2×10^{-4}		English and Carroll (2001)	Q	230, 260
	4.5×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	3.5×10^{-4}		Duchowicz et al. (2020)	?	185, 21
	3.5×10^{-4}		Abraham et al. (1990)	?	
1-iodoheptane	2.6×10^{-4}		Abraham (1984)	V	
$C_7H_{15}I$	1.1×10^{-3}		Keshavarz et al. (2022)	Q	
[4282-40-0]	1.2×10^{-3}		Duchowicz et al. (2020)	Q	184
LMHCYRULPLGEEZ-UHFFFAOYSA-N	3.1×10^{-4}		Raventos-Duran et al. (2010)	Q	242, 243
	3.1×10^{-4}		Raventos-Duran et al. (2010)	Q	244
	3.1×10^{-4}		Raventos-Duran et al. (2010)	Q	245
	6.7×10^{-4}		Hilal et al. (2008)	Q	
	9.7×10^{-5}		Modarresi et al. (2007)	Q	67
	3.1×10^{-4}		English and Carroll (2001)	Q	230, 231
	3.5×10^{-4}		Nirmalakhandan et al. (1997)	Q	
	2.5×10^{-4}		Duchowicz et al. (2020)	?	185, 21
	2.5×10^{-4}		Abraham et al. (1990)	?	
iodocyclohexane	3.9×10^{-3}		Hilal et al. (2008)	Q	
$C_6H_{11}I$					
[626-62-0]					
FUCOMWZKWIEKRK-UHFFFAOYSA-N					

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Table A8.1: Iodocarbons (C, H, O, Cl, I) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-iodo-1-propene C_3H_5I [556-56-9] HFEHLDPGIKPNKL-UHFFFAOYSA-N	3.8×10^{-3}		Hilal et al. (2008)	Q	
1-iodocyclohexene C_6H_9I [17497-53-9] CAROGICRCNKEOD-UHFFFAOYSA-N	4.1×10^{-3}		Hilal et al. (2008)	Q	
iodobenzene C_6H_5I [591-50-4] SNHMUERNLJLMHN-UHFFFAOYSA-N	7.7×10^{-3}		Mackay and Shiu (1981)	L	
	7.6×10^{-3}		Li and Carr (1993)	M	
	1.2×10^{-2}		Duchowicz et al. (2020)	V	186
	1.2×10^{-2}		HSDB (2015)	V	
	7.9×10^{-3}		Schüürmann (2000)	V	
	1.3×10^{-2}		Mackay et al. (1993)	V	
	6.9×10^{-3}		Yaws (2003)	X	237
	8.6×10^{-3}		Duchowicz et al. (2020)	Q	
	7.7×10^{-3}		Li et al. (2014)	Q	241
	8.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	242, 243
	2.0×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	7.8×10^{-3}		Raventos-Duran et al. (2010)	Q	245
	6.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.4×10^{-2}		Hilal et al. (2008)	Q	
	6.9×10^{-3}		Modarresi et al. (2007)	Q	67
	7.7×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	8.3×10^{-3}		Yao et al. (2002)	Q	229
	2.3×10^{-3}		English and Carroll (2001)	Q	230, 231
	6.4×10^{-3}		Katritzky et al. (1998)	Q	
	3.8×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	7.0×10^{-3}		Yaws (1999)	?	21
	7.4×10^{-3}		Yaws and Yang (1992)	?	21
	7.7×10^{-3}		Abraham et al. (1990)	?	
			Brockbank (2013)	W	798
iodoacetic acid $C_2H_3IO_2$ [64-69-7] JDNTWHVOXJZDSN-UHFFFAOYSA-N	2.4×10^{2}		HSDB (2015)	Q	99
2-iodophenol C_6H_5IO [533-58-4] KQDJTBPASNJQFQ-UHFFFAOYSA-N	1.4×10^{1}		Abraham et al. (1994a)	R	
	6.9		Hilal et al. (2008)	Q	
	1.4×10^{1}		Yaffe et al. (2003)	Q	248, 249
	1.5×10^{1}		English and Carroll (2001)	Q	230, 231
	1.6×10^{2}		Nirmalakhandan et al. (1997)	Q	

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Table A8.1: Iodocarbons (C, H, O, Cl, I) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3-iodophenol C_6H_5IO [626-02-8] FXTKWBZFNQHAAO-UHFFFAOYSA-N	7.0×10^{1}		Hilal et al. (2008)	Q	
4-iodophenol C_6H_5IO [540-38-5] VSMDINRNYYEDRN-UHFFFAOYSA-N	4.6×10^{1}		Hilal et al. (2008)	Q	
erythrosine $C_{20}H_8I_4O_5$ [16423-68-0] OALHHIHQOFIMEF-UHFFFAOYSA-N	3.9×10^{13} 2.3×10^{8} 8.6×10^{10} 5.1×10^{9}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
4-hydroxy-3,5-diiodo-benzonitrile $C_7H_3I_2NO$ (ioxynil) [1689-83-4] NRXQIUSYPAHGNM-UHFFFAOYSA-N	1.3×10^{2} 1.8×10^{4}		Mackay et al. (2006d) HSDB (2015)	V Q	 99
3-iodo-2-propynyl butylcarbamate $C_8H_{12}INO_2$ [55406-53-6] WYVVKGNFXHOCQV-UHFFFAOYSA-N	8.2×10^{1}		HSDB (2015)	V	
diatrizoic acid $C_{11}H_9I_3N_2O_4$ [117-96-4] YVPYQUNUQOZFHG-UHFFFAOYSA-N	3.5×10^{12} 5.4×10^{8} 1.2×10^{17} 3.3×10^{16}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
iothalamic acid $C_{11}H_9I_3N_2O_4$ [2276-90-6] UXIGWFXRQKWHHA-UHFFFAOYSA-N	4.4×10^{12} 4.8×10^{9} 4.2×10^{16} 1.9×10^{16}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
benodanil $C_{13}H_{10}INO$ [15310-01-7] LJOZMWRYMKECFF-UHFFFAOYSA-N	6.2×10^{5} $>2.3\times10^{10}$		Mackay et al. (2006d) MacBean (2012a)	V ?	
proquinazid $C_{14}H_{17}IN_2O_2$ [189278-12-4] FLVBXVXXXMLMOX-UHFFFAOYSA-N	3.3×10^{1}		Maniere et al. (2011)	?	165
iopamidol $C_{17}H_{22}I_3N_3O_8$ [60166-93-0] XQZXYNRDCRIARQ-LURJTMIESA-N	9.0×10^{19}		HSDB (2015)	Q	99

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Table A8.1: Iodocarbons (C, H, O, Cl, I) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ioxaglic acid	2.7×10^{35}		Zhang et al. (2010)	Q	287, 288
$C_{24}H_{21}I_6N_5O_8$	1.4×10^{27}		Zhang et al. (2010)	Q	287, 289
[59017-64-0]	2.0×10^{29}		Zhang et al. (2010)	Q	287, 290
TYYBFXNZMFNZJT-UHFFFAOYSA-N	7.2×10^{38}		Zhang et al. (2010)	Q	287, 291
perfluorohexyl iodide	4.6×10^{-4}	8200	Abusallout et al. (2022)	M	
$C_6F_{13}I$					
[355-43-1]					
BULLJMKUVKYZDJ-UHFFFAOYSA-N					
1,1,1,2,2,3,3-heptafluoro-5-iodopentane	4.6×10^{-6}		Zhang et al. (2010)	Q	287, 288
$C_5H_4F_7I$	1.2×10^{-4}		Zhang et al. (2010)	Q	287, 289
[68188-12-5]	3.8×10^{-4}		Zhang et al. (2010)	Q	287, 290
TZNRRNKRZXHADL-UHFFFAOYSA-N	5.0×10^{-6}		Zhang et al. (2010)	Q	287, 291
1-fluoro-4-iodobenzene	4.5×10^{-3}		Ebert et al. (2023)	?	316
C_6H_4FI					
[352-34-1]					
KGNQDBQYEBMPFZ-UHFFFAOYSA-N					
5-diethylamiloride	8.8×10^{-7}		Zhang et al. (2010)	Q	287, 288
$C_6H_4F_9I$	5.6×10^{-5}		Zhang et al. (2010)	Q	287, 289
[2043-55-2]	1.9×10^{-4}		Zhang et al. (2010)	Q	287, 290
CXHFIVFPHDGZIS-UHFFFAOYSA-N	1.0×10^{-6}		Zhang et al. (2010)	Q	287, 291
1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-8-iodooctane	1.3×10^{-3}		Abusallout et al. (2022)	M	
$C_8H_4F_{13}I$	3.2×10^{-8}		Zhang et al. (2010)	Q	287, 288
[2043-57-4]	3.4×10^{-6}		Zhang et al. (2010)	Q	287, 289
NVVZEKTVIXIUKW-UHFFFAOYSA-N	5.4×10^{-5}		Zhang et al. (2010)	Q	287, 290
	4.3×10^{-8}		Zhang et al. (2010)	Q	287, 291
1H,2H-perfluoro-1-iodooct-1-ene	8.4×10^{-4}		Abusallout et al. (2022)	M	
$C_8H_2F_{13}I$					
[150223-14-6]					
WDWNMIBWWPZNJK-OWOJBTEDSA-N					
1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-10-iododecane	1.2×10^{-9}		Zhang et al. (2010)	Q	287, 288
$C_{10}H_4F_{17}I$	7.7×10^{-8}		Zhang et al. (2010)	Q	287, 289
[2043-53-0]	2.0×10^{-5}		Zhang et al. (2010)	Q	287, 290
XVKJSLBVVRCOIT-UHFFFAOYSA-N	2.3×10^{-9}		Zhang et al. (2010)	Q	287, 291
chloroiodomethane	8.4×10^{-3}	5100	Burkholder et al. (2019)	L	70
CH_2ClI	8.4×10^{-3}	5100	Burkholder et al. (2015)	L	70
[593-71-5]	8.3×10^{-3}	6200	Ooki and Yokouchi (2011)	M	70
PJGJQVRXEUVAFT-UHFFFAOYSA-N	9.1×10^{-3}	4100	Moore et al. (1995)	M	799, 70
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	271, 243
	2.5×10^{-2}		Raventos-Duran et al. (2010)	Q	244
	4.9×10^{-3}		Raventos-Duran et al. (2010)	Q	245

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Table A8.1: Iodocarbons (C, H, O, Cl, I) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.0×10^{-2} 5.0×10^{-4}		Hilal et al. (2008) Modarresi et al. (2007)	Q Q	 67
1-chloro-4-iodobenzene C_6H_4ClI [637-87-6] GWQSENYKCGJTRI-UHFFFAOYSA-N	6.9×10^{-3}		Ebert et al. (2023)	?	316
bromoiodomethane CH_2BrI [557-68-6] TUDWMIUPYRKEFN-UHFFFAOYSA-N	2.0×10^{-2}		Karagodin-Doyennel et al. (2021)	E	800
1-bromo-4-iodobenzene C_6H_4BrI [589-87-7] UCCUXODGPMAHRL-UHFFFAOYSA-N	1.5×10^{-2}		Ebert et al. (2023)	?	316

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A9 Organic species with sulfur (S)

A9.1 Sulfur (C, H, O, N, Cl, S)

Table A9.1: Sulfur (C, H, O, N, Cl, S)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^\ominus$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methanethiol	3.8×10^{-3}	3400	Burkholder et al. (2019)	L	
CH_3SH	3.8×10^{-3}	3400	Burkholder et al. (2015)	L	
(methyl mercaptan)	3.8×10^{-3}	3400	Sander et al. (2011)	L	
[74-93-1]	3.8×10^{-3}	3400	Sander et al. (2006)	L	
LSDPWZHWYPCBBB-UHFFFAOYSA-N	2.8×10^{-3}	2900	Plyasunova et al. (2004)	L	
	2.8×10^{-3}	3100	Staudinger and Roberts (2001)	L	
	2.0×10^{-3}	2800	De Bruyn et al. (1995b)	M	
	2.3×10^{-3}	2700	Tsuji et al. (1990)	M	62
	3.9×10^{-3}	3400	Przyjazny et al. (1983)	M	
	3.3×10^{-3}		Hine and Weimar (1965)	M	
	3.2×10^{-3}		Duchowicz et al. (2020)	V	186
	3.2×10^{-3}		HSDB (2015)	V	
	3.3×10^{-3}		Hine and Mookerjee (1975)	V	
	2.4×10^{-3}		Yaws (2003)	X	237
	2.6×10^{-3}	1600	Goldstein (1982)	X	298
	1.4×10^{-1}		Duchowicz et al. (2020)	Q	
	2.3×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
	3.5×10^{-3}		Hilal et al. (2008)	Q	
		3300	Kühne et al. (2005)	Q	
	4.1×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.0×10^{-2}		Yao et al. (2002)	Q	229
	2.1×10^{-3}		Katritzky et al. (1998)	Q	
	2.9×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	7.0×10^{-3}		Russell et al. (1992)	Q	279
	4.0×10^{-3}		Suzuki et al. (1992)	Q	232
		3400	Kühne et al. (2005)	?	
	2.4×10^{-3}		Yaws et al. (2003)	?	21
	5.1×10^{-3}		Yaws (1999)	?	21, 80
	4.0×10^{-3}		Abraham et al. (1990)	?	
ethanethiol	2.8×10^{-3}	3700	Burkholder et al. (2019)	L	
C_2H_5SH	2.8×10^{-3}	3700	Burkholder et al. (2015)	L	
(ethyl mercaptan)	2.8×10^{-3}	3700	Sander et al. (2011)	L	
[75-08-1]	2.8×10^{-3}	3700	Sander et al. (2006)	L	
DNJIEGIFACGWOD-UHFFFAOYSA-N	2.3×10^{-3}	3500	Plyasunova et al. (2004)	L	
	2.4×10^{-3}	2800	Jou et al. (2021)	M	
	2.8×10^{-3}	3700	Przyjazny et al. (1983)	M	
	2.2×10^{-3}		Vitenberg et al. (1975)	M	
	3.4×10^{-3}		Mackay et al. (2006d)	V	
	3.4×10^{-3}		Mackay et al. (1995)	V	
	3.4×10^{-3}		Hwang et al. (1992)	V	
	3.6×10^{-3}		Hine and Mookerjee (1975)	V	

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	3.4×10^{-3}		Yaws (2003)	X	237
	1.8×10^{-3}		Hayer et al. (2022)	Q	20
	1.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
	3.9×10^{-3}		Hilal et al. (2008)	Q	
	5.6×10^{-3}		Modarresi et al. (2007)	Q	67
		3600	Kühne et al. (2005)	Q	
	2.2×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	5.8×10^{-3}		Yao et al. (2002)	Q	229
	3.6×10^{-3}		English and Carroll (2001)	Q	230, 231
	2.9×10^{-3}		Katritzky et al. (1998)	Q	
	1.9×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	1.0×10^{-2}		Russell et al. (1992)	Q	279
	2.9×10^{-3}		Suzuki et al. (1992)	Q	232
		3700	Kühne et al. (2005)	?	
	3.4×10^{-3}		Yaws et al. (2003)	?	21
	3.4×10^{-3}		Yaws (1999)	?	21
	3.4×10^{-3}		Yaws and Yang (1992)	?	21
	2.8×10^{-3}		Abraham et al. (1990)	?	
1,2-ethanedithiol $C_2H_6S_2$ [540-63-6] VYMPLPIFKRHAAC-UHFFFAOYSA-N	8.2×10^{-2}		HSDB (2015)	Q	99
thiirane C_2H_4S (ethylene sulfide) [420-12-2] VOVUARRWDCVURC-UHFFFAOYSA-N	2.8×10^{-2}		HSDB (2015)	Q	99
1-propanethiol C_3H_7SH (propyl mercaptan) [107-03-9] SUVIGLJNEAMWEG-UHFFFAOYSA-N	1.7×10^{-3}	3600	Plyasunova et al. (2004)	L	
	1.8×10^{-3}	4100	Haimi et al. (2006)	M	801
	1.7×10^{-3}	3100	Coquelet and Richon (2005)	M	
	2.4×10^{-3}	3900	Przyjazny et al. (1983)	M	
	9.0×10^{-4}		Mazza (1980)	M	
	2.4×10^{-3}		Yaws et al. (2003)	V	802
	2.4×10^{-3}		Yaws (2003)	X	237
	1.6×10^{-2}		Keshavarz et al. (2022)	Q	
	4.7×10^{-2}		Duchowicz et al. (2020)	Q	299
	8.2×10^{-4}		Gharagheizi et al. (2012)	Q	
	2.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
	3.4×10^{-3}		Hilal et al. (2008)	Q	
		4000	Kühne et al. (2005)	Q	
	3.9×10^{-3}		Yao et al. (2002)	Q	229, 267
	2.9×10^{-3}		English and Carroll (2001)	Q	230, 260
	1.5×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	2.4×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		3800	Kühne et al. (2005)	?	

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{-3}		Yaws (1999)	?	21
	2.4×10^{-3}		Abraham et al. (1990)	?	
2-propanethiol	1.3×10^{-3}	3700	Brockbank (2013)	L	1
C_3H_8S	1.6×10^{-3}	4300	Zin et al. (2016)	M	803
(isopropyl mercaptan)	1.3×10^{-3}	3800	Haimi et al. (2006)	M	804
[75-33-2]	2.2×10^{-3}		Yaws et al. (2003)	V	802
KJRCEJOSASVSRA-UHFFFAOYSA-N	2.2×10^{-3}		Yaws (2003)	X	237
	2.1×10^{-3}		HSDB (2015)	Q	99
	1.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	2.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.1×10^{-3}		Hilal et al. (2008)	Q	
	2.9×10^{-3}		Yao et al. (2002)	Q	229
	2.4×10^{-3}		Yaws (1999)	?	21
1-butanethiol	1.5×10^{-3}	4300	Brockbank (2013)	L	1
C_4H_9SH	1.4×10^{-3}	4400	Plyasunova et al. (2004)	L	
(butyl mercaptan)	1.5×10^{-3}	4300	Haimi et al. (2006)	M	805
[109-79-5]	1.5×10^{-3}	3600	Coquelet and Richon (2005)	M	
WQAQPCDUOCURKW-UHFFFAOYSA-N	2.2×10^{-3}	4100	Przyjazny et al. (1983)	M	
	1.1×10^{-3}		Mackay et al. (2006d)	V	
	1.1×10^{-3}		Mackay et al. (1995)	V	
	1.4×10^{-3}		Hwang et al. (1992)	V	
	1.1×10^{-3}		Yaws (2003)	X	258
	1.1×10^{-3}		Yaws (2003)	X	237
	1.8×10^{-3}		Dupeux et al. (2022)	Q	259
	2.2×10^{-2}		Keshavarz et al. (2022)	Q	
	4.8×10^{-2}		Duchowicz et al. (2020)	Q	299
	6.1×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.7×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.7×10^{-3}		Hilal et al. (2008)	Q	
	3.4×10^{-3}		Modarresi et al. (2007)	Q	67
		4300	Kühne et al. (2005)	Q	
	2.2×10^{-3}		Yaffe et al. (2003)	Q	248, 272
	3.2×10^{-3}		Yao et al. (2002)	Q	229
	2.3×10^{-3}		English and Carroll (2001)	Q	230, 231
	2.5×10^{-3}		Katritzky et al. (1998)	Q	
	1.2×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	2.2×10^{-3}		Duchowicz et al. (2020)	?	185, 21
	1.1×10^{-3}		Bartelt-Hunt et al. (2008)	?	21
		4200	Kühne et al. (2005)	?	
	1.1×10^{-3}		Yaws et al. (2003)	?	21
	1.1×10^{-3}		Yaws (1999)	?	21
	1.1×10^{-3}		Yaws and Yang (1992)	?	21
	2.2×10^{-3}		Abraham et al. (1990)	?	

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-butanethiol	1.3×10^{-3}		Plyasunova et al. (2004)	L	
$C_4H_{10}S$	1.4×10^{-3}		Duchowicz et al. (2020)	V	186
(*sec*-butyl mercaptan)	1.4×10^{-3}		HSDB (2015)	V	
[513-53-1]	1.9×10^{-3}		Yaws et al. (2003)	V	802
LOCHFZBWPCLPAN-UHFFFAOYSA-N	1.9×10^{-3}		Yaws (2003)	X	237
	1.9×10^{-2}		Duchowicz et al. (2020)	Q	
	9.4×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.8×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.7×10^{-3}		Modarresi et al. (2007)	Q	67
	2.0×10^{-3}		Yao et al. (2002)	Q	229
	1.5×10^{-3}		Yaws (1999)	?	21
2-methyl-1-propanethiol	1.0×10^{-3}	3600	Zin et al. (2016)	M	806
$C_4H_{10}S$	1.9×10^{-3}		Yaws et al. (2003)	V	802
(isobutyl mercaptan)	1.9×10^{-3}		Yaws (2003)	X	237
[513-44-0]	3.3×10^{-4}		Gharagheizi et al. (2012)	Q	
BDFAOUQQXJIZDG-UHFFFAOYSA-N	2.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.4×10^{-3}		Hilal et al. (2008)	Q	
	2.0×10^{-3}		Yao et al. (2002)	Q	229, 267
	1.4×10^{-3}		Yaws (1999)	?	21
2-methyl-2-propanethiol	4.5×10^{-4}		Plyasunova et al. (2004)	L	
$C_4H_{10}S$	1.9×10^{-3}		Yaws et al. (2003)	V	802
(*tert*-butyl mercaptan)	1.9×10^{-3}		Yaws (2003)	X	237
[75-66-1]	1.6×10^{-3}		HSDB (2015)	Q	99
WMXCDAVJEZZYLT-UHFFFAOYSA-N	1.6×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
	6.1×10^{-4}		Hilal et al. (2008)	Q	
	1.1×10^{-3}		Yao et al. (2002)	Q	229
	1.8×10^{-3}		Yaws (1999)	?	21
1,4-dithiane	2.4×10^{-1}		Duchowicz et al. (2020)	V	186
$C_4H_8S_2$	2.3×10^{-1}		HSDB (2015)	V	
[505-29-3]	6.9		Duchowicz et al. (2020)	Q	
LOZWAPSEEHRYPG-UHFFFAOYSA-N					
1-pentanethiol	8.7×10^{-4}		Plyasunova et al. (2004)	L	
$C_5H_{11}SH$	8.2×10^{-4}		Duchowicz et al. (2020)	V	186
(pentyl mercaptan)	8.2×10^{-4}		HSDB (2015)	V	
[110-66-7]	1.4×10^{-3}		Yaws et al. (2003)	V	802
ZRKMQKLGEQPLNS-UHFFFAOYSA-N	7.3×10^{-4}		Amoore and Buttery (1978)	V	
	1.4×10^{-3}		Yaws (2003)	X	237
	4.8×10^{-2}		Duchowicz et al. (2020)	Q	
	4.6×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.3×10^{-3}		Hilal et al. (2008)	Q	
	2.5×10^{-3}		Modarresi et al. (2007)	Q	67
	1.6×10^{-3}		Yao et al. (2002)	Q	229, 267
	7.1×10^{-4}		Yaws (1999)	?	21

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,2-dimethyl-1-propanethiol	1.5×10^{-3}		Yaws et al. (2003)	V	802
$C_5H_{12}S$	1.5×10^{-3}		Yaws (2003)	X	237
[1679-08-9]	1.1×10^{-4}		Gharagheizi et al. (2012)	Q	
LSUXMVNABVPWMF-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
2-methyl-1-butanethiol	1.5×10^{-3}		Yaws et al. (2003)	V	802
$C_5H_{12}S$	1.5×10^{-3}		Yaws (2003)	X	237
[1878-18-8]	2.6×10^{-4}		Gharagheizi et al. (2012)	Q	
WGQKBCSACFQGQY-UHFFFAOYSA-N	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
2-methyl-2-butanethiol	1.5×10^{-3}		Yaws et al. (2003)	V	802
$C_5H_{12}S$	1.5×10^{-3}		Yaws (2003)	X	237
[1679-09-0]	8.6×10^{-4}		Gharagheizi et al. (2012)	Q	
IQIBYAHJXQVQGB-UHFFFAOYSA-N	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
	8.9×10^{-4}		Yao et al. (2002)	Q	229, 807
	1.0×10^{-3}		Yaws (1999)	?	21
2-pentanethiol	1.5×10^{-3}		Yaws et al. (2003)	V	802
$C_5H_{12}S$	1.5×10^{-3}		Yaws (2003)	X	258
[2084-19-7]	1.5×10^{-3}		Yaws (2003)	X	237
QUSTYFNPKBDELJ-UHFFFAOYSA-N	1.0×10^{-3}		Dupeux et al. (2022)	Q	259
	6.3×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
3-pentanethiol	1.5×10^{-3}		Yaws et al. (2003)	V	802
$C_5H_{12}S$	1.5×10^{-3}		Yaws (2003)	X	237
[616-31-9]	4.5×10^{-4}		Gharagheizi et al. (2012)	Q	
WICKAMSPKJXSGN-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
3-methyl-1-butanethiol	9.5×10^{-4}		Plyasunova et al. (2004)	L	
$C_5H_{12}S$	1.5×10^{-3}		Yaws et al. (2003)	V	802
[541-31-1]	1.5×10^{-3}		Yaws (2003)	X	237
GIJGXNFNUUFEGH-UHFFFAOYSA-N	3.7×10^{-4}		Gharagheizi et al. (2012)	Q	
	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
3-methyl-2-butanethiol	1.5×10^{-3}		Yaws et al. (2003)	V	802
$C_5H_{12}S$	1.5×10^{-3}		Yaws (2003)	X	237
[2084-18-6]	4.0×10^{-4}		Gharagheizi et al. (2012)	Q	
BFLXFRNPNMTTAA-UHFFFAOYSA-N	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
1-hexanethiol	5.2×10^{-4}		Plyasunova et al. (2004)	L	
$C_6H_{14}S$	1.1×10^{-3}		Yaws et al. (2003)	V	802
(hexyl mercaptan)	1.1×10^{-3}		Yaws (2003)	X	237
[111-31-9]	3.5×10^{-4}		Gharagheizi et al. (2012)	Q	
PMBXCGGQNSVESQ-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.9×10^{-3}		Hilal et al. (2008)	Q	
	1.4×10^{-3}		Yao et al. (2002)	Q	229
	4.5×10^{-4}		Yaws (1999)	?	21

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-hexanethiol	1.2×10^{-3}		Yaws et al. (2003)	V	802
$C_6H_{14}S$	1.2×10^{-3}		Yaws (2003)	X	237
[1679-06-7]	4.9×10^{-4}		Gharagheizi et al. (2012)	Q	
ABNPJVOPTXYSQW-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
1-heptanethiol	4.2×10^{-4}		Plyasunova et al. (2004)	L	
$C_7H_{16}S$	4.0×10^{-4}		Duchowicz et al. (2020)	V	186
(heptyl mercaptan)	9.5×10^{-4}		Yaws et al. (2003)	V	802
[1639-09-4]	8.2×10^{-4}		Yaws (2003)	X	237
VPIAKHNXCOTPAY-UHFFFAOYSA-N	4.8×10^{-2}		Duchowicz et al. (2020)	Q	
	2.7×10^{-4}		Gharagheizi et al. (2012)	Q	
	8.4×10^{-4}		Gharagheizi et al. (2010)	Q	246
	2.7×10^{-3}		Hilal et al. (2008)	Q	
	1.2×10^{-3}		Yao et al. (2002)	Q	229, 267
	3.3×10^{-4}		Yaws (1999)	?	21
2-heptanethiol	1.3×10^{-3}		Yaws et al. (2003)	V	802
$C_7H_{16}S$	8.2×10^{-4}		Yaws (2003)	X	237
[628-00-2]	4.1×10^{-4}		Gharagheizi et al. (2012)	Q	
DAZNOIJJVKASGS-UHFFFAOYSA-N	8.3×10^{-4}		Gharagheizi et al. (2010)	Q	246
1-octanethiol	7.1×10^{-4}		Yaws et al. (2003)	V	802
$C_8H_{18}S$	6.9×10^{-4}		Yaws (2003)	X	237
(octyl mercaptan)	4.3×10^{-4}		HSDB (2015)	Q	99
[111-88-6]	2.0×10^{-4}		Gharagheizi et al. (2012)	Q	
KZCOBXFFBQJQHH-UHFFFAOYSA-N	7.4×10^{-4}		Gharagheizi et al. (2010)	Q	246
	1.3×10^{-3}		Hilal et al. (2008)	Q	
	1.1×10^{-3}		Yao et al. (2002)	Q	229
	3.0×10^{-4}		Yaws (1999)	?	21
tert-octanethiol	2.0×10^{-3}		Yaws et al. (2003)	V	802
$C_8H_{18}S$	6.2×10^{-4}		Yaws (2003)	X	237
(*tert*-octyl mercaptan)	5.2×10^{-4}		HSDB (2015)	Q	99
[141-59-3]	2.8×10^{-4}		Gharagheizi et al. (2012)	Q	
QZLAEIZEPJAELS-UHFFFAOYSA-N	6.6×10^{-4}		Gharagheizi et al. (2010)	Q	246
	4.2×10^{-4}		Yao et al. (2002)	Q	229
	2.6×10^{-4}		Yaws (1999)	?	21
2-octanethiol	9.9×10^{-4}		Yaws et al. (2003)	V	802
$C_8H_{18}S$	6.6×10^{-4}		Yaws (2003)	X	237
[3001-66-9]	3.0×10^{-4}		Gharagheizi et al. (2012)	Q	
BZXFEMZFRLXGCY-UHFFFAOYSA-N	6.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
1-nonanethiol	5.7×10^{-4}		Yaws et al. (2003)	V	802
$C_9H_{20}S$	6.7×10^{-4}		Yaws (2003)	X	237
(nonyl mercaptan)	1.5×10^{-4}		Gharagheizi et al. (2012)	Q	
[1455-21-6]	7.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
ZVEZMVFBMOOHAT-UHFFFAOYSA-N	1.2×10^{-3}		Hilal et al. (2008)	Q	
	8.9×10^{-4}		Yao et al. (2002)	Q	229, 267
	3.7×10^{-4}		Yaws (1999)	?	21

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-nonanethiol	7.7×10^{-4}		Yaws et al. (2003)	V	802
$C_9H_{20}S$	5.1×10^{-4}		Yaws (2003)	X	237
[13281-11-3]	2.3×10^{-4}		Gharagheizi et al. (2012)	Q	
UOMSUBPWUZCGQU-UHFFFAOYSA-N	6.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
1-decanethiol	5.0×10^{-4}		Yaws et al. (2003)	V	802
$C_{10}H_{22}S$	8.1×10^{-4}		Yaws (2003)	X	237
(decyl mercaptan)	1.6×10^{-4}		Gharagheizi et al. (2012)	Q	
[143-10-2]	7.7×10^{-4}		Gharagheizi et al. (2010)	Q	246
VTXVGVNLYGSIAR-UHFFFAOYSA-N	9.9×10^{-4}		Hilal et al. (2008)	Q	
	8.2×10^{-4}		Yao et al. (2002)	Q	229
	6.5×10^{-4}		Yaws (1999)	?	21
2-decanethiol	6.5×10^{-4}		Yaws et al. (2003)	V	802
$C_{10}H_{22}S$	4.4×10^{-4}		Yaws (2003)	X	237
[13402-60-3]	2.5×10^{-4}		Gharagheizi et al. (2012)	Q	
NWKXKAHGQAWFQP-UHFFFAOYSA-N	5.8×10^{-4}		Gharagheizi et al. (2010)	Q	246
1-undecanethiol	4.9×10^{-4}		Yaws et al. (2003)	V	802
$C_{11}H_{24}S$	2.6×10^{-3}		Yaws (2003)	X	237
(undecyl mercaptan)	9.3×10^{-4}		Gharagheizi et al. (2010)	Q	246
[5332-52-5]	6.7×10^{-4}		Yao et al. (2002)	Q	229
CCIDWXHLGNEQSL-UHFFFAOYSA-N	3.4×10^{-3}		Yaws (1999)	?	21
2-undecanethiol	6.1×10^{-4}		Yaws et al. (2003)	V	802
$C_{11}H_{24}S$	6.6×10^{-4}		Yaws (2003)	X	237
[62155-02-6]	2.9×10^{-4}		Gharagheizi et al. (2012)	Q	
KRMLVHZORKTOLI-UHFFFAOYSA-N	6.0×10^{-4}		Gharagheizi et al. (2010)	Q	246
1-dodecanethiol	5.3×10^{-4}		Yaws et al. (2003)	V	802
$C_{12}H_{26}S$	5.8×10^{-4}		Yaws (2003)	X	237
(dodecyl mercaptan)	1.7×10^{-4}		HSDB (2015)	Q	99
[112-55-0]	1.9×10^{-4}		Gharagheizi et al. (2012)	Q	
WNAHIZMDSQCWRP-UHFFFAOYSA-N	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
	5.3×10^{-4}		Yao et al. (2002)	Q	229
	1.4×10^{-3}		Yaws (1999)	?	21
2-dodecanethiol	6.3×10^{-4}		Yaws et al. (2003)	V	802
$C_{12}H_{26}S$	7.2×10^{-4}		Yaws (2003)	X	237
[14402-50-7]	3.0×10^{-4}		Gharagheizi et al. (2012)	Q	
UROXMPKAGAWKPP-UHFFFAOYSA-N	6.9×10^{-4}		Gharagheizi et al. (2010)	Q	246
5-propyl-5-nonanethiol	1.7×10^{-4}		Zhang et al. (2010)	Q	287, 288
$C_{12}H_{26}S$	5.8×10^{-4}		Zhang et al. (2010)	Q	287, 289
BGQHJKADBZPYGJ-UHFFFAOYSA-N	2.4×10^{-3}		Zhang et al. (2010)	Q	287, 290
	9.7×10^{-5}		Zhang et al. (2010)	Q	287, 291

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-tridecanethiol	6.4×10^{-4}		Yaws et al. (2003)	V	802
$C_{13}H_{28}S$	2.8×10^{-3}		Yaws (2003)	X	237
[19484-26-5]	2.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
IPBROXKVGHZHJV-UHFFFAOYSA-N					
2-tridecanethiol	7.3×10^{-4}		Yaws et al. (2003)	V	802
$C_{13}H_{28}S$	9.6×10^{-4}		Yaws (2003)	X	237
[62155-03-7]	3.2×10^{-4}		Gharagheizi et al. (2012)	Q	
ZAPRCDVCNIREGW-UHFFFAOYSA-N	9.0×10^{-4}		Gharagheizi et al. (2010)	Q	246
1-tetradecanethiol	8.5×10^{-4}		Yaws et al. (2003)	V	802
$C_{14}H_{30}S$	5.1×10^{-3}		Yaws (2003)	X	237
[2079-95-0]	4.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
GEKDEMKPCKTKEC-UHFFFAOYSA-N					
2-tetradecanethiol	9.2×10^{-4}		Yaws et al. (2003)	V	802
$C_{14}H_{30}S$	1.5×10^{-3}		Yaws (2003)	X	237
[62155-04-8]	3.4×10^{-4}		Gharagheizi et al. (2012)	Q	
YESAYZVWGLMPDY-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
dimethyl sulfide	5.3×10^{-3}	3500	Burkholder et al. (2019)	L	
CH_3SCH_3	5.3×10^{-3}	3500	Burkholder et al. (2015)	L	
(DMS)	5.4×10^{-3}	3500	Brockbank (2013)	L	1
[75-18-3]	5.6×10^{-3}	3500	Warneck and Williams (2012)	L	
QMMFVYPAHWMCMS-UHFFFAOYSA-N	5.3×10^{-3}	3500	Sander et al. (2011)	L	
	5.3×10^{-3}	3500	Sander et al. (2006)	L	
	5.3×10^{-3}	3800	Plyasunova et al. (2004)	L	
	5.2×10^{-3}	3600	Fogg and Sangster (2003)	L	
	5.3×10^{-3}	3500	Staudinger and Roberts (2001)	L	
	4.7×10^{-3}	4700	Bruneel et al. (2016)	M	
	4.6×10^{-3}		Schuhfried et al. (2011)	M	
	4.8×10^{-3}	2800	Falabella (2007)	M	11, 338
	5.2×10^{-3}	3600	Coquelet and Richon (2005)	M	
	5.5×10^{-3}	3800	Iliuta and Larachi (2005a)	M	
	4.9×10^{-3}		Straver and de Loos (2005)	M	
	6.4×10^{-3}	4100	Barcellos da Rosa et al. (2003)	M	
	4.9×10^{-3}		Pollien et al. (2003)	M	
	6.4×10^{-3}		van Ruth et al. (2002)	M	14
	7.2×10^{-3}		van Ruth and Villeneuve (2002)	M	14, 361
	4.7×10^{-3}	3700	Gershenzon et al. (2001)	M	
	4.9×10^{-3}		van Ruth et al. (2001)	M	14
	1.6×10^{-2}		Marin et al. (1999)	M	
	4.2×10^{-3}	4300	Wong and Wang (1997)	M	
	4.7×10^{-3}	3100	De Bruyn et al. (1995b)	M	
	5.7×10^{-3}	2700	Tsuji et al. (1990)	M	62
	5.5×10^{-3}	3500	Dacey et al. (1984)	M	
	5.6×10^{-3}	4000	Przyjazny et al. (1983)	M	
	6.1×10^{-3}		Vitenberg et al. (1975)	M	12
	1.6×10^{-3}		Lovelock et al. (1972)	M	

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
			Mackay et al. (2006d)	V	558
	4.2×10^{-3}		Marin et al. (1999)	V	
	1.3×10^{-1}		Mackay et al. (1995)	V	
	5.4×10^{-3}		Hine and Mookerjee (1975)	V	
	5.5×10^{-3}		Hine and Weimar (1965)	V	
	7.0×10^{-3}		Vitenberg et al. (1975)	R	12
	6.0×10^{-3}	3700	Bagno et al. (1991)	T	473
	5.5×10^{-3}		Yaws (2003)	X	237
	6.1×10^{-3}		Gaffney and Senum (1984)	X	389
	4.4×10^{-3}		Cline and Bates (1983)	C	70
	2.3×10^{-3}		Keshavarz et al. (2022)	Q	
	1.7×10^{-1}		Duchowicz et al. (2020)	Q	184
	1.7×10^{-3}		Wang et al. (2017)	Q	80, 238
	1.7×10^{-2}		Wang et al. (2017)	Q	80, 239
	4.9×10^{-3}		Wang et al. (2017)	Q	80, 240
	1.9×10^{-3}		Gharagheizi et al. (2012)	Q	
	8.7×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	3.3×10^{-3}		Modarresi et al. (2007)	Q	67
	7.2×10^{-3}		Hertel et al. (2007)	Q	467
		3100	Kühne et al. (2005)	Q	
	6.2×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	4.8×10^{-3}		English and Carroll (2001)	Q	230, 231
	5.0×10^{-3}		Marin et al. (1999)	Q	
	3.1×10^{-3}		Katritzky et al. (1998)	Q	
	6.5×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	7.9×10^{-4}		Russell et al. (1992)	Q	279
	6.4×10^{-3}		Suzuki et al. (1992)	Q	232
	6.1×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		3500	Kühne et al. (2005)	?	
	5.5×10^{-3}		Yaws et al. (2003)	?	21
	4.9×10^{-3}		Yaws (1999)	?	21
	1.7×10^{-3}		Abraham et al. (1990)	?	
ethyl methyl sulfide	4.2×10^{-3}		Burkholder et al. (2019)	L	
$C_2H_5SCH_3$	4.2×10^{-3}		Burkholder et al. (2015)	L	
[624-89-5]	4.2×10^{-3}		Schuhfried et al. (2011)	M	
WXEHBUMAEPOYKP-UHFFFAOYSA-N	5.4×10^{-3}		Yaws et al. (2003)	V	802
	5.1×10^{-3}		Bagno et al. (1991)	T	473
	5.4×10^{-3}		Yaws (2003)	X	237
	2.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	5.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
	8.6×10^{-3}		Hilal et al. (2008)	Q	
	5.1×10^{-3}		Yao et al. (2002)	Q	229
	3.5×10^{-3}		English and Carroll (2001)	Q	230, 231
	4.4×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	5.0×10^{-3}		Yaws (1999)	?	21

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
diethyl sulfide	3.5×10^{-3}		Burkholder et al. (2019)	L	
$C_2H_5SC_2H_5$	3.5×10^{-3}		Burkholder et al. (2015)	L	
[352-93-2]	4.7×10^{-3}	4800	Plyasunova et al. (2004)	L	
LJSQFQKUNVCTIA-UHFFFAOYSA-N	3.5×10^{-3}		Schuhfried et al. (2011)	M	
	5.4×10^{-3}	4900	Przyjazny et al. (1983)	M	
	5.1×10^{-1}		Mackay et al. (2006d)	V	
	4.5×10^{-3}		Hine and Mookerjee (1975)	V	
	4.5×10^{-3}		Yaws (2003)	X	237
	4.3×10^{-3}		Keshavarz et al. (2022)	Q	
	2.0×10^{-2}		Duchowicz et al. (2020)	Q	184
	3.4×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.7×10^{-3}		Gharagheizi et al. (2010)	Q	246
	6.0×10^{-3}		Hilal et al. (2008)	Q	
	3.6×10^{-3}		Modarresi et al. (2007)	Q	67
	4.8×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	4.0×10^{-3}		Yao et al. (2002)	Q	229
	4.6×10^{-3}		English and Carroll (2001)	Q	230, 274
	2.6×10^{-3}		Katritzky et al. (1998)	Q	
	2.9×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	1.5×10^{-3}		Russell et al. (1992)	Q	279
	3.9×10^{-3}		Suzuki et al. (1992)	Q	232
	5.9×10^{-3}		Duchowicz et al. (2020)	?	185, 21
	1.1×10^{-2}		Yaws et al. (2003)	?	21
	4.4×10^{-3}		Yaws (1999)	?	21, 12
	5.7×10^{-3}		Yaws and Yang (1992)	?	21, 12
	4.7×10^{-3}		Abraham et al. (1990)	?	
methyl isopropyl sulfide	4.5×10^{-3}		Yaws et al. (2003)	V	802
$C_4H_{10}S$	4.5×10^{-3}		Yaws (2003)	X	237
[1551-21-9]	2.7×10^{-3}		Gharagheizi et al. (2012)	Q	
ROSSIHMZZJOVOU-UHFFFAOYSA-N	4.6×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.6×10^{-3}		Yao et al. (2002)	Q	229
	3.5×10^{-3}		Yaws (1999)	?	21
methyl propyl sulfide	4.3×10^{-3}		Plyasunova et al. (2004)	L	
$C_4H_{10}S$	4.3×10^{-3}		Mazza (1980)	M	
[3877-15-4]	4.5×10^{-3}		Yaws et al. (2003)	V	802
ZOASGOXWEHUTKZ-UHFFFAOYSA-N	4.5×10^{-3}		Yaws (2003)	X	237
	1.1×10^{-3}		Gharagheizi et al. (2012)	Q	
	4.2×10^{-3}		Gharagheizi et al. (2010)	Q	246
	4.1×10^{-3}		Yao et al. (2002)	Q	229
	3.1×10^{-3}		Yaws (1999)	?	21
tetrahydrothiophene	2.2×10^{-3}		Yaws et al. (2003)	V	802
C_4H_8S	1.7×10^{-2}		Gharagheizi et al. (2012)	Q	
[110-01-0]					
RAOIDOHSFRTOEL-UHFFFAOYSA-N					

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-methyl-3-thiapentane	3.7×10^{-3}		Yaws et al. (2003)	V	802
$C_5H_{12}S$	3.7×10^{-3}		Yaws (2003)	X	237
[5145-99-3]	3.7×10^{-3}		Gharagheizi et al. (2012)	Q	
NZUQQADVSXWVNW-UHFFFAOYSA-N	3.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
3,3-dimethyl-2-thiabutane	3.6×10^{-3}		Yaws et al. (2003)	V	802
$C_5H_{12}S$	3.6×10^{-3}		Yaws (2003)	X	237
[6163-64-0]	2.9×10^{-3}		Gharagheizi et al. (2012)	Q	
CJFVCTVYZFTORU-UHFFFAOYSA-N	3.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
3-methyl-2-thiapentane	3.6×10^{-3}		Yaws et al. (2003)	V	802
$C_5H_{12}S$	3.5×10^{-3}		Yaws (2003)	X	237
[10359-64-5]	1.3×10^{-3}		Gharagheizi et al. (2012)	Q	
IJRCRFQMYAJPPO-UHFFFAOYSA-N	3.6×10^{-3}		Gharagheizi et al. (2010)	Q	246
4-methyl-2-thiapentane	3.5×10^{-3}		Yaws et al. (2003)	V	802
$C_5H_{12}S$	3.5×10^{-3}		Yaws (2003)	X	237
[5008-69-5]	4.3×10^{-4}		Gharagheizi et al. (2012)	Q	
UYVGFIKOUAFDOZ-UHFFFAOYSA-N	4.2×10^{-3}		Gharagheizi et al. (2010)	Q	246
ethyl propyl sulfide	3.5×10^{-3}		Yaws et al. (2003)	V	802
$C_5H_{12}S$	3.5×10^{-3}		Yaws (2003)	X	237
[4110-50-3]	1.6×10^{-3}		Gharagheizi et al. (2012)	Q	
ZDDDFDQTSXYYSE-UHFFFAOYSA-N	2.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.1×10^{-3}		Yao et al. (2002)	Q	229
	1.9×10^{-3}		Yaws (1999)	?	21
methyl butyl sulfide	3.4×10^{-3}		Yaws et al. (2003)	V	802
$C_5H_{12}S$	3.4×10^{-3}		Yaws (2003)	X	237
[628-29-5]	8.6×10^{-4}		Gharagheizi et al. (2012)	Q	
WCXXISMIJBRDQK-UHFFFAOYSA-N	3.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
	2.2×10^{-3}		Yao et al. (2002)	Q	229
	1.8×10^{-3}		Yaws (1999)	?	21
dipropyl sulfide	3.3×10^{-3}	5700	Plyasunova et al. (2004)	L	
$C_3H_7SC_3H_7$	3.3×10^{-3}	4500	Przyjazny et al. (1983)	M	
[111-47-7]	2.7×10^{-3}		Yaws et al. (2003)	V	802
ZERULLAPCVRMCO-UHFFFAOYSA-N	2.7×10^{-3}		Yaws (2003)	X	237
	7.8×10^{-3}		Keshavarz et al. (2022)	Q	
	2.0×10^{-2}		Duchowicz et al. (2020)	Q	299
	8.9×10^{-4}		Gharagheizi et al. (2012)	Q	
	2.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
	3.4×10^{-3}		Hilal et al. (2008)	Q	
		4500	Kühne et al. (2005)	Q	
	4.8×10^{-3}		Yaffe et al. (2003)	Q	248, 272
	1.9×10^{-3}		Yao et al. (2002)	Q	229
	3.1×10^{-3}		English and Carroll (2001)	Q	230, 231
	1.8×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	3.0×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4500	Kühne et al. (2005)	?	

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.2×10^{-3}		Yaws (1999)	?	21
	3.5×10^{-3}		Abraham et al. (1990)	?	
di-(2-propyl)-sulfide	2.8×10^{-3}	4900	Brockbank (2013)	L	1
$(C_3H_7)_2S$	3.0×10^{-3}		Plyasunova et al. (2004)	L	
(diisopropyl sulfide)	3.0×10^{-3}	5000	Przyjazny et al. (1983)	M	
[625-80-9]	2.9×10^{-3}		Yaws et al. (2003)	V	802
XYWDPYKBIRQXQS-UHFFFAOYSA-N	2.9×10^{-3}		Yaws (2003)	X	237
	7.8×10^{-3}		Keshavarz et al. (2022)	Q	
	3.1×10^{-3}		Duchowicz et al. (2020)	Q	
	4.8×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.2×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.6×10^{-3}		Hilal et al. (2008)	Q	
		4500	Kühne et al. (2005)	Q	
	3.1×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	1.1×10^{-3}		Yao et al. (2002)	Q	229
	1.2×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	3.0×10^{-3}		Duchowicz et al. (2020)	?	185, 21
		4200	Kühne et al. (2005)	?	
	1.5×10^{-3}		Yaws (1999)	?	21
	3.1×10^{-3}		Abraham et al. (1990)	?	
2,2-dimethyl-3-thiapentane	2.8×10^{-3}		Yaws et al. (2003)	V	802
$C_6H_{14}S$	2.8×10^{-3}		Yaws (2003)	X	237
[14290-92-7]	4.9×10^{-3}		Gharagheizi et al. (2012)	Q	
GZJUDUMQICJSFJ-UHFFFAOYSA-N	2.8×10^{-3}		Gharagheizi et al. (2010)	Q	246
2-methyl-3-thiahexane	2.8×10^{-3}		Yaws et al. (2003)	V	802
$C_6H_{14}S$	2.7×10^{-3}		Yaws (2003)	X	237
[5008-73-1]	2.1×10^{-3}		Gharagheizi et al. (2012)	Q	
BDFDQOJJDDORSR-UHFFFAOYSA-N	2.6×10^{-3}		Gharagheizi et al. (2010)	Q	246
3,3-dimethyl-2-thiapentane	2.7×10^{-3}		Yaws et al. (2003)	V	802
$C_6H_{14}S$	2.7×10^{-3}		Yaws (2003)	X	237
[13286-92-5]	1.9×10^{-3}		Gharagheizi et al. (2012)	Q	
SJOHDSPLOVBXOF-UHFFFAOYSA-N	3.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
3,4-dimethyl-2-thiapentane	2.9×10^{-3}		Yaws et al. (2003)	V	802
$C_6H_{14}S$	2.9×10^{-3}		Yaws (2003)	X	237
[53897-51-1]	6.1×10^{-4}		Gharagheizi et al. (2012)	Q	
AUNQXXJGFDKEMS-UHFFFAOYSA-N	3.2×10^{-3}		Gharagheizi et al. (2010)	Q	246
3-ethyl-2-thiapentane	3.0×10^{-3}		Yaws et al. (2003)	V	802
$C_6H_{14}S$	3.0×10^{-3}		Yaws (2003)	X	237
[57093-84-2]	6.6×10^{-4}		Gharagheizi et al. (2012)	Q	
ZQOHJVSSVAWXQZ-UHFFFAOYSA-N	2.8×10^{-3}		Gharagheizi et al. (2010)	Q	246

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

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3-methyl-2-thiahexane	2.8×10^{-3}		Yaws et al. (2003)	V	802
$C_6H_{14}S$	2.7×10^{-3}		Yaws (2003)	X	237
[13286-91-4]	1.2×10^{-3}		Gharagheizi et al. (2012)	Q	
WGBHWWSSUGCSCP-UHFFFAOYSA-N	2.6×10^{-3}		Gharagheizi et al. (2010)	Q	246
4,4-dimethyl-2-thiapentane	2.7×10^{-3}		Yaws et al. (2003)	V	802
$C_6H_{14}S$	2.7×10^{-3}		Yaws (2003)	X	237
[6079-57-8]	3.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
YUFAJXXIXSYTMS-UHFFFAOYSA-N					
4-methyl-2-thiahexane	2.7×10^{-3}		Yaws et al. (2003)	V	802
$C_6H_{14}S$	2.7×10^{-3}		Yaws (2003)	X	237
[15013-37-3]	3.9×10^{-4}		Gharagheizi et al. (2012)	Q	
XMOUDDXUCXXDTJ-UHFFFAOYSA-N	2.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
4-methyl-3-thiahexane	2.7×10^{-3}		Yaws et al. (2003)	V	802
$C_6H_{14}S$	2.7×10^{-3}		Yaws (2003)	X	237
[5008-72-0]	2.2×10^{-3}		Gharagheizi et al. (2012)	Q	
JFNGZXUPUVUYST-UHFFFAOYSA-N	2.6×10^{-3}		Gharagheizi et al. (2010)	Q	246
5-methyl-2-thiahexane	2.8×10^{-3}		Yaws et al. (2003)	V	802
$C_6H_{14}S$	2.8×10^{-3}		Yaws (2003)	X	237
[13286-90-3]	5.4×10^{-4}		Gharagheizi et al. (2012)	Q	
ABIKQXWLJOURPN-UHFFFAOYSA-N	2.7×10^{-3}		Gharagheizi et al. (2010)	Q	246
5-methyl-3-thiahexane	2.7×10^{-3}		Yaws et al. (2003)	V	802
$C_6H_{14}S$	2.7×10^{-3}		Yaws (2003)	X	237
[1613-45-2]	7.1×10^{-4}		Gharagheizi et al. (2012)	Q	
OIRKGXWQBSPXLQ-UHFFFAOYSA-N	2.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
ethyl butyl sulfide	2.6×10^{-3}		Yaws et al. (2003)	V	802
$C_6H_{14}S$	2.6×10^{-3}		Yaws (2003)	X	237
[638-46-0]	1.2×10^{-3}		Gharagheizi et al. (2012)	Q	
XJIRSLHMKBUGMR-UHFFFAOYSA-N	2.2×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.9×10^{-3}		Yao et al. (2002)	Q	229
	1.2×10^{-3}		Yaws (1999)	?	21
methyl pentyl sulfide	3.8×10^{-3}		Yaws et al. (2003)	V	802
$C_6H_{14}S$	3.8×10^{-3}		Yaws (2003)	X	237
[1741-83-9]	2.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
FOJGPFUFFHWGFQ-UHFFFAOYSA-N					
ethyl pentyl sulfide	1.0×10^{-3}		Yaws et al. (2003)	V	802
$C_7H_{16}S$	9.6×10^{-4}		Yaws (2003)	X	237
[26158-99-6]	1.1×10^{-3}		Gharagheizi et al. (2012)	Q	
SOGIWVXLDPPMMF-UHFFFAOYSA-N	1.8×10^{-3}		Gharagheizi et al. (2010)	Q	246
methyl hexyl sulfide	1.0×10^{-3}		Yaws et al. (2003)	V	802
$C_7H_{16}S$	9.6×10^{-4}		Yaws (2003)	X	237
[20291-60-5]	5.2×10^{-4}		Gharagheizi et al. (2012)	Q	
LZRXQHHKXDXOIC-UHFFFAOYSA-N	1.8×10^{-3}		Gharagheizi et al. (2010)	Q	246

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

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propyl butyl sulfide	1.0×10^{-3}		Yaws et al. (2003)	V	802
$C_7H_{16}S$	9.6×10^{-4}		Yaws (2003)	X	237
[1613-46-3]	7.6×10^{-4}		Gharagheizi et al. (2012)	Q	
ZBRWJPVULTZZCE-UHFFFAOYSA-N	1.8×10^{-3}		Gharagheizi et al. (2010)	Q	246
dibutyl sulfide	1.3×10^{-3}		Yaws et al. (2003)	V	802
$C_8H_{18}S$	1.3×10^{-3}		Yaws (2003)	X	237
[544-40-1]	3.9×10^{-4}		Gharagheizi et al. (2012)	Q	
HTIRHQRTDBPHNZ-UHFFFAOYSA-N	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
ethyl hexyl sulfide	6.2×10^{-4}		Yaws et al. (2003)	V	802
$C_8H_{18}S$	6.2×10^{-4}		Yaws (2003)	X	237
[7309-44-6]	8.7×10^{-4}		Gharagheizi et al. (2012)	Q	
MGVUJBCOCITTRS-UHFFFAOYSA-N	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
methyl heptyl sulfide	6.2×10^{-4}		Yaws et al. (2003)	V	802
$C_8H_{18}S$	6.2×10^{-4}		Yaws (2003)	X	237
[20291-61-6]	4.0×10^{-4}		Gharagheizi et al. (2012)	Q	
FJDWJOQOEZRIDJ-UHFFFAOYSA-N	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
propyl pentyl sulfide	6.2×10^{-4}		Yaws et al. (2003)	V	802
$C_8H_{18}S$	6.2×10^{-4}		Yaws (2003)	X	237
[42841-80-5]	5.9×10^{-4}		Gharagheizi et al. (2012)	Q	
MJRCCWJSYFOGBX-UHFFFAOYSA-N	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
butyl pentyl sulfide	9.8×10^{-4}		Yaws et al. (2003)	V	802
$C_9H_{20}S$	9.7×10^{-4}		Yaws (2003)	X	237
[24768-42-1]	7.0×10^{-4}		Gharagheizi et al. (2012)	Q	
RNEUXBDXTNIASG-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
ethyl heptyl sulfide	9.8×10^{-4}		Yaws et al. (2003)	V	802
$C_9H_{20}S$	9.7×10^{-4}		Yaws (2003)	X	237
[24768-44-3]	1.0×10^{-3}		Gharagheizi et al. (2012)	Q	
PYPULUCCVXMPFP-UHFFFAOYSA-N	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
methyl octyl sulfide	9.8×10^{-4}		Yaws et al. (2003)	V	802
$C_9H_{20}S$	9.7×10^{-4}		Yaws (2003)	X	237
[3698-95-1]	4.7×10^{-4}		Gharagheizi et al. (2012)	Q	
AHCJTMBRROLNHV-UHFFFAOYSA-N	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
propyl hexyl sulfide	9.8×10^{-4}		Yaws et al. (2003)	V	802
$C_9H_{20}S$	9.7×10^{-4}		Yaws (2003)	X	237
[24768-43-2]	7.0×10^{-4}		Gharagheizi et al. (2012)	Q	
ABZLKKGJOVPBBL-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
butyl hexyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	802
$C_{10}H_{22}S$	1.6×10^{-3}		Yaws (2003)	X	237
[16967-04-7]	8.1×10^{-4}		Gharagheizi et al. (2012)	Q	
YZUHMAFUXBPUKH-UHFFFAOYSA-N	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	246

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

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dipentyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	802
$C_{10}H_{22}S$	1.6×10^{-3}		Yaws (2003)	X	237
[872-10-6]	8.1×10^{-4}		Gharagheizi et al. (2012)	Q	
JOZDADPMWLVEJK-UHFFFAOYSA-N	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
ethyl octyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	802
$C_{10}H_{22}S$	1.6×10^{-3}		Yaws (2003)	X	237
[3698-94-0]	1.2×10^{-3}		Gharagheizi et al. (2012)	Q	
WAITXWGCJQLPGH-UHFFFAOYSA-N	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
methyl nonyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	802
$C_{10}H_{22}S$	1.6×10^{-3}		Yaws (2003)	X	237
[59973-07-8]	3.6×10^{-4}		Gharagheizi et al. (2012)	Q	
FCRSULZJMFDBIK-UHFFFAOYSA-N	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
propyl heptyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	802
$C_{10}H_{22}S$	1.6×10^{-3}		Yaws (2003)	X	237
[24768-46-5]	8.1×10^{-4}		Gharagheizi et al. (2012)	Q	
PCPVCHFKVPNTBH-UHFFFAOYSA-N	1.3×10^{-3}		Gharagheizi et al. (2010)	Q	246
butyl heptyl sulfide	1.7×10^{-3}		Yaws et al. (2003)	V	802
$C_{11}H_{24}S$	1.7×10^{-3}		Yaws (2003)	X	237
[40813-84-1]	9.1×10^{-4}		Gharagheizi et al. (2012)	Q	
HYUPOCGXBZUYFY-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
ethyl nonyl sulfide	1.7×10^{-3}		Yaws et al. (2003)	V	802
$C_{11}H_{24}S$	1.7×10^{-3}		Yaws (2003)	X	237
[59973-08-9]	8.8×10^{-4}		Gharagheizi et al. (2012)	Q	
LUAABLIRQSWMGZ-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
methyl decyl sulfide	1.7×10^{-3}		Yaws et al. (2003)	V	802
$C_{11}H_{24}S$	1.7×10^{-3}		Yaws (2003)	X	237
[22438-39-7]	4.1×10^{-4}		Gharagheizi et al. (2012)	Q	
HKGUUZAACYBIID-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
propyl octyl sulfide	1.7×10^{-3}		Yaws et al. (2003)	V	802
$C_{11}H_{24}S$	1.7×10^{-3}		Yaws (2003)	X	237
[3698-93-9]	9.1×10^{-4}		Gharagheizi et al. (2012)	Q	
GPJXDRJGQAKGLH-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
butyl octyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	802
$C_{12}H_{26}S$	1.5×10^{-3}		Yaws (2003)	X	237
[16900-07-5]	1.0×10^{-3}		Gharagheizi et al. (2012)	Q	
UNIAPWPIAGJFDG-UHFFFAOYSA-N	1.8×10^{-3}		Gharagheizi et al. (2010)	Q	246
dihexyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	802
$C_{12}H_{26}S$	1.5×10^{-3}		Yaws (2003)	X	237
[6294-31-1]	1.0×10^{-3}		Gharagheizi et al. (2012)	Q	
LHNRHYOMDUJLLM-UHFFFAOYSA-N	1.8×10^{-3}		Gharagheizi et al. (2010)	Q	246

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ethyl decyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	802
$C_{12}H_{26}S$	1.5×10^{-3}		Yaws (2003)	X	237
[19313-61-2]	9.7×10^{-4}		Gharagheizi et al. (2012)	Q	
VSSRSPLEFYQIEK-UHFFFAOYSA-N	1.8×10^{-3}		Gharagheizi et al. (2010)	Q	246
methyl undecyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	802
$C_{12}H_{26}S$	1.5×10^{-3}		Yaws (2003)	X	237
[7289-44-3]	4.5×10^{-4}		Gharagheizi et al. (2012)	Q	
HDOADYQJIBYVGE-UHFFFAOYSA-N	1.7×10^{-3}		Gharagheizi et al. (2010)	Q	246
propyl nonyl sulfide	1.6×10^{-3}		Yaws et al. (2003)	V	802
$C_{12}H_{26}S$	1.5×10^{-3}		Yaws (2003)	X	237
[62103-66-6]	6.6×10^{-4}		Gharagheizi et al. (2012)	Q	
AQAOPNMAEGBYHI-UHFFFAOYSA-N	1.8×10^{-3}		Gharagheizi et al. (2010)	Q	246
butyl nonyl sulfide	1.8×10^{-3}		Yaws et al. (2003)	V	802
$C_{13}H_{28}S$	1.8×10^{-3}		Yaws (2003)	X	237
[66577-32-0]	7.1×10^{-4}		Gharagheizi et al. (2012)	Q	
FWRIVMHSSSZAFD-UHFFFAOYSA-N	2.6×10^{-3}		Gharagheizi et al. (2010)	Q	246
ethyl undecyl sulfide	1.8×10^{-3}		Yaws et al. (2003)	V	802
$C_{13}H_{28}S$	1.8×10^{-3}		Yaws (2003)	X	237
[66577-30-8]	1.0×10^{-3}		Gharagheizi et al. (2012)	Q	
OSWITQLVZPPUIR-UHFFFAOYSA-N	2.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
methyl dodecyl sulfide	1.8×10^{-3}		Yaws et al. (2003)	V	802
$C_{13}H_{28}S$	1.8×10^{-3}		Yaws (2003)	X	237
[3698-89-3]	4.8×10^{-4}		Gharagheizi et al. (2012)	Q	
KJWHJDGMOQJLGF-UHFFFAOYSA-N	2.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
propyl decyl sulfide	1.8×10^{-3}		Yaws et al. (2003)	V	802
$C_{13}H_{28}S$	1.8×10^{-3}		Yaws (2003)	X	237
[66577-31-9]	7.1×10^{-4}		Gharagheizi et al. (2012)	Q	
HPJCKXDELORROO-UHFFFAOYSA-N	2.6×10^{-3}		Gharagheizi et al. (2010)	Q	246
butyl decyl sulfide	2.6×10^{-3}		Yaws et al. (2003)	V	802
$C_{14}H_{30}S$	2.6×10^{-3}		Yaws (2003)	X	237
[19313-57-6]	7.5×10^{-4}		Gharagheizi et al. (2012)	Q	
CLBLVLKZMJDLOT-UHFFFAOYSA-N	4.7×10^{-3}		Gharagheizi et al. (2010)	Q	246
diheptyl sulfide	2.6×10^{-3}		Yaws et al. (2003)	V	802
$C_{14}H_{30}S$	2.6×10^{-3}		Yaws (2003)	X	237
[629-65-2]	1.2×10^{-3}		Gharagheizi et al. (2012)	Q	
LEMIDOZYVQXGLI-UHFFFAOYSA-N	4.7×10^{-3}		Gharagheizi et al. (2010)	Q	246
ethyl dodecyl sulfide	2.6×10^{-3}		Yaws et al. (2003)	V	802
$C_{14}H_{30}S$	2.6×10^{-3}		Yaws (2003)	X	237
[2851-83-4]	1.1×10^{-3}		Gharagheizi et al. (2012)	Q	
QECBTJWQRXCSCU-UHFFFAOYSA-N	4.4×10^{-3}		Gharagheizi et al. (2010)	Q	246

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methyl tridecyl sulfide	2.6×10^{-3}		Yaws et al. (2003)	V	802
$C_{14}H_{30}S$	2.6×10^{-3}		Yaws (2003)	X	237
[62155-09-3]	5.1×10^{-4}		Gharagheizi et al. (2012)	Q	
QVXOOYOFFITGCV-UHFFFAOYSA-N	4.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
propyl undecyl sulfide	2.6×10^{-3}		Yaws et al. (2003)	V	802
$C_{14}H_{30}S$	2.6×10^{-3}		Yaws (2003)	X	237
[66826-84-4]	7.5×10^{-4}		Gharagheizi et al. (2012)	Q	
ITNOZFAANYXVSG-UHFFFAOYSA-N	4.7×10^{-3}		Gharagheizi et al. (2010)	Q	246
dimethyl disulfide	5.8×10^{-3}		Burkholder et al. (2019)	L	
CH_3SSCH_3	5.8×10^{-3}		Burkholder et al. (2015)	L	
[624-92-0]	8.3×10^{-3}	3700	Brockbank (2013)	L	1
WQOXQRCZOLPYPM-UHFFFAOYSA-N	7.4×10^{-3}	4200	Plyasunova et al. (2004)	L	
	6.7×10^{-3}	5200	Bruneel et al. (2016)	M	
	5.8×10^{-3}		Schuhfried et al. (2011)	M	
	6.5×10^{-3}	3200	Falabella (2007)	M	11, 338
	9.1×10^{-3}	4100	Iliuta and Larachi (2005b)	M	
	7.8×10^{-3}		Souchon et al. (2004)	M	
	5.9×10^{-3}		Pollien et al. (2003)	M	
	3.6×10^{-3}		McIntosh and Heffron (2000)	M	14
	9.4×10^{-3}	4300	Przyjazny et al. (1983)	M	
	8.6×10^{-3}		Mazza (1980)	M	
	8.3×10^{-3}		Vitenberg et al. (1975)	M	12
	1.7×10^{-2}		Mackay et al. (2006d)	V	
	1.7×10^{-2}		Mackay et al. (1995)	V	
	9.0×10^{-3}		Vitenberg et al. (1975)	R	12
	3.0×10^{-2}		Hilal et al. (2008)	Q	
	8.7×10^{-2}		Modarresi et al. (2007)	Q	67
		1700	Kühne et al. (2005)	Q	
	4.6×10^{-3}		Nirmalakhandan et al. (1997)	Q	
		1600	Kühne et al. (2005)	?	
	9.0×10^{-3}		Abraham et al. (1990)	?	
diethyl disulfide	3.7×10^{-3}		Burkholder et al. (2019)	L	
$C_2H_5SSC_2H_5$	3.7×10^{-3}		Burkholder et al. (2015)	L	
[110-81-6]	4.0×10^{-3}	4900	Plyasunova et al. (2004)	L	
CETBSQOFQKLHHZ-UHFFFAOYSA-N	3.7×10^{-3}		Schuhfried et al. (2011)	M	
	6.3×10^{-3}	4300	Przyjazny et al. (1983)	M	
	4.7×10^{-3}		Vitenberg et al. (1975)	M	12
	1.2×10^{-2}		Hilal et al. (2008)	Q	
	3.7×10^{-2}		Modarresi et al. (2007)	Q	67
	2.3×10^{-3}		Nirmalakhandan et al. (1997)	Q	
	6.4×10^{-3}		Abraham et al. (1990)	?	
dipropyl disulfide	2.2×10^{-3}	5400	Plyasunova et al. (2004)	L	
$C_3H_7SSC_3H_7$	2.4×10^{-3}		Schuhfried et al. (2011)	M	
[629-19-6]	1.8×10^{-2}		Mazza (1980)	M	
ALVPFGSHPUPROW-UHFFFAOYSA-N					

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
carbon disulfide	6.1×10^{-4}	4300	Burkholder et al. (2019)	L	
CS_2	6.1×10^{-4}	4300	Burkholder et al. (2015)	L	
[75-15-0]	6.1×10^{-4}	3900	Warneck and Williams (2012)	L	
QGJOPFRUJISHPQ-UHFFFAOYSA-N	6.1×10^{-4}	4300	Sander et al. (2011)	L	
	6.1×10^{-4}	4300	Sander et al. (2006)	L	
	5.5×10^{-4}	3700	Plyasunova et al. (2004)	L	
	5.7×10^{-4}	3800	Hiatt (2013)	M	
	5.4×10^{-4}	2800	De Bruyn et al. (1995b)	M	
	6.2×10^{-4}	3800	Elliott (1989)	M	
	5.4×10^{-4}	4300	Rex (1906)	M	
	5.7×10^{-4}		Mackay et al. (2006d)	V	
	5.7×10^{-4}		Mackay et al. (1995)	V	
	8.0×10^{-4}		Hwang et al. (1992)	V	
	4.5×10^{-4}	4100	Winkler (1906)	V	
	5.1×10^{-4}		Yaws (2003)	X	237
	7.5×10^{-4}	1200	Goldstein (1982)	X	298
	5.0×10^{-4}		Hayer et al. (2022)	Q	20
	1.3×10^{-2}		Gharagheizi et al. (2012)	Q	
	5.1×10^{-4}		Gharagheizi et al. (2010)	Q	246
	9.4×10^{-5}		Yaws (1999)	?	21
	3.2×10^{-4}		Abraham and Weathersby (1994)	?	21
	5.1×10^{-4}		Yaws and Yang (1992)	?	21
			Schäfer and Lax (1962)	?	808
			Booth and Jolley (1943)	?	809
			Booth and Jolley (1943)	?	810
2,3,4-trithiapentane	1.2×10^{-2}		Plyasunova et al. (2004)	L	
$C_2H_6S_3$	1.4×10^{-2}		Souchon et al. (2004)	M	
(dimethyl trisulfide)	2.1×10^{-2}		Roberts and Pollien (1997)	M	
[3658-80-8]					
YWHLKYXPLRWGSE-UHFFFAOYSA-N					
dicyclohexyldisulfide	2.5×10^{-3}		HSDB (2015)	Q	99
$C_{12}H_{22}S_2$					
[2550-40-5]					
ODHAQPXNQDBHSH-UHFFFAOYSA-N					
allyl mercaptan	1.2×10^{-2}		Hilal et al. (2008)	Q	
C_3H_6S					
[870-23-5]					
ULIKDJVNUXNQHS-UHFFFAOYSA-N					
3,3'-thiobis-1-propene	4.1×10^{-3}		Lindinger et al. (1998)	M	811
$(C_3H_5)_2S$	7.1×10^{-3}		Mazza (1980)	M	
(diallyl sulfide)	7.6×10^{-3}		HSDB (2015)	Q	99
[592-88-1]	9.9×10^{-3}		Hilal et al. (2008)	Q	
UBJVUCKUDDKUJF-UHFFFAOYSA-N					

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
allyl methyl sulfide	4.2×10^{-3}		Burkholder et al. (2019)	L	
$CH_2CHCH_2SCH_3$	4.2×10^{-3}		Burkholder et al. (2015)	L	
(2-propenyl methyl sulfide)	4.2×10^{-3}		Schuhfried et al. (2011)	M	
[10152-76-8]	5.0×10^{-3}		Mazza (1980)	M	
NVLPQIPTCCLBEU-UHFFFAOYSA-N					
thiophene	4.1×10^{-3}	4300	Haimi et al. (2006)	M	812
C_4H_4S	4.4×10^{-3}	4000	Przyjazny et al. (1983)	M	
[110-02-1]	3.4×10^{-3}		HSDB (2015)	V	
YTPLMLYBLZKORZ-UHFFFAOYSA-N			Mackay et al. (2006d)	V	558
	4.5×10^{-3}		Mackay et al. (1995)	V	
	3.4×10^{-3}		Yaws (2003)	X	237
	8.2×10^{-3}		Gharagheizi et al. (2012)	Q	
	3.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.4×10^{-3}		Hilal et al. (2008)	Q	
	9.8×10^{-3}		Modarresi et al. (2007)	Q	67
		2800	Kühne et al. (2005)	Q	
	3.4×10^{-3}		Yaffe et al. (2003)	Q	248, 249
	9.3×10^{-3}		Yao et al. (2002)	Q	229, 267
	8.8×10^{-3}		English and Carroll (2001)	Q	230, 231
	6.9×10^{-4}		Katritzky et al. (1998)	Q	
	4.5×10^{-3}		Mackay et al. (2006d)	?	
		1900	Kühne et al. (2005)	?	
	3.4×10^{-3}		Yaws et al. (2003)	?	21
	3.4×10^{-3}		Yaws (1999)	?	21
	3.4×10^{-3}		Yaws and Yang (1992)	?	21
	4.4×10^{-3}		Abraham et al. (1990)	?	
2-methylthiophene	4.1×10^{-3}	4300	Brockbank (2013)	L	1
$CH_3C_4H_3S$	4.1×10^{-3}	4300	Przyjazny et al. (1983)	M	
[554-14-3]	2.2×10^{-3}		Yaws et al. (2003)	V	802
XQQBUAPQHNYYRS-UHFFFAOYSA-N	1.9×10^{-3}		Yaws (2003)	X	237
	2.9×10^{-2}		Keshavarz et al. (2022)	Q	
	2.7×10^{-2}		Duchowicz et al. (2020)	Q	
	1.1×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.4×10^{-3}		Hilal et al. (2008)	Q	
	8.0×10^{-3}		English and Carroll (2001)	Q	230, 231
	4.1×10^{-3}		Duchowicz et al. (2020)	?	185, 21
	4.1×10^{-3}		Abraham et al. (1990)	?	
3-methylthiophene	1.4×10^{-3}		Duchowicz et al. (2020)	V	186
$CH_3C_4H_3S$	1.4×10^{-3}		Yaws (2003)	X	237
[616-44-4]	2.7×10^{-2}		Duchowicz et al. (2020)	Q	
QENGPZGAWFQWCZ-UHFFFAOYSA-N	4.0×10^{-3}		Gharagheizi et al. (2012)	Q	
	1.9×10^{-3}		Gharagheizi et al. (2010)	Q	246
	1.7×10^{-3}		Hilal et al. (2008)	Q	
	8.2×10^{-3}		Modarresi et al. (2007)	Q	67
	1.4×10^{-3}		Yaffe et al. (2003)	Q	248, 249

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.8×10^{-3}		Katritzky et al. (1998)	Q	
	1.4×10^{-3}		Yaws et al. (2003)	?	21
propyl allyl disulfide $C_6H_{12}S_2$ [2179-59-1] FCSSPCOFDUKHPV-UHFFFAOYSA-N	3.5×10^{-3}		HSDB (2015)	Q	99
4,5-dithia-1,7-octadiene $C_6H_{10}S_2$ (diallyl disulfide) [2179-57-9] PFRGXCVKLLPLIP-UHFFFAOYSA-N	7.5×10^{-3}		Mazza (1980)	M	
2,3-dimethylthiophene	1.5×10^{-3}		Yaws et al. (2003)	V	802
C_6H_8S	1.3×10^{-3}		Yaws (2003)	X	237
[632-16-6]	4.8×10^{-3}		Gharagheizi et al. (2012)	Q	
BZYUMXXOAYSFOW-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
2,4-dimethylthiophene	1.5×10^{-3}		Yaws et al. (2003)	V	802
C_6H_8S	1.3×10^{-3}		Yaws (2003)	X	237
[638-00-6]	4.7×10^{-3}		Gharagheizi et al. (2012)	Q	
CPULIKNSOUFMPL-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
2,5-dimethylthiophene	3.7×10^{-3}		Mazza (1980)	M	
C_6H_8S	1.6×10^{-3}		Yaws et al. (2003)	V	802
[638-02-8]	1.4×10^{-3}		Yaws (2003)	X	237
GWQOOADXMVQEFT-UHFFFAOYSA-N	1.3×10^{-2}		Gharagheizi et al. (2012)	Q	
	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
2-ethylthiophene	1.4×10^{-3}		Yaws (2003)	X	237
C_6H_8S	3.9×10^{-3}		Gharagheizi et al. (2012)	Q	
[872-55-9]	1.5×10^{-3}		Gharagheizi et al. (2010)	Q	246
JCCCMAAJYSNBPR-UHFFFAOYSA-N	1.9×10^{-3}		Yaws et al. (2003)	?	21
3,4-dimethylthiophene	1.5×10^{-3}		Yaws et al. (2003)	V	802
C_6H_8S	1.2×10^{-3}		Yaws (2003)	X	237
[632-15-5]	1.7×10^{-3}		Gharagheizi et al. (2012)	Q	
GPSFYJDZKSRMKZ-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
3-ethylthiophene	1.6×10^{-3}		Yaws et al. (2003)	V	802
C_6H_8S	1.4×10^{-3}		Yaws (2003)	X	237
[1795-01-3]	1.9×10^{-3}		Gharagheizi et al. (2012)	Q	
SLDBAXYJAIRQMX-UHFFFAOYSA-N	1.4×10^{-3}		Gharagheizi et al. (2010)	Q	246
2,3,4-trimethylthiophene	1.3×10^{-3}		Yaws et al. (2003)	V	802
$C_7H_{10}S$	1.1×10^{-3}		Yaws (2003)	X	237
[1795-04-6]	2.9×10^{-3}		Gharagheizi et al. (2012)	Q	
MAVVDCDMBKFUES-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	246

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2,3,5-trimethylthiophene	1.1×10^{-3}		Yaws et al. (2003)	V	802
$C_7H_{10}S$	9.3×10^{-4}		Yaws (2003)	X	237
[1795-05-7]	7.2×10^{-3}		Gharagheizi et al. (2012)	Q	
QKZJQIHBRCFDGQ-UHFFFAOYSA-N	9.7×10^{-4}		Gharagheizi et al. (2010)	Q	246
2-isopropylthiophene	1.3×10^{-3}		Yaws et al. (2003)	V	802
$C_7H_{10}S$	1.1×10^{-3}		Yaws (2003)	X	237
[4095-22-1]	1.8×10^{-3}		Gharagheizi et al. (2012)	Q	
LOXBELRNKUFSRD-UHFFFAOYSA-N	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
2-methyl-3-ethylthiophene	1.2×10^{-3}		Yaws et al. (2003)	V	802
$C_7H_{10}S$	1.0×10^{-3}		Yaws (2003)	X	237
[53119-51-0]	2.8×10^{-3}		Gharagheizi et al. (2012)	Q	
RBRAJDCWXUJHIY-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
2-methyl-4-ethylthiophene	1.1×10^{-3}		Yaws et al. (2003)	V	802
$C_7H_{10}S$	9.6×10^{-4}		Yaws (2003)	X	237
[13678-54-1]	3.3×10^{-3}		Gharagheizi et al. (2012)	Q	
KIWVMUQUYOKTKU-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
2-methyl-5-ethylthiophene	1.2×10^{-3}		Yaws et al. (2003)	V	802
$C_7H_{10}S$	9.9×10^{-4}		Yaws (2003)	X	237
[40323-88-4]	6.6×10^{-3}		Gharagheizi et al. (2012)	Q	
VOIVNYVBGCJFRW-UHFFFAOYSA-N	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
2-propylthiophene	1.2×10^{-3}		Yaws et al. (2003)	V	802
$C_7H_{10}S$	1.0×10^{-3}		Yaws (2003)	X	237
[1551-27-5]	3.1×10^{-3}		Gharagheizi et al. (2012)	Q	
BTXIJTYYMLCUHI-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
3-isopropylthiophene	1.1×10^{-3}		Yaws et al. (2003)	V	802
$C_7H_{10}S$	9.7×10^{-4}		Yaws (2003)	X	237
[29488-27-5]	1.4×10^{-3}		Gharagheizi et al. (2012)	Q	
LJPDBPCGTFTUDE-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
3-methyl-2-ethylthiophene	1.2×10^{-3}		Yaws et al. (2003)	V	802
$C_7H_{10}S$	9.8×10^{-4}		Yaws (2003)	X	237
[31805-48-8]	2.1×10^{-3}		Gharagheizi et al. (2012)	Q	
VVSCPYCHXFEKLF-UHFFFAOYSA-N	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
3-methyl-4-ethylthiophene	1.3×10^{-3}		Yaws et al. (2003)	V	802
$C_7H_{10}S$	1.1×10^{-3}		Yaws (2003)	X	237
[66577-03-5]	8.1×10^{-4}		Gharagheizi et al. (2012)	Q	
QMHNYDJBWOPGHE-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
3-methyl-5-ethylthiophene	1.3×10^{-3}		Yaws et al. (2003)	V	802
$C_7H_{10}S$	1.1×10^{-3}		Yaws (2003)	X	237
(2-ethyl-4-methylthiophene)	1.8×10^{-3}		Gharagheizi et al. (2012)	Q	
[66577-04-6]	1.1×10^{-3}		Gharagheizi et al. (2010)	Q	246
NZOYEHPXDWJOCD-UHFFFAOYSA-N					

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

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3-propylthiophene	1.2×10^{-3}		Yaws et al. (2003)	V	802
$C_7H_{10}S$	9.9×10^{-4}		Yaws (2003)	X	237
[1518-75-8]	1.5×10^{-3}		Gharagheizi et al. (2012)	Q	
QZNFRMXKQCIPQY-UHFFFAOYSA-N	1.0×10^{-3}		Gharagheizi et al. (2010)	Q	246
benzenethiol	2.9×10^{-2}		Duchowicz et al. (2020)	V	186
C_6H_5SH	2.9×10^{-2}		HSDB (2015)	V	
(thiophenol)	3.0×10^{-2}		Hine and Mookerjee (1975)	V	
[108-98-5]	3.0×10^{-2}		Hine and Weimar (1965)	V	
RMVRSNDYEFQCLF-UHFFFAOYSA-N	3.0×10^{-2}		Schüürmann (2000)	C	21
	3.2×10^{-1}		Duchowicz et al. (2020)	Q	
	4.1×10^{-2}		Hilal et al. (2008)	Q	
	2.6×10^{-2}		Modarresi et al. (2007)	Q	67
	2.9×10^{-2}		Yaffe et al. (2003)	Q	248, 249
	1.6×10^{-2}		English and Carroll (2001)	Q	230, 231
	1.8×10^{-2}		Katritzky et al. (1998)	Q	
	1.0×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	3.0×10^{-2}		Suzuki et al. (1992)	Q	232
	3.0×10^{-2}		Abraham et al. (1990)	?	
methyl phenyl sulfide	4.0×10^{-2}		Hine and Mookerjee (1975)	V	
$C_6H_5SCH_3$	4.1×10^{-2}		Hine and Weimar (1965)	V	
(thioanisole)	5.8×10^{-2}		Hilal et al. (2008)	Q	
[100-68-5]	4.3×10^{-2}		Yaffe et al. (2003)	Q	248, 249
HNKJADCVZUBCPG-UHFFFAOYSA-N	2.3×10^{-2}		Nirmalakhandan et al. (1997)	Q	
	4.0×10^{-2}		Suzuki et al. (1992)	Q	232
2-methylbenzenethiol C_7H_8S (2-thiocresol) [137-06-4] LXUNZSDDXMPKLP-UHFFFAOYSA-N	2.7×10^{-2}		HSDB (2015)	Q	99
3-methylbenzenethiol C_7H_8S (3-thiocresol) [108-40-7] WRXOZRLZDJAYDR-UHFFFAOYSA-N	2.7×10^{-2}		HSDB (2015)	Q	99
4-methylbenzenethiol C_7H_8S (4-thiocresol) [106-45-6] WLHCBQAPPJAULW-UHFFFAOYSA-N	2.7×10^{-2}		HSDB (2015)	Q	99
benzenemethanethiol C_7H_8S [100-53-8] UENWRTRMUIOCKN-UHFFFAOYSA-N	4.7×10^{-2}		HSDB (2015)	Q	99

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

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benzo[*b*]thiophene			Mackay et al. (2006d)	V	558
C_8H_6S	4.1×10^{-2}		Mackay et al. (1995)	V	
[95-15-8]	3.6×10^{-2}		Smith and Bomberger (1980)	V	24
FCEHBMOGCRZNNI-UHFFFAOYSA-N	3.0×10^{-2}		Yaws (1999)	?	21, 12
dibenzothiophene	2.9×10^{-1}		Duchowicz et al. (2020)	V	186
$C_{12}H_8S$	2.9×10^{-1}		HSDB (2015)	V	
[132-65-0]	2.3×10^{-2}		Mackay et al. (2006d)	V	
IYYZUPMFVPLQIF-UHFFFAOYSA-N	2.3×10^{-2}		Mackay et al. (1995)	V	
	2.3×10^{-2}		Smith and Bomberger (1980)	V	24
	1.2		Duchowicz et al. (2020)	Q	
	3.3×10^{-1}		Parnis et al. (2015)	Q	369
thianthrene	4.0		Abraham et al. (2019)	Q	
$C_{12}H_8S_2$					
[92-85-3]					
GVIJJXMXTUZIOD-UHFFFAOYSA-N					
2-methyldibenzothiophene	2.7×10^{-1}		Parnis et al. (2015)	Q	369
$C_{13}H_{10}S$					
[20928-02-3]					
VHUXLBLPAMBOJS-UHFFFAOYSA-N					
2,3-dimethyldibenzothiophene	3.1×10^{-1}		Parnis et al. (2015)	Q	369
$C_{14}H_{12}S$					
[31317-17-6]					
KEIKATUAMBEIQN-UHFFFAOYSA-N					
2,8-dimethyldibenzothiophene	2.4×10^{-1}		Parnis et al. (2015)	Q	369
$C_{14}H_{12}S$					
[1207-15-4]					
RRYWCJRYULRSJM-UHFFFAOYSA-N					
benzyl sulfide	1.9		HSDB (2015)	Q	99
$C_{14}H_{14}S$					
[538-74-9]					
LUFPJJNWMYZRQE-UHFFFAOYSA-N					
2,3,7-trimethyldibenzothiophene	2.7×10^{-1}		Parnis et al. (2015)	Q	369
$C_{15}H_{14}S$					
HJSMFSZKADBZIO-UHFFFAOYSA-N					
2,3,8-trimethyldibenzothiophene	2.7×10^{-1}		Parnis et al. (2015)	Q	369
$C_{15}H_{14}S$					
QSOGKFSFLARZIE-UHFFFAOYSA-N					
2,4,7-trimethyldibenzothiophene	1.9×10^{-1}		Parnis et al. (2015)	Q	369
$C_{15}H_{14}S$					
[216983-03-8]					
YDWNRDFOOADVGC-UHFFFAOYSA-N					

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4,6-diethyldibenzothiophene $C_{16}H_{16}S$ [132034-91-4] UMQGGSYHJPHWFV-UHFFFAOYSA-N	1.3×10^{-1}		Parnis et al. (2015)	Q	369
2-butyldibenzothiophene $C_{16}H_{16}S$ [147792-31-2] BEQMTJNPMZQPKZ-UHFFFAOYSA-N	1.6×10^{-1}		Parnis et al. (2015)	Q	369
carbon oxide sulfide	2.0×10^{-4}	3500	Burkholder et al. (2019)	L	
OCS	2.0×10^{-4}	3500	Burkholder et al. (2015)	L	
(carbonyl sulfide)	2.1×10^{-4}	3300	Warneck and Williams (2012)	L	
[463-58-1]	2.0×10^{-4}	3500	Sander et al. (2011)	L	
JJWKPURADFRFRB-UHFFFAOYSA-N	2.0×10^{-4}	3500	Sander et al. (2006)	L	
	2.1×10^{-4}	3000	Wilhelm et al. (1977)	L	
	2.2×10^{-4}	2100	De Bruyn et al. (1995b)	M	
	1.5×10^{-4}	3800	Johnson and Harrison (1986)	M	70
	1.5×10^{-4}	3500	Hoyt (1982)	M	70
	2.4×10^{-4}		Stock and Kuß (1917)	M	
	2.1×10^{-4}	3300	Winkler (1907)	M	
	2.1×10^{-4}	3300	Winkler (1906)	M	
	3.4×10^{-4}		Hempel (1901)	M	619
	1.6×10^{-5}		Duchowicz et al. (2020)	V	186
	1.6×10^{-5}		HSDB (2015)	V	
	1.9×10^{-4}		Yaws (2003)	X	237
	2.0×10^{-4}		Hayer et al. (2022)	Q	20
	5.4		Duchowicz et al. (2020)	Q	
	2.0×10^{-4}		Ghargheizi et al. (2010)	Q	246
		2900	Kühne et al. (2005)	Q	
		3300	Kühne et al. (2005)	?	
	2.0×10^{-4}		Yaws (1999)	?	21
	2.1×10^{-4}	3000	Yaws et al. (1999)	?	21
	1.9×10^{-4}		Yaws and Yang (1992)	?	21
methanesulfonic acid			Brimblecombe and Clegg (1988)	T	813
CH_3SO_3H	7.3×10^{3}		Wang et al. (2017)	Q	80, 238
(MSA)	1.2×10^{6}		Wang et al. (2017)	Q	80, 239
[75-75-2]	5.0×10^{5}		Wang et al. (2017)	Q	80, 240
AFVFQIVMOAPDHO-UHFFFAOYSA-N					
MCM:CH3SO2OOH	1.9×10^{5}		Wang et al. (2017)	Q	80, 238
CH_4O_4S	1.0×10^{7}		Wang et al. (2017)	Q	80, 239
BENVNICSYZXTGE-UHFFFAOYSA-N	1.8×10^{4}		Wang et al. (2017)	Q	80, 240
MCM:CH3SOOOH	4.3×10^{7}		Wang et al. (2017)	Q	80, 238
CH_4O_3S	5.6×10^{6}		Wang et al. (2017)	Q	80, 239
IZTYBZWDPIUSAG-UHFFFAOYSA-N	2.7×10^{3}		Wang et al. (2017)	Q	80, 240

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
MCM:MSIA CH_4O_2S XNEFVTBPCXGIRX-UHFFFAOYSA-N	1.6×10^{6} 8.0×10^{3} 3.6×10^{5}		Wang et al. (2017) Wang et al. (2017) Wang et al. (2017)	Q Q Q	80, 238 80, 239 80, 240
sulfuric acid, dimethyl ester $C_2H_6O_4S$ (dimethyl sulfate) [77-78-1] VAYGXNSJCAHWJZ-UHFFFAOYSA-N	6.9 2.5		Hilal et al. (2008) Yaws (1999)	Q ?	 21, 28
dimethylsulfoxide CH_3SOCH_3 (DMSO) [67-68-5] IAZDPXIOMUYVGZ-UHFFFAOYSA-N	9.8×10^{2} 9.8×10^{2} 8.0×10^{3} 9.8×10^{2} 9.8×10^{2} $>9.9\times10^{3}$ 9.4×10^{2} 4.4 4.4 1.0×10^{4} 1.4×10^{1} 2.0×10^{2} 1.3×10^{2} 4.6×10^{2} 3.9×10^{4} 2.0×10^{5} 4.3×10^{3} 6.7×10^{3} 6.5×10^{3} 	7800 1300 8700 3100 4100 	Burkholder et al. (2019) Burkholder et al. (2015) Brockbank (2013) Sander et al. (2011) Sander et al. (2006) Lee and Zhou (1994) Watts and Brimblecombe (1987) Mackay et al. (2006d) Mackay et al. (1995) Bagno et al. (1991) Betterton (1992) Keshavarz et al. (2022) Duchowicz et al. (2020) Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) Hilal et al. (2008) Kühne et al. (2005) Taft et al. (1985) Duchowicz et al. (2020) Kühne et al. (2005) Fogg and Sangster (2003)	L L L L L M M V V T C Q Q Q Q Q Q Q Q ? ? ?	 1 473 80, 238 80, 239 80, 240 185, 21 814
dimethylsulfone $CH_3SO_2CH_3$ (DMSO2) [67-71-0] HHVIBTZHLRERCL-UHFFFAOYSA-N	5.0×10^{-3} 5.0×10^{-3} 4.0 3.3×10^{4} 1.8×10^{5} $>4.9\times10^{2}$		Mackay et al. (2006d) Mackay et al. (1995) Wang et al. (2017) Wang et al. (2017) Wang et al. (2017) De Bruyn et al. (1994)	V V Q Q Q E	 80, 238 80, 239 80, 240
mercaptoacetic acid $C_2H_4O_2S$ [68-11-1] CWERGRDVMFNCDR-UHFFFAOYSA-N	5.2×10^{2}		HSDB (2015)	Q	99
2-mercaptoethanol C_2H_6OS [60-24-2] DGVVWUTYPXICAM-UHFFFAOYSA-N	5.5×10^{1} 5.5×10^{1} 1.0×10^{2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methanesulfonic acid, methyl ester $C_2H_6O_3S$ [66-27-3] MBABOKRGFJTBAE-UHFFFAOYSA-N	2.5		HSDB (2015)	Q	99
MCM:CH3SCH2OOH	1.1×10^{2}		Wang et al. (2017)	Q	80, 238
$C_2H_6O_2S$	1.4×10^{2}		Wang et al. (2017)	Q	80, 239
LDZPECMXMDESRV-UHFFFAOYSA-N	9.8		Wang et al. (2017)	Q	80, 240
MCM:DMSO2OOH	2.6×10^{5}		Wang et al. (2017)	Q	80, 238
$C_2H_6O_4S$	6.5×10^{6}		Wang et al. (2017)	Q	80, 239
GCLQZLAJAMWHPS-UHFFFAOYSA-N	6.8×10^{5}		Wang et al. (2017)	Q	80, 240
MCM:CH3SCH2OH	4.2		Wang et al. (2017)	Q	80, 238
C_2H_6OS	7.6×10^{1}		Wang et al. (2017)	Q	80, 239
ZSSFPSNLAUYOFG-UHFFFAOYSA-N	1.1×10^{1}		Wang et al. (2017)	Q	80, 240
MCM:DMSO2OH	1.0×10^{4}		Wang et al. (2017)	Q	80, 238
$C_2H_6O_3S$	5.6×10^{6}		Wang et al. (2017)	Q	80, 239
ICHBUPLXTAHKLA-UHFFFAOYSA-N	5.8×10^{6}		Wang et al. (2017)	Q	80, 240
MCM:CH3SCHO	1.3		Wang et al. (2017)	Q	80, 238
C_2H_4OS	1.5×10^{-1}		Wang et al. (2017)	Q	80, 239
LFJRGYNYRORDDM-UHFFFAOYSA-N	4.8×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:CH3SO2CHO	3.1×10^{3}		Wang et al. (2017)	Q	80, 238
$C_2H_4O_3S$	3.6×10^{2}		Wang et al. (2017)	Q	80, 239
LUGQISNSRPQOGS-UHFFFAOYSA-N	2.2×10^{2}		Wang et al. (2017)	Q	80, 240
mercaptoacetic acid, methyl ester $C_3H_6O_2S$ (methyl thioglycolate) [2365-48-2] MKIJJIMOAABWGF-UHFFFAOYSA-N	1.6		HSDB (2015)	Q	99
1,3-propane sultone $C_3H_6O_3S$ [1120-71-4] FSSPGSAQUIYDCN-UHFFFAOYSA-N	1.6×10^{3}		Ebert et al. (2023)	?	316
methanesulfonic acid, ethyl ester	3.8×10^{1}		Duchowicz et al. (2020)	V	186
$C_3H_8O_3S$	2.8×10^{-2}		Duchowicz et al. (2020)	Q	
[62-50-0]	1.8		HSDB (2015)	Q	99
PLUBXMRUUVWRLT-UHFFFAOYSA-N					
2,3-dimercapto-1-propanol	1.1×10^{3}		Duchowicz et al. (2020)	V	186
$C_3H_8OS_2$	4.1×10^{3}		Duchowicz et al. (2020)	Q	
[59-52-9]					
WQABCVAJNWAXTE-UHFFFAOYSA-N					

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
divinyl sulfoxide C_4H_6OS (vinyl sulfoxide) [1115-15-7] HQSMEHLVLOGBCK-UHFFFAOYSA-N	2.5×10^{1}		HSDB (2015)	Q	99
divinyl sulphone $C_4H_6O_2S$ [77-77-0] AFOSIXZFDONLBT-UHFFFAOYSA-N	2.0×10^{-1}		HSDB (2015)	Q	99
2,5-dihydrothiophene sulfone $C_4H_6O_2S$ (2,5-dihydrothiophene 1,1-dioxide) [77-79-2] MBDNRNMVTZADMQ-UHFFFAOYSA-N	2.3		HSDB (2015)	Q	99
thiodiacetic acid $C_4H_6O_4S$ [123-93-3] UVZICZIVKIMRNE-UHFFFAOYSA-N	2.2×10^{8}		HSDB (2015)	Q	99
thiophene, tetrahydro-, 1,1-dioxide $C_4H_8O_2S$ (sulfolane) [126-33-0] HXJUTPCZVOIRIF-UHFFFAOYSA-N	2.1		HSDB (2015)	Q	99
2-(ethylthio)ethanol $C_4H_{10}OS$ [110-77-0] LNRIEBFNWGMXKP-UHFFFAOYSA-N	1.9×10^{2}		HSDB (2015)	Q	99
thiodiglycol $C_4H_{10}O_2S$ [111-48-8] YODZTKMDCQEPHD-UHFFFAOYSA-N	5.2×10^{3}		HSDB (2015)	Q	99
methanesulfonic acid, 1-methylethyl ester $C_4H_{10}O_3S$ [926-06-7] SWWHCQCMVCPLEQ-UHFFFAOYSA-N	1.4		HSDB (2015)	Q	99
diethyl sulfate $C_4H_{10}O_4S$ [64-67-5] DENRZWYUOJLTMF-UHFFFAOYSA-N	1.6		Ebert et al. (2023)	?	316

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
S-methyl butanethioate $C_5H_{10}OS$ [2432-51-1] GRLJIIJNZJVMGP-UHFFFAOYSA-N	2.6×10^{-2}		Souchon et al. (2004)	M	
4-hydroxybenzenesulfonic acid $C_6H_6O_4S$ [98-67-9] FEPBITJSIHRMRT-UHFFFAOYSA-N	3.8×10^{7}		HSDB (2015)	Q	99
benzenesulfonic acid $C_6H_6O_3S$ [98-11-3] SRSXLGNVWSONIS-UHFFFAOYSA-N	3.9×10^{3}		HSDB (2015)	Q	99
dimethipin $C_6H_{10}O_4S_2$ [55290-64-7] PHVNLLCAQHGNKU-UHFFFAOYSA-N	4.3×10^{5} 7.0×10^{5} 4.3×10^{5}		Duchowicz et al. (2020) Duchowicz et al. (2020) MacBean (2012a)	V Q ?	186
4-methylbenzenesulfonic acid $C_7H_8O_3S$ [104-15-4] JOXIMZWYDAKGHI-UHFFFAOYSA-N	3.6×10^{3}		HSDB (2015)	Q	99
phenylmethanesulfonic acid $C_7H_8O_3S$ (benzylsulfonic acid) [100-87-8] NIXKBAZVOQAHGC-UHFFFAOYSA-N	9.9×10^{3}		HSDB (2015)	Q	99
isoprothiolane $C_{12}H_{18}O_4S_2$ [50512-35-1] UFHLMYOGRXOCSL-UHFFFAOYSA-N	9.8×10^{-2} 2.8×10^{3}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
4,4'-sulfonyldiphenol $C_{12}H_{10}O_4S$ (bisphenol S) [80-09-1] VPWNQTHUCYMVMZ-UHFFFAOYSA-N	3.7×10^{9}		HSDB (2015)	Q	447
benfuresate $C_{12}H_{16}O_4S$ [68505-69-1] QGQSRQPXXMTJCM-UHFFFAOYSA-N	3.7×10^{2}		Ebert et al. (2023)	?	318

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
lauryl sulfate $C_{12}H_{26}O_4S$ (dodecyl sulfate) [151-41-7] MOTZDAYCYVMXPC-UHFFFAOYSA-N	5.5×10^{1}		HSDB (2015)	Q	99
ethofumesate	2.7×10^{2}		Duchowicz et al. (2020)	V	186
$C_{13}H_{18}O_5S$	2.7×10^{2}		HSDB (2015)	V	
[26225-79-6]	4.5×10^{1}		Barcelo and Hennion (1997)	X	567
IRCMYGHHKLLGHV-UHFFFAOYSA-N	7.7		Duchowicz et al. (2020)	Q	
	1.1×10^{2}		Goodarzi et al. (2010)	Q	568, 569
	2.7×10^{2}		Maniere et al. (2011)	?	165
1,1'-sulfonylbis(4-(1-methylethyl)-benzene	1.0×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_{18}H_{22}O_2S$	2.9×10^{3}		Zhang et al. (2010)	Q	287, 289
[57913-35-6]	6.7×10^{4}		Zhang et al. (2010)	Q	287, 290
PKQWGBLKCJIMDP-UHFFFAOYSA-N	3.1×10^{2}		Zhang et al. (2010)	Q	287, 291
propargite	1.5×10^{1}		Duchowicz et al. (2020)	V	186
$C_{19}H_{26}O_4S$	1.5×10^{1}		HSDB (2015)	V	
[2312-35-8]	1.0×10^{2}		Duchowicz et al. (2020)	Q	
ZYHMJXZULPZUED-UHFFFAOYSA-N					
kadethrin $C_{23}H_{24}O_4S$ [58769-20-3] UGWALRUNBSBTGI-QJLCOAGJSA-N	1.2×10^{4}		HSDB (2015)	Q	99
spironolactone $C_{24}H_{32}O_4S$ [52-01-7] LXMSZDCAJNLERA-PJKOONHHSA-N	9.0×10^{4}		HSDB (2015)	Q	99
2,2'-thiobis(4-(1,1,3,3-tetramethylbutyl)phenol)	4.5×10^{5}		Zhang et al. (2010)	Q	287, 288
$C_{28}H_{42}O_2S$	1.2×10^{4}		Zhang et al. (2010)	Q	287, 289
[3294-03-9]	2.2×10^{7}		Zhang et al. (2010)	Q	287, 290
WQYFETFRIRDUPJ-UHFFFAOYSA-N	1.8×10^{5}		Zhang et al. (2010)	Q	287, 291
propanoic acid, 3,3'-thiobis-, didodecyl ester $C_{30}H_{58}O_4S$ (dilauryl thiodipropionate) [123-28-4] GHKOFFNLGXMVNJ-UHFFFAOYSA-N	2.5		HSDB (2015)	Q	447
dioctadecyl 3,3'-thiodipropionate $C_{42}H_{82}O_4S$ [693-36-7] PWWSSIYVTQUJQQ-UHFFFAOYSA-N	8.2×10^{-2}		HSDB (2015)	Q	447

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methyl isothiocyanate CH_3NCS [556-61-6] LGDSHSYDSCRFAB-UHFFFAOYSA-N	1.7×10^{-1} 1.7×10^{-1} 1.7×10^{-1} 1.6×10^{-1} 2.2×10^{-1} 2.2×10^{-1} 2.1 1.8×10^{-2}		Burkholder et al. (2019) Burkholder et al. (2015) Sander et al. (2011) Worthington and Wade (2007) Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Modarresi et al. (2007)	L L L M V V Q Q	 186 67
thiourea CH_4N_2S [62-56-6] UMGDCJDMYOKAJW-UHFFFAOYSA-N	5.0×10^{3} 4.9×10^{3} 1.7×10^{5}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
hydrazinecarbothioamide CH_5N_3S (1-amino-2-thiourea) [79-19-6] BRWIZMBXBAOCCF-UHFFFAOYSA-N	1.5×10^{4}		HSDB (2015)	Q	99
thiocyanic acid, methyl ester C_2H_3NS [556-64-9] VYHVQEYOFIYNJP-UHFFFAOYSA-N	2.2×10^{-1}		HSDB (2015)	Q	99
ethanethioamide C_2H_5NS (thioacetamide) [62-55-5] YUKQRDCYNOVPGJ-UHFFFAOYSA-N	1.5		HSDB (2015)	Q	99
mercaptamine C_2H_7NS (cysteamine) [60-23-1] UFULAYFCSOUIOV-UHFFFAOYSA-N	2.7×10^{1}		HSDB (2015)	Q	99
thiocyanic acid, ethyl ester C_3H_5NS [542-90-5] WFCLYEAZTHWNEH-UHFFFAOYSA-N	1.7×10^{-1}		HSDB (2015)	Q	99
2-imidazolidinethione $C_3H_6N_2S$ (ethylene thiourea) [96-45-7] PDQAZBWRQCGBEV-UHFFFAOYSA-N	2.9×10^{1}		HSDB (2015)	Q	99

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ethylthiourea $C_3H_8N_2S$ [625-53-6] GMEHFXXZSWDEDB-UHFFFAOYSA-N	4.2×10^{2}		HSDB (2015)	Q	99
allyl isothiocyanate C_4H_5NS [57-06-7] ZOJBYZNEUISWFT-UHFFFAOYSA-N	2.1×10^{-2} 4.1×10^{-2} 4.1×10^{-2} 2.7 2.3×10^{-1}		Souchon et al. (2004) Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Modarresi et al. (2007)	M V V Q Q	 186 67
dazomet $C_5H_{10}N_2S_2$ [533-74-4] QAYICIQNSGETAS-UHFFFAOYSA-N	2.0×10^{4} 4.6×10^{4} 3.7×10^{4} 3.7×10^{5} 2.0×10^{4}		Duchowicz et al. (2020) Mackay et al. (2006d) MacBean (2012b) Duchowicz et al. (2020) Maniere et al. (2011)	V V X Q ?	186 350 12, 165
N,N'-diethylthiourea $C_5H_{12}N_2S$ [105-55-5] FLVIGYVXZHLUHP-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	99
tetramethylthiourea $C_5H_{12}N_2S$ [2782-91-4] MNOILHPDHOHILI-UHFFFAOYSA-N	8.5×10^{2}		HSDB (2015)	Q	99
thiram $C_6H_{12}N_2S_4$ [137-26-8] KUAZQDVKQLNFPE-UHFFFAOYSA-N	9.3×10^{1} 3.0×10^{1}		Mackay et al. (2006d) MacBean (2012b)	V X	 350
bis(dimethylthiocarbamyl) sulfide $C_6H_{12}N_2S_3$ (bis(dimethylthiocarbamoyl) sulfide) [97-74-5] REQPQFUJGGOFQL-UHFFFAOYSA-N	5.8×10^{-1}		HSDB (2015)	Q	99
benzothiazole C_7H_5NS [95-16-9] IOJUPLGTWVMSFF-UHFFFAOYSA-N	2.7×10^{1} 2.7×10^{1} 2.8 1.1×10^{1} 2.0		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	99 287, 288 287, 289 287, 290 287, 291
2-mercaptobenzothiazole $C_7H_5NS_2$ [149-30-4] YXIWHUQXZSMYRE-UHFFFAOYSA-N	2.7×10^{2} 2.7×10^{2} 2.8×10^{3} 2.2×10^{2} 2.1×10^{1}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	99 287, 288 287, 289 287, 290 287, 291

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-benzothiazolamine $C_7H_6N_2S$ [136-95-8] UHGULLIUJBCTEF-UHFFFAOYSA-N	7.6×10^4		HSDB (2015)	Q	99
phenylthiourea $C_7H_8N_2S$ [103-85-5] FULZLIGZKMKICU-UHFFFAOYSA-N	9.9×10^4		HSDB (2015)	Q	99
aziprotryn $C_7H_{11}N_7S$ [4658-28-0] AFIIBUOYKYSPKB-UHFFFAOYSA-N	4.0×10^2 9.2×10^2		Abraham et al. (2007) MacBean (2012a)	Q ?	
isothiocyanatobenzene C_7H_5NS [103-72-0] QKFJKGMPGYROCL-UHFFFAOYSA-N	3.3×10^{-3} 5.1		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
simetryn $C_8H_{15}N_5S$ [1014-70-6] MGLWZSOBALDPEK-UHFFFAOYSA-N	2.2×10^4 2.2×10^4 3.8×10^6 2.9×10^4 1.0×10^4		Duchowicz et al. (2020) Mackay et al. (2006d) Duchowicz et al. (2020) Hilal et al. (2008) Abraham et al. (2007)	V V Q Q Q	186
desmetryn $C_8H_{15}N_5S$ [1014-69-3] HCRWJJJUKUVORR-UHFFFAOYSA-N	2.1×10^4 5.0×10^7 2.2×10^4 2.0×10^4 1.4×10^9 3.9×10^7 2.1×10^4		HSDB (2015) Delgado and Alderete (2003) Hilal et al. (2008) Abraham et al. (2007) Delgado and Alderete (2003) Delgado and Alderete (2003) MacBean (2012a)	V C Q Q Q Q ?	
thioquinox $C_9H_4N_2S_3$ [93-75-4] ILERPRJWJPJZDN-UHFFFAOYSA-N	1.3×10^2		HSDB (2015)	Q	99
thiocyanic acid, (2-benzothiazolylthio)methyl ester $C_9H_6N_2S_3$ [21564-17-0] TUBQDCKAWGHZPF-UHFFFAOYSA-N	1.5×10^6		HSDB (2015)	Q	99

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
ametryn	2.1×10^{1}		Chao et al. (2017)	M	
$C_9H_{17}N_5S$	4.1×10^{3}		HSDB (2015)	V	
[834-12-8]	8.1×10^{3}		Mackay et al. (2006d)	V	
RQVYBGPQFYCBGX-UHFFFAOYSA-N	8.3×10^{3}		Suntio et al. (1988)	V	12
	8.2×10^{1}		Barcelo and Hennion (1997)	X	567
	4.1×10^{3}		Delgado and Alderete (2003)	C	
	1.3×10^{2}		Goodarzi et al. (2010)	Q	568
	1.2×10^{4}		Hilal et al. (2008)	Q	
	5.1×10^{3}		Abraham et al. (2007)	Q	
	8.9×10^{7}		Delgado and Alderete (2003)	Q	
	1.1×10^{7}		Delgado and Alderete (2003)	Q	
cimetidine	1.0×10^{10}		HSDB (2015)	Q	99
$C_{10}H_{16}N_6S$					
[51481-61-9]					
AQIXAKUUQRKLND-UHFFFAOYSA-N					
prometryn	8.2×10^{2}		HSDB (2015)	V	
$C_{10}H_{19}N_5S$	2.0×10^{3}		Mackay et al. (2006d)	V	
[7287-19-6]	2.0×10^{3}		Suntio et al. (1988)	V	12
AAEVYOVXGOFMJO-UHFFFAOYSA-N	2.0×10^{1}		Barcelo and Hennion (1997)	X	567
	2.9×10^{6}		Delgado and Alderete (2003)	C	
	7.6×10^{2}		Delgado and Alderete (2003)	C	
	2.5×10^{2}		Goodarzi et al. (2010)	Q	568
	7.5×10^{2}		Hilal et al. (2008)	Q	
	2.5×10^{3}		Abraham et al. (2007)	Q	
	5.1×10^{6}		Delgado and Alderete (2003)	Q	
	1.4×10^{6}		Delgado and Alderete (2003)	Q	
terbutryn	4.7×10^{2}		HSDB (2015)	V	
$C_{10}H_{19}N_5S$	7.0×10^{2}		Mackay et al. (2006d)	V	
[886-50-0]	7.7×10^{2}		Suntio et al. (1988)	V	12
IROINLKCQGIITA-UHFFFAOYSA-N	7.6		Barcelo and Hennion (1997)	X	567
	1.2×10^{6}		Delgado and Alderete (2003)	C	
	8.7×10^{2}		Delgado and Alderete (2003)	C	
	1.7×10^{2}		Goodarzi et al. (2010)	Q	568
	4.5×10^{3}		Hilal et al. (2008)	Q	
	1.6×10^{3}		Abraham et al. (2007)	Q	
	5.1×10^{6}		Delgado and Alderete (2003)	Q	
	1.4×10^{6}		Delgado and Alderete (2003)	Q	
disulfiram	1.2×10^{-1}		HSDB (2015)	Q	99
$C_{10}H_{20}N_2S_4$					
[97-77-8]					
AUZONCFQVSMFAP-UHFFFAOYSA-N					

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1-naphthalenylthiourea $C_{11}H_{10}N_2S$ [86-88-4] PIVQQUNOTICCSA-UHFFFAOYSA-N	1.2×10^{3}		HSDB (2015)	Q	99
4,4'-thiobisbenzenamine $C_{12}H_{12}N_2S$ (bis(4-aminophenyl) sulfide) [139-65-1] ICNFHJVPAJKPHW-UHFFFAOYSA-N	2.5×10^{6}		HSDB (2015)	Q	99
dipropetryn $C_{11}H_{19}N_5S$ [4147-51-7] NPWMZOGDXOFZIN-UHFFFAOYSA-N	6.0×10^{2} 1.6×10^{3} 6.5×10^{2}		Hilal et al. (2008) Abraham et al. (2007) MacBean (2012a)	Q Q ?	
dimethametryn $C_{11}H_{21}N_5S$ [22936-75-0] IKYICRRUVNIHPP-UHFFFAOYSA-N	8.2×10^{3} 1.0×10^{3}		Hilal et al. (2008) Abraham et al. (2007)	Q Q	
phenothiazine $C_{12}H_9NS$ [92-84-2] WJFKNYWRSNBZNX-UHFFFAOYSA-N	1.0×10^{2} 3.5×10^{2} 3.5×10^{2} 6.9×10^{2} 9.7×10^{1} 4.3×10^{2}		Abraham et al. (2019) HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q Q	 99 287, 288 287, 289 287, 290 287, 291
cymiazole $C_{12}H_{14}N_2S$ [61676-87-7] YUAUPYJCVKNAEC-UHFFFAOYSA-N	1.5×10^{2}		Ebert et al. (2023)	?	318
2,2'-dithiobisbenzothiazole $C_{14}H_8N_2S_4$ (2,2'-dibenzothiazyl disulfide) [120-78-5] AFZSMODLJJCVPP-UHFFFAOYSA-N	4.2×10^{7}		HSDB (2015)	Q	99
methapyrilene $C_{14}H_{19}N_3S$ [91-80-5] HNJJXZKZRAWDPF-UHFFFAOYSA-N	3.6×10^{1}		HSDB (2015)	V	
olanzapine $C_{17}H_{20}N_4S$ [132539-06-1] KVWDHTXUZHCGIO-UHFFFAOYSA-N	1.3×10^{9}		HSDB (2015)	Q	99

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-(1,1-dimethylethyl)bis(2-benzothiazolesulfen)amide	2.4×10^{8}		Zhang et al. (2010)	Q	287, 288
$C_{18}H_{17}N_3S_4$	1.7×10^{3}		Zhang et al. (2010)	Q	287, 289
[3741-80-8]	2.3×10^{3}		Zhang et al. (2010)	Q	287, 290
VILGDADBAQFRJE-UHFFFAOYSA-N	3.9×10^{8}		Zhang et al. (2010)	Q	287, 291
buthiobate	3.4×10^{1}		Ebert et al. (2023)	?	318
$C_{21}H_{28}N_2S_2$					
[51308-54-4]					
ZZVVDIVWGXTDRQ-UHFFFAOYSA-N					
MCM:CH3SO4NO2	7.8×10^{3}		Wang et al. (2017)	Q	80, 238
CH_3NO_6S	1.6×10^{4}		Wang et al. (2017)	Q	80, 239
IMLJWBRSRKRPAQ-UHFFFAOYSA-N	3.2×10^{-2}		Wang et al. (2017)	Q	80, 240
MCM:CH3SOO2NO2	1.7×10^{6}		Wang et al. (2017)	Q	80, 238
CH_3NO_5S	3.9×10^{8}		Wang et al. (2017)	Q	80, 239
PGTDFOBGUOOGGZ-UHFFFAOYSA-N	8.3×10^{-2}		Wang et al. (2017)	Q	80, 240
taurine	5.8×10^{6}		HSDB (2015)	Q	447
$C_2H_7NO_3S$					
[107-35-7]					
XOAAWQZATWQOTB-UHFFFAOYSA-N					
2-amino-5-nitrothiazole	1.9×10^{6}		HSDB (2015)	Q	99
$C_3H_3N_3O_2S$					
[121-66-4]					
MIHADVKEHAFNPG-UHFFFAOYSA-N					
N-(aminothioxomethyl)acetamide	3.8×10^{5}		HSDB (2015)	Q	99
$C_3H_6N_2OS$					
(1-acetyl-2-thiourea)					
[591-08-2]					
IPCRBOOJBPETMF-UHFFFAOYSA-N					
acesulfame	1.0×10^{3}		HSDB (2015)	Q	99
$C_4H_5NO_4S$					
[33665-90-6]					
YGCFIWIQZPHFLU-UHFFFAOYSA-N					
methomyl	2.0×10^{2}		Chao et al. (2017)	M	
$C_5H_{10}N_2O_2S$	5.0×10^{5}		Duchowicz et al. (2020)	V	186
[16752-77-5]	5.2×10^{5}		HSDB (2015)	V	
UHXUZOCRWCRNSJ-UHFFFAOYSA-N	5.3×10^{4}		Mackay et al. (2006d)	V	
	1.5×10^{4}		Suntio et al. (1988)	V	12
	1.5×10^{2}		Barcelo and Hennion (1997)	X	567
	1.0×10^{4}		Duchowicz et al. (2020)	Q	
	1.3×10^{2}		Goodarzi et al. (2010)	Q	568, 569

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-aminobenzenesulfonic acid $C_6H_7NO_3S$ (sulfanilic acid) [121-57-3] HVBSAKJJOYLTQU-UHFFFAOYSA-N	1.1×10^{7}		HSDB (2015)	Q	447
sulfanilamide $C_6H_8N_2O_2S$ [63-74-1] FDDDEECHVMSUSB-UHFFFAOYSA-N	6.6×10^{4}		HSDB (2015)	Q	99
nithiazide $C_6H_8N_4O_3S$ [139-94-6] FQSUTLQHSDLLAN-UHFFFAOYSA-N	6.2×10^{9}		HSDB (2015)	Q	99
2-methylbenzenesulfonamide $C_7H_9NO_2S$ (*o*-toluenesulfonamide) [88-19-7] YCMLQMDWSXFTIF-UHFFFAOYSA-N	2.1×10^{1}		HSDB (2015)	Q	99
4-methylbenzenesulfonamide $C_7H_9NO_2S$ (*p*-toluenesulfonamide) [70-55-3] LMYRWZFENFIFIT-UHFFFAOYSA-N	2.1×10^{1}		HSDB (2015)	Q	99
ethidimuron $C_7H_{12}N_4O_3S_2$ [30043-49-3] KCOCSOWTADCKOL-UHFFFAOYSA-N	1.4×10^{8}		MacBean (2012a)	?	
oxamyl $C_7H_{13}N_3O_3S$ [23135-22-0] KZAUOCCYDRDERY-UITAMQMPSA-N	4.2×10^{4}		Duchowicz et al. (2020)	V	186
	4.2×10^{4}		HSDB (2015)	V	
	4.2×10^{4}		Mackay et al. (2006d)	V	
	3.8×10^{3}		Suntio et al. (1988)	V	12
	3.8×10^{1}		Barcelo and Hennion (1997)	X	567
	3.4×10^{7}		Duchowicz et al. (2020)	Q	
	6.4×10^{1}		Goodarzi et al. (2010)	Q	568
	2.0×10^{7}		Maniere et al. (2011)	?	165
aldicarb $C_7H_{14}N_2O_2S$ [116-06-3] QGLZXHRNAYXIBU-WEVVVXLNSA-N	6.9×10^{3}		Duchowicz et al. (2020)	V	186
	6.6×10^{3}		HSDB (2015)	V	
	7.9×10^{3}		Mackay et al. (2006d)	V	
	3.1×10^{3}		Suntio et al. (1988)	V	12
	3.1×10^{1}		Barcelo and Hennion (1997)	X	567
	1.9		Suntio et al. (1988)	C	12
	8.0×10^{3}		Duchowicz et al. (2020)	Q	
	2.6×10^{1}		Goodarzi et al. (2010)	Q	568, 571

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
aldicarb sulfoxide $C_7H_{14}N_2O_3S$ [1646-87-3] BXPMAGSOWXBZHS-UHFFFAOYSA-N	1.0×10^4 4.2×10^6		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
aldicarb sulfone $C_7H_{14}N_2O_4S$ [1646-88-4] YRRKLBAKDXSTNC-UHFFFAOYSA-N	2.9×10^3 4.4×10^6 3.7×10^3		Duchowicz et al. (2020) Duchowicz et al. (2020) MacBean (2012a)	V Q ?	186
butocarboxim $C_7H_{14}N_2O_2S$ [34681-10-2] SFNPDDSJBGRXLW-UHFFFAOYSA-N	1.7×10^4 1.7×10^4		HSDB (2015) MacBean (2012a)	V ?	
butoxycarboxim $C_7H_{14}N_2O_4S$ [34681-23-7] CTJBHIROCMPUKL-UHFFFAOYSA-N	3.5×10^6		HSDB (2015)	V	
saccharin $C_7H_5NO_3S$ [81-07-2] CVHZOJJKTDOEJC-UHFFFAOYSA-N	8.2×10^3		HSDB (2015)	Q	99
acibenzolar-S-methyl $C_8H_6N_2OS_2$ [135158-54-2] UELITFHSCLAHKR-UHFFFAOYSA-N	8.3×10^1 8.2×10^1 1.5×10^6 7.7×10^1		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Maniere et al. (2011)	V V Q ?	186 241, 165
quinomethionate $C_8H_6N_2OS_2$ [2439-01-2] FBQQHUGEACOBDN-UHFFFAOYSA-N	1.6×10^2 1.6×10^2		HSDB (2015) MacBean (2012a)	V ?	
nifurthiazole $C_8H_6N_4O_4S$ [3570-75-0] DUWYZHLZDVCZIO-UHFFFAOYSA-N	1.3×10^{12}		HSDB (2015)	Q	99
4-methylbenzenesulfonyl isocyanate $C_8H_7NO_3S$ [4083-64-1] VLJQDHDVZJXNQL-UHFFFAOYSA-N	1.7×10^{-1} 3.2×10^1 6.7 4.0×10^4		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
tinidazole $C_8H_{13}N_3O_4S$ [19387-91-8] HJLSLZFTEKNLFI-UHFFFAOYSA-N	1.9×10^5		HSDB (2015)	Q	99

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
metribuzin $C_8H_{14}N_4OS$ [21087-64-9] FOXFZRUHNHCZPX-UHFFFAOYSA-N	8.2×10^4 5.0×10^4		HSDB (2015) Maniere et al. (2011)	V ?	 241, 165
tricyclazole $C_9H_7N_3S$ [41814-78-2] DQJCHOQLCLEDLL-UHFFFAOYSA-N	3.2×10^5 3.2×10^5 5.5×10^5		Duchowicz et al. (2020) Mackay et al. (2006d) Duchowicz et al. (2020)	V V Q	186
benzthiazuron $C_9H_9N_3OS$ [1929-88-0] DTCJYIIKPVRVDD-UHFFFAOYSA-N	1.9×10^6		Ebert et al. (2023)	?	365
thidiazuron $C_9H_8N_4OS$ [51707-55-2] HFCYZXMHUIHAQI-UHFFFAOYSA-N	3.0×10^7		HSDB (2015)	V	
sulfathiazole $C_9H_9N_3O_2S_2$ [72-14-0] JNMRHUJNCSQMMB-UHFFFAOYSA-N	1.7×10^8		HSDB (2015)	Q	99
sulfamethizole $C_9H_{10}N_4O_2S_2$ [144-82-1] VACCAVUAMIDAGB-UHFFFAOYSA-N	3.8×10^8		HSDB (2015)	Q	99
ethiozin $C_9H_{16}N_4OS$ [64529-56-2] ADZSGNDOZREKJK-UHFFFAOYSA-N	2.0×10^2		MacBean (2012a)	?	
tebuthiuron $C_9H_{16}N_4OS$ [34014-18-1] HBPDKDSFLXWOAE-UHFFFAOYSA-N	6.9×10^4 3.2×10^4 8.2×10^4		Keshavarz et al. (2022) Duchowicz et al. (2020) Duchowicz et al. (2020)	Q Q ?	 185, 21
molinate $C_9H_{17}NOS$ [2212-67-1] DEDOPGXGGQYYMW-UHFFFAOYSA-N	7.7 2.2 1.7 6.9 1.1×10^1 1.0×10^1 7.6 7.3 2.3	 7300 	Watanabe (1993) Sagebiel et al. (1992) Sagebiel et al. (1992) Mackay et al. (2006d) Sagebiel et al. (1992) Woodrow et al. (1990) Armbrust (2000) Hilal et al. (2008) Modarresi et al. (2007)	M M M V V V C Q Q	 12 12 67

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
thiofanox	1.1×10^{3}		Duchowicz et al. (2020)	V	186
$C_9H_{18}N_2O_2S$	3.4×10^{3}		Duchowicz et al. (2020)	Q	
[39196-18-4]					
FZSVSABTBYGOQH-UHFFFAOYSA-N					
amidosulfuron	6.4×10^{5}		Maniere et al. (2011)	?	12, 493, 165
$C_9H_{15}N_5O_7S_2$	1.9×10^{3}		Maniere et al. (2011)	?	12, 577, 165
[120923-37-7]	1.5×10^{5}		Maniere et al. (2011)	?	12, 573, 165
CTTHWASMBLQOFR-UHFFFAOYSA-N					
S-ethyl dipropylthiocarbamate	5.6×10^{-1}	9100	Reyes-Pérez et al. (2008)	M	
$C_9H_{19}NOS$	3.8×10^{-2}	4800	Breiter et al. (1998)	M	
(eptam; EPTC)	6.2×10^{-1}		HSDB (2015)	V	
[759-94-4]	9.8×10^{-1}		Mackay et al. (2006d)	V	
GUVLYNGULCJVDO-UHFFFAOYSA-N	4.2×10^{-1}		Breiter et al. (1998)	V	
	9.8×10^{-1}		Suntio et al. (1988)	V	12
	7.4×10^{-1}		Burkhard and Guth (1981)	V	
	1.0×10^{-2}		Barcelo and Hennion (1997)	X	567
	1.1×10^{-2}		Goodarzi et al. (2010)	Q	568
	8.2×10^{-1}		Hilal et al. (2008)	Q	
	1.2		Modarresi et al. (2007)	Q	67
		4800	Kühne et al. (2005)	Q	
		4800	Kühne et al. (2005)	?	
thiabendazole	4.7×10^{5}		Duchowicz et al. (2020)	V	186
$C_{10}H_7N_3S$	4.7×10^{5}		HSDB (2015)	V	
[148-79-8]	4.7×10^{5}		Mackay et al. (2006d)	V	
WJCNZQLZVWNLKY-UHFFFAOYSA-N	1.3×10^{5}		Duchowicz et al. (2020)	Q	
	2.7×10^{5}		Maniere et al. (2011)	?	241, 165
benzo[*b*]thiophene-4-ol, methylcarbamate	5.8×10^{3}		HSDB (2015)	Q	99
$C_{10}H_9NO_2S$					
(mobam)					
[1079-33-0]					
BOTUVXISJHKZKJ-UHFFFAOYSA-N					
sulfamethoxazole	1.5×10^{7}		HSDB (2015)	Q	99
$C_{10}H_{11}N_3O_3S$					
[723-46-6]					
JLKIGFTWXXRPMT-UHFFFAOYSA-N					
bentazone	4.5×10^{3}		HSDB (2015)	V	
$C_{10}H_{12}N_2O_3S$	1.3×10^{2}		Barcelo and Hennion (1997)	X	567
[25057-89-0]	3.6×10^{2}		Goodarzi et al. (2010)	Q	568, 569
ZOMSMJKLGFBRBS-UHFFFAOYSA-N	1.4×10^{4}		Maniere et al. (2011)	?	12, 165
	4.7×10^{5}		Maniere et al. (2011)	?	12, 165

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
buthidazole $C_{10}H_{16}N_4O_2S$ [55511-98-3] SWMGXKSQWDSBKV-UHFFFAOYSA-N	4.8×10^{6}		MacBean (2012a)	?	
thiodicarb $C_{10}H_{18}N_4O_4S_3$ [59669-26-0] XDOTVMNBCQVZKG-UHFFFAOYSA-N	1.1×10^{1} 2.3×10^{1}		HSDB (2015) Mackay et al. (2006d)	V V	
pebulate $C_{10}H_{21}NOS$ [1114-71-2] SGEJQUSYQTVSIU-UHFFFAOYSA-N	4.1×10^{-2} 3.8×10^{-1} 8.6×10^{-2} 8.4×10^{-4} 6.6×10^{-3} 6.4×10^{-1} 8.9×10^{-1} $>2.3\times10^{10}$		HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Goodarzi et al. (2010) Hilal et al. (2008) Modarresi et al. (2007) MacBean (2012a)	V V V X Q Q Q ?	 12 567 568 67
vernolate $C_{10}H_{21}NOS$ [1929-77-7] OKUGPJPKMAEJOE-UHFFFAOYSA-N	3.2×10^{-1} 4.9×10^{-1} 4.9×10^{-1} 4.8×10^{-3} 2.9×10^{-3} 6.5×10^{-1} 9.0×10^{-1}		HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Goodarzi et al. (2010) Hilal et al. (2008) Modarresi et al. (2007)	V V V X Q Q Q	 12 567 568 67
biotin $C_{10}H_{16}N_2O_3S$ [58-85-5] YBJHBAHKTGYVGT-ZKWXMUAHSA-N	5.6×10^{2}		Abraham et al. (2019)	Q	
methabenzthiazuron $C_{10}H_{11}N_3OS$ [18691-97-9] RRVIAQKBTUQODI-UHFFFAOYSA-N	1.8×10^{4} 6.6×10^{4}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
sulfisoxazole $C_{11}H_{13}N_3O_3S$ [127-69-5] NHUHCSRWZMLRLA-UHFFFAOYSA-N	6.2×10^{6}		HSDB (2015)	Q	99
ethiofencarb $C_{11}H_{15}NO_2S$ [29973-13-5] HEZNVIYQEUHLNI-UHFFFAOYSA-N	8.6×10^{3} 8.2×10^{3} 7.7×10^{2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methiocarb	8.3		Mackay et al. (2006d)	V	
$C_{11}H_{15}NO_2S$	8.4×10^3		MacBean (2012b)	X	350
[2032-65-7]					
YFBPRJGDJKVWAH-UHFFFAOYSA-N					
cycloate	1.9		HSDB (2015)	V	
$C_{11}H_{21}NOS$	3.7		Hilal et al. (2008)	Q	
[1134-23-2]	3.2		Modarresi et al. (2007)	Q	67
DFCAFRGABIXSDS-UHFFFAOYSA-N					
methoprotryn	3.1×10^4		HSDB (2015)	V	
$C_{11}H_{21}N_5OS$	1.5×10^5		Hilal et al. (2008)	Q	
[841-06-5]	2.0×10^5		Abraham et al. (2007)	Q	
DDUIUBPJPOKOMV-UHFFFAOYSA-N	3.1×10^4		MacBean (2012a)	?	
butylate	1.2×10^{-1}		HSDB (2015)	V	
$C_{11}H_{23}NOS$			Mackay et al. (2006d)	V	558
[2008-41-5]	1.8		Suntio et al. (1988)	V	12
BMTAFVWTTFSTOG-UHFFFAOYSA-N	1.8×10^{-2}		Barcelo and Hennion (1997)	X	567
	2.1×10^{-1}		Goodarzi et al. (2010)	Q	568
	5.8×10^{-1}		Hilal et al. (2008)	Q	
	6.0×10^{-1}		Modarresi et al. (2007)	Q	67
2-octyl-3(2H)-isothiazolone	4.8×10^2		Duchowicz et al. (2020)	V	186
$C_{11}H_{19}NOS$	1.8		Duchowicz et al. (2020)	Q	
[26530-20-1]					
JPMIIZHYYWMHDT-UHFFFAOYSA-N					
metsulfovax	9.2×10^5		Ebert et al. (2023)	?	318
$C_{12}H_{12}N_2OS$					
[21452-18-6]					
UDSJPFPDKCMYBD-UHFFFAOYSA-N					
carboxin	3.1×10^4		Duchowicz et al. (2020)	V	186
$C_{12}H_{13}NO_2S$	3.1×10^4		HSDB (2015)	V	
[5234-68-4]	6.4×10^4		Mackay et al. (2006d)	V	
GYSSRZJIHXQEHQ-UHFFFAOYSA-N	7.6×10^2		Duchowicz et al. (2020)	Q	
	3.1×10^4		Maniere et al. (2011)	?	241, 165
oxycarboxin	9.3×10^5		Duchowicz et al. (2020)	V	186
$C_{12}H_{13}NO_4S$	9.0×10^5		HSDB (2015)	V	
[5259-88-1]	2.8×10^3		Mackay et al. (2006d)	V	
AMEKQAFGQBKLKX-UHFFFAOYSA-N	5.3×10^5		Duchowicz et al. (2020)	Q	
thifensulfuron-methyl	3.4×10^8		HSDB (2015)	V	
$C_{12}H_{13}N_5O_6S_2$	1.0×10^{14}		Maniere et al. (2011)	?	241, 493, 165
[79277-27-3]	3.6×10^{12}		Maniere et al. (2011)	?	241, 570, 165
AHTPATJNIAFOLR-UHFFFAOYSA-N					

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

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sulfamethazine $C_{12}H_{14}N_4O_2S$ [57-68-1] ASWVTGNCAZCNNR-UHFFFAOYSA-N	3.2×10^{7}		HSDB (2015)	Q	99
thiophanate-methyl $C_{12}H_{14}N_4O_4S_2$ [23564-05-8] QGHREAKMXXNCOA-UHFFFAOYSA-N	8.2×10^{3} 7.9×10^{2} 6.0×10^{3}		HSDB (2015) Mackay et al. (2006d) Maniere et al. (2011)	V V ?	 241, 165
4,4'- oxydi(benzenesulphonohydrazide) $C_{12}H_{14}N_4O_5S_2$ [80-51-3] NBOCQTNZUPTTEI-UHFFFAOYSA-N	7.8×10^{11}		HSDB (2015)	Q	99
albendazole $C_{12}H_{15}N_3O_2S$ [54965-21-8] HXHWSAZORRCQMX-UHFFFAOYSA-N	1.3×10^{8}		HSDB (2015)	Q	99
oryzalin $C_{12}H_{18}N_4O_6S$ [19044-88-3] UNAHYJYOSSSJHH-UHFFFAOYSA-N	5.2×10^{3} 5.3×10^{3} 3.6×10^{7} 2.5×10^{8} 3.0×10^{7}		HSDB (2015) Mackay et al. (2006d) Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011)	V V ? ? ?	 12, 570, 165 12, 572, 165 12, 493, 165
STK366145 $C_{12}H_{19}N_3O_3S$ (N-(2-ethyl(3-methyl-4-nitrosophenyl)amino)ethyl)-methanesulfonamide) [56046-62-9] XWQURWIJAIIPQP-UHFFFAOYSA-N	9.9×10^{4}		HSDB (2015)	V	
isomethiozin $C_{12}H_{20}N_4OS$ [57052-04-7] MZTLOILRKLUURT-UHFFFAOYSA-N	7.9×10^{2}		MacBean (2012a)	?	

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
thiencarbazone-methyl	2.1×10^{12}		Maniere et al. (2011)	?	241, 815, 165
$C_{12}H_{14}N_4O_7S_2$	5.0×10^{12}		Maniere et al. (2011)	?	241, 577, 165
[317815-83-1]	1.3×10^{13}		Maniere et al. (2011)	?	241, 493, 165
XSKZXGDFSCCXQX-UHFFFAOYSA-N	1.2×10^{13}		Maniere et al. (2011)	?	241, 573, 165
2,8-dinitrodibenzothiophene $C_{12}H_6N_2O_4S$ [109041-38-5] VMQHOWOVMXIROE-UHFFFAOYSA-N	4.0×10^{4}		Parnis et al. (2015)	Q	369
2-nitrodibenzothiophene $C_{12}H_7NO_2S$ [6639-36-7] GXLYVLHWXVRVKI-UHFFFAOYSA-N	1.2×10^{2}		Parnis et al. (2015)	Q	369
azimsulfuron	2.0×10^{9}		Maniere et al. (2011)	?	241, 493, 165
$C_{13}H_{16}N_{10}O_5S$	1.2×10^{8}		Maniere et al. (2011)	?	241, 570, 165
[120162-55-2]	1.1×10^{10}		Maniere et al. (2011)	?	241, 573, 165
MAHPNPYYQAIOJN-UHFFFAOYSA-N					
fenothiocarb $C_{13}H_{19}NO_2S$ [62850-32-2] HMIBKHHNXANVHR-UHFFFAOYSA-N	5.3×10^{2}		Ebert et al. (2023)	?	316
isobornyl thiocyanoacetate $C_{13}H_{19}NO_2S$ [115-31-1] IXEVGHXRXDBAOB-RUETXSTFSA-N	3.8×10^{1}		HSDB (2015)	Q	99
nitralin	1.4×10^{3}		HSDB (2015)	V	
$C_{13}H_{19}N_3O_6S$	7.2×10^{-3}		Mackay et al. (2006d)	V	
[4726-14-1]	7.2×10^{-3}		Suntio et al. (1988)	V	12
UMKANAFDOQQUKE-UHFFFAOYSA-N					
bupirimate	6.9×10^{2}		Duchowicz et al. (2020)	V	186
$C_{13}H_{24}N_4O_3S$	1.0×10^{2}		Mackay et al. (2006d)	V	
[41483-43-6]	1.5×10^{3}		Duchowicz et al. (2020)	Q	
DSKJPMWIHSOYEA-UHFFFAOYSA-N	7.4×10^{-1}		Maniere et al. (2011)	?	12, 165
timolol $C_{13}H_{24}N_4O_3S$ [26839-75-8] BLJRIMJGRPQVNF-JTQLQIEISA-N	2.3×10^{11}		HSDB (2015)	Q	99

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triazamate $C_{13}H_{22}N_4O_3S$ [112143-82-5] NKNFWVNSBIXGLL-UHFFFAOYSA-N	8.6×10^4 1.2×10^5		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
dithianone $C_{14}H_4N_2O_2S_2$ [3347-22-6] PYZSVQVRHDXQSL-UHFFFAOYSA-N	1.7×10^5 7.4×10^6		HSDB (2015) Mackay et al. (2006d) Maniere et al. (2011)	V V ?	 558 12, 165
N-(cyclohexylthio)phthalimide $C_{14}H_{15}NO_2S$ [17796-82-6] UEZWYKZHXASYJN-UHFFFAOYSA-N	1.5×10^2		HSDB (2015)	Q	99
metsulfuron-methyl $C_{14}H_{15}N_5O_6S$ [74223-64-6] RSMUVYRMZCOLBH-UHFFFAOYSA-N	7.5×10^{10} 2.1×10^8		HSDB (2015) Maniere et al. (2011)	V ?	 241, 165
rimsulfuron $C_{14}H_{17}N_5O_7S_2$ [122931-48-0] MEFOUWRMVYJCQC-UHFFFAOYSA-N	1.5×10^4 9.1×10^6 2.2×10^5 1.2×10^7		HSDB (2015) Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011)	V ? ? ?	 573, 165 570, 165 493, 165
thiophanate $C_{14}H_{18}N_4O_4S_2$ [23564-06-9] YFNCATAIYKQPOO-UHFFFAOYSA-N	1.9×10^7		HSDB (2015)	Q	99
sumatriptan $C_{14}H_{21}N_3O_2S$ [103628-46-2] KQKPFRSPSRPDEB-UHFFFAOYSA-N	2.2×10^8		HSDB (2015)	Q	99
mesotrione $C_{14}H_{13}NO_7S$ [104206-82-8] KPUREKXXPHOJQT-UHFFFAOYSA-N	$>2.0\times10^6$		Maniere et al. (2011)	?	12, 165
prosulfocarb $C_{14}H_{21}NOS$ [52888-80-9] NQLVQOSNDJXLKG-UHFFFAOYSA-N	7.6×10^2 9.5×10^1 6.6×10^1		Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011)	V Q ?	186 12, 165
pyriftalid $C_{15}H_{14}N_2O_4S$ [135186-78-6] RRKHIAYNPVQKEF-UHFFFAOYSA-N	2.5×10^5		Ebert et al. (2023)	?	318

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nicosulfuron $C_{15}H_{18}N_6O_6S$ [111991-09-4] RTCOGUMHFFWOJV-UHFFFAOYSA-N	6.8×10^{10}		Maniere et al. (2011)	?	12, 165
sulfometuron methyl $C_{15}H_{16}N_4O_5S$ [74222-97-2] ZDXMLEQEMNLCQG-UHFFFAOYSA-N	8.2×10^{12} 1.9×10^{8}		Armbrust (2000) HSDB (2015)	C Q	 99
tribenuron-methyl $C_{15}H_{17}N_5O_6S$ [101200-48-0] VLCQZHSMCYCDJL-UHFFFAOYSA-N	9.7×10^{7} 6.1×10^{7} 8.4×10^{8} 9.7×10^{7} 1.1×10^{9} $>7.5\times10^{9}$		MacBean (2012b) Keshavarz et al. (2022) Duchowicz et al. (2020) Duchowicz et al. (2020) Maniere et al. (2011) Maniere et al. (2011)	X Q Q ? ? ?	350 185, 21 241, 570, 165 241, 573, 165
ethametsulfuron-methyl $C_{15}H_{18}N_6O_6S$ [97780-06-8] ZINJLDJMHCUBIP-UHFFFAOYSA-N	2.1×10^{9}		Ebert et al. (2023)	?	318
propoxycarbazone $C_{15}H_{18}N_4O_7S$ [145026-81-9] JTHMVYBOQLDDIY-UHFFFAOYSA-N	7.0×10^{11}		HSDB (2015)	Q	99
dimepiperate $C_{15}H_{21}NOS$ [61432-55-1] BWUPSGJXXPATLU-UHFFFAOYSA-N	2.8×10^{2}		Ebert et al. (2023)	?	318
esprocarb $C_{15}H_{23}NOS$ [85785-20-2] BXEHUCNTIZGSOJ-UHFFFAOYSA-N	1.8×10^{1} 1.5×10^{1}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
valdecoxib $C_{16}H_{14}N_2O_3S$ [181695-72-7] LNPDTQAFDNKSHK-UHFFFAOYSA-N	4.5×10^{5}		HSDB (2015)	Q	99
topramezone $C_{16}H_{17}N_3O_5S$ [210631-68-8] BPPVUXSMLBXYGG-UHFFFAOYSA-N	1.0×10^{12}		HSDB (2015)	Q	99

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

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sulfosulfuron	4.3×10^5		HSDB (2015)	V	
$C_{16}H_{18}N_6O_7S_2$	3.4×10^7		Maniere et al. (2011)	?	12, 573, 165
[141776-32-1]	1.2×10^6		Maniere et al. (2011)	?	12, 570, 165
RBSXHDIPCIWOMG-UHFFFAOYSA-N	1.1×10^8		Maniere et al. (2011)	?	12, 493, 165
orthosulfamuron $C_{16}H_{20}N_6O_6S$ [213464-77-8] UCDPMNSCCRBWIC-UHFFFAOYSA-N	1.3×10^4		HSDB (2015)	V	
cafenstrole $C_{16}H_{22}N_4O_3S$ [125306-83-4] HFEJHAAIJZXXRE-UHFFFAOYSA-N	8.0×10^5		Ebert et al. (2023)	?	318
buprofezin	2.4		Duchowicz et al. (2020)	V	186
$C_{16}H_{23}N_3OS$	2.3		HSDB (2015)	V	
[69327-76-0]	2.5×10^2		Duchowicz et al. (2020)	Q	
PRLVTUNWOQKEAI-UHFFFAOYSA-N					
bensulfuron methyl	7.0×10^{10}		Armbrust (2000)	C	
$C_{16}H_{18}N_4O_7S$	2.5×10^{12}		Maniere et al. (2011)	?	573, 165
[83055-99-6]	5.0×10^{10}		Maniere et al. (2011)	?	493, 165
XMQFTWRPUQYINF-UHFFFAOYSA-N	1.7×10^9		Maniere et al. (2011)	?	570, 165
mefenacet	2.1×10^4		Duchowicz et al. (2020)	V	186
$C_{16}H_{14}N_2O_2S$	3.4×10^4		Duchowicz et al. (2020)	Q	
[73250-68-7]					
XIGAUIHYSDTJHW-UHFFFAOYSA-N					
alanycarb	1.1×10^4		Duchowicz et al. (2020)	V	186
$C_{17}H_{25}N_3O_4S_2$	1.8×10^5		Duchowicz et al. (2020)	Q	
[83130-01-2]					
GMAUQNJOSOMMHI-JXAWBTAJSA-N					
fenamidone $C_{17}H_{17}N_3OS$ [161326-34-7] LMVPQMGRYSRMIW-KRWDZBQOSA-N	8.6×10^4		Ebert et al. (2023)	?	365
esomeprazole $C_{17}H_{19}N_3O_3S$ [119141-88-7] SUBDBMMJDZJVOS-UHFFFAOYSA-N	3.3×10^{13}		HSDB (2015)	Q	99

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
foramsulfuron $C_{17}H_{20}N_6O_7S$ [173159-57-4] PXDNXJSDGQBLKS-UHFFFAOYSA-N	1.7×10^{11} 1.7×10^{11}		HSDB (2015) Maniere et al. (2011)	V ?	 12, 165
sethoxydim $C_{17}H_{29}NO_3S$ [74051-80-2] NMHGOXYVOKDNHF-UHFFFAOYSA-N	4.5×10^{5}		HSDB (2015)	Q	99
mesosulfuron-methyl $C_{17}H_{21}N_5O_9S_2$ [208465-21-8] NIFKBBMCXCMCAO-UHFFFAOYSA-N	9.0×10^{10} 8.7×10^{12} 2.7×10^{11} 4.1×10^{9}		HSDB (2015) Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011)	V ? ? ?	 12, 573, 165 12, 493, 165 12, 570, 165
cycloxydim $C_{17}H_{27}NO_3S$ [101205-02-1] HAHCNFVGRVWFIP-VKAVYKQESA-N	1.6×10^{4}		Maniere et al. (2011)	?	12, 165
fenpyrazamine $C_{17}H_{21}N_3O_2S$ [473798-59-3] UTOHZQYBSYOOGC-UHFFFAOYSA-N	6.2×10^{3}		Maniere et al. (2011)	?	12, 165
cyprosulfamide $C_{18}H_{18}N_2O_5S$ [221667-31-8] OAWUUPVZMNKZRY-UHFFFAOYSA-N	7.0×10^{6} 9.1×10^{2} 2.9×10^{5}		Maniere et al. (2011) Maniere et al. (2011) Maniere et al. (2011)	? ? ?	241, 573, 165 241, 577, 165 241, 493, 165
rosiglitazone $C_{18}H_{19}N_3O_3S$ [122320-73-4] YASAKCUCGLMORW-UHFFFAOYSA-N	5.8×10^{8}		HSDB (2015)	Q	99
rabeprazole $C_{18}H_{21}N_3O_3S$ [117976-89-3] YREYEVIYCVEVJK-UHFFFAOYSA-N	8.2×10^{11}		HSDB (2015)	Q	99
pyributicarb $C_{18}H_{22}N_2O_2S$ [88678-67-5] VTRWMTJQBQJKQH-UHFFFAOYSA-N	4.3×10^{1}		Ebert et al. (2023)	?	318

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
furathiocarb $C_{18}H_{26}N_2O_5S$ [65907-30-4] HAWJXYBZNNRMNO-UHFFFAOYSA-N	7.6×10^{3}		HSDB (2015)	V	
lincomycin $C_{18}H_{34}N_2O_6S$ [154-21-2] OJMMVQQUTAEWLP-UHFFFAOYSA-N	3.3×10^{17}		HSDB (2015)	Q	99
pioglitazone $C_{19}H_{20}N_2O_3S$ [111025-46-8] HYAFETHFCAUJAY-UHFFFAOYSA-N	5.8×10^{6}		HSDB (2015)	Q	99
isofetamid $C_{20}H_{25}NO_3S$ [875915-78-9] WMKZDPFZIZQROT-UHFFFAOYSA-N	3.5×10^{4}		Ebert et al. (2023)	?	318
tamsulosin $C_{20}H_{28}N_2O_5S$ [106133-20-4] DRHKJLXJIQTDTD-OAHLLOKOSA-N	2.0×10^{9}		HSDB (2015)	Q	99
carbosulfan $C_{20}H_{32}N_2O_3S$ [55285-14-8] JLQUFIHWVLZVTJ-UHFFFAOYSA-N	1.9×10^{1} 1.7		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
sufentanil $C_{22}H_{30}N_2O_2S$ [56030-54-7] GGCSSNBKKAUURC-UHFFFAOYSA-N	2.4×10^{9}		HSDB (2015)	Q	99
sildenafil $C_{22}H_{30}N_6O_4S$ [139755-83-2] BNRNXUUZRGQAQC-UHFFFAOYSA-N	1.4×10^{15}		HSDB (2015)	Q	99
benfuracarb $C_{20}H_{30}N_2O_5S$ [82560-54-1] FYZBOYWSHKHDMT-UHFFFAOYSA-N	4.9×10^{2}		Ebert et al. (2023)	?	318
tirofiban $C_{22}H_{36}N_2O_5S$ [144494-65-5] COKMIXFXJJXBQG-NRFANRHFSA-N	1.3×10^{9}		HSDB (2015)	Q	99

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
vardenafil $C_{23}H_{32}N_6O_4S$ [224785-90-4] SECKRCOLJRRGGV-UHFFFAOYSA-N	5.2×10^{15}		HSDB (2015)	Q	99
taurocholic acid $C_{26}H_{45}NO_7S$ [81-24-3] WBWWGRHZICKQGZ-HZAMXZRMSA-N	1.9×10^{15}		HSDB (2015)	Q	447
dalfopristin $C_{34}H_{50}N_4O_9S$ [112362-50-2] SUYRLXYYZQTJHF-FUODUHIRSA-N	2.2×10^{24}		HSDB (2015)	Q	99
C.I. acid green 3 $C_{37}H_{37}N_2O_6S_2$ [4680-78-8] SRRJCDUOSQWHGS-UHFFFAOYSA-O	2.0×10^{23}		HSDB (2015)	Q	447
tinopal $C_{40}H_{40}N_{12}O_8S_2$ [24231-46-7] YGUMVDWOQQJBGA-VAWYXSNFSA-N	1.2×10^{38} 1.4×10^{40} 4.2×10^{26} 2.2×10^{37}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
quinupristin $C_{53}H_{67}N_9O_{10}S$ [120138-50-3] WTHRRGMBUAHGNI-UHFFFAOYSA-N	4.9×10^{22}		HSDB (2015)	Q	99
3,3,4,4,4-pentafluorobutane-1-thiol $C_4H_5F_5S$ [68140-18-1] WEILNYJKAUGBAU-UHFFFAOYSA-N	5.2×10^{-5} 1.4×10^{-3} 1.5×10^{-3} 1.2×10^{-5}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
3,3,4,4,5,5,6,6,6-nonafluoro-1-hexanethiol $C_6H_5F_9S$ [68140-20-5] GQJXVHYUQPXZOL-UHFFFAOYSA-N	1.9×10^{-6} 4.7×10^{-4} 3.1×10^{-4} 1.9×10^{-6}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
3,3,4,4,5,5,7,7,8,8,9,9,10,10,10-pentadecafluoro-1-decanethiol $C_{10}H_7F_{15}S$ [68140-21-6] ROKKEEDUUQVHFZ-UHFFFAOYSA-N	9.7×10^{-9} 6.5×10^{-6} 8.6×10^{-4} 1.3×10^{-8}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
3,3,4,4,5,5-hexafluoro-1-(3,3,4,4,5,5-hexafluorohexyldisulfanyl)hexane	1.2×10^{-7}		Zhang et al. (2010)	Q	287, 288
$C_{12}H_{14}F_{12}S_2$	9.0×10^{-6}		Zhang et al. (2010)	Q	287, 289
[118400-71-8]	1.9×10^{-2}		Zhang et al. (2010)	Q	287, 290
CIZUOSOWGOENRE-UHFFFAOYSA-N	3.5×10^{-7}		Zhang et al. (2010)	Q	287, 291
methanesulfonyl fluoride	1.6×10^{-1}		Ebert et al. (2023)	?	318
CH_3FO_2S					
[558-25-8]					
KNWQLFOXPQZGPX-UHFFFAOYSA-N					
perfluorobutane sulfonic acid	2.0		Plassmann et al. (2011)	E	
$C_4HF_9O_3S$					
(PFBS)					
[375-73-5]					
JGTNAGYHADQMCM-UHFFFAOYSA-N					
4-(pentafluorosulfanyl)phenol	4.0×10^{1}		Ebert et al. (2023)	?	371
$C_6H_5F_5OS$					
[774-94-7]					
XHJLGVIUMCBMHL-UHFFFAOYSA-N					
1H,1H,2H,2H-perfluorohexane sulfonic acid	4.5×10^{-3}		Abusallout et al. (2022)	M	
$C_6H_5F_9O_3S$					
(4:2 FTS)					
[757124-72-4]					
TXGIGTRUEITPSC-UHFFFAOYSA-N					
perfluorohexane sulfonic acid	5.1×10^{-1}		Plassmann et al. (2011)	E	
$C_6HF_{13}O_3S$					
(PFHxS)					
[355-46-4]					
QZHDEAJFRJCDMF-UHFFFAOYSA-N					
1H,1H,2H,2H-perfluorooctane sulfonic acid	2.1×10^{-3}	11000	Abusallout et al. (2022)	M	
$C_8H_5F_{13}O_3S$					
(6:2 FTS)					
[27619-97-2]					
VIONGDJUYAYOPU-UHFFFAOYSA-N					
perfluorooctane sulfonic acid	9.0×10^{-4}		Zhang et al. (2010)	Q	287, 288
$C_8HF_{17}O_3S$	8.6×10^{-3}		Zhang et al. (2010)	Q	287, 289
(PFOS)	1.6×10^{-1}		Zhang et al. (2010)	Q	287, 290
[1763-23-1]	9.9×10^{-3}		Zhang et al. (2010)	Q	287, 291
YFSUTJLHUFNCNZ-UHFFFAOYSA-N	1.0×10^{-1}		Arp et al. (2006)	Q	633
	4.6×10^{-3}		Arp et al. (2006)	Q	634

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
heptadecafluorooctanesulphonyl fluoride $C_8F_{18}O_2S$ (perfluorooctylsulfonyl fluoride) [307-35-7] BHFJBHMTEDLICO-UHFFFAOYSA-N	1.5×10^{-7}		HSDB (2015)	Q	99
1H,1H,2H,2H-perfluorodecane sulfonic acid $C_{10}H_5F_{17}O_3S$ (8:2 FTS) [39108-34-4] ALVYVCQIFHTIRD-UHFFFAOYSA-N	2.2×10^{-3}		Abusallout et al. (2022)	M	
fluticasone $C_{22}H_{27}F_3O_4S$ [90566-53-3] MGNNYOODZCAHBA-GQKYHHCASA-N	4.3×10^{3}		HSDB (2015)	Q	99
3-aminophenylsulfur pentafluoride $C_6H_6F_5NS$ [2993-22-8] NUFLICUHOXHWER-UHFFFAOYSA-N	6.4		Ebert et al. (2023)	?	371
4-aminophenylsulfur pentafluoride $C_6H_6F_5NS$ [2993-24-0] MZGZUHNSMNNSRJ-UHFFFAOYSA-N	4.0		Ebert et al. (2023)	?	371
flubenzimine $C_{17}H_{10}F_6N_4S$ [37893-02-0] IZFZCMFMJKDHJZ-UHFFFAOYSA-N	$>2.3\times10^{10}$		MacBean (2012a)	?	
thiazafluron $C_6H_7F_3N_4OS$ [25366-23-8] BBJPZPLAZVZTGR-UHFFFAOYSA-N	3.2×10^{4}		MacBean (2012a)	?	
4-nitrophenylsulfur pentafluoride $C_6H_4F_5NO_2S$ [2613-27-6] AGNCKMHGYZKMLN-UHFFFAOYSA-N	1.6×10^{-1}		Ebert et al. (2023)	?	371
undecafluoro-N-methyl-1-pentanesulfonamide	3.5×10^{-4}		Zhang et al. (2010)	Q	287, 288
$C_6H_4F_{11}NO_2S$	4.4×10^{-2}		Zhang et al. (2010)	Q	287, 289
[68298-13-5]	5.6×10^{-4}		Zhang et al. (2010)	Q	287, 290
BKKNDZBSSSAGIB-UHFFFAOYSA-N	6.2×10^{-1}		Zhang et al. (2010)	Q	287, 291

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
1,1,2,2,3,3,4,4,4-nonafluoro-N-(2-hydroxyethyl)-N-methylbutane-1-sulfonamide	1.8×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_7H_8F_9NO_3S$	1.1×10^{1}		Zhang et al. (2010)	Q	287, 289
[34454-97-2]	4.6×10^{-1}		Zhang et al. (2010)	Q	287, 290
DSRUAYIFDCHEEV-UHFFFAOYSA-N	2.7×10^{2}		Zhang et al. (2010)	Q	287, 291
tridecafluoro-N-methyl-1-hexanesulfonamide	6.7×10^{-5}		Zhang et al. (2010)	Q	287, 288
$C_7H_4F_{13}NO_2S$	9.2×10^{-3}		Zhang et al. (2010)	Q	287, 289
[68259-15-4]	2.5×10^{-4}		Zhang et al. (2010)	Q	287, 290
HPPDPHZGXWMRHN-UHFFFAOYSA-N	1.2×10^{-1}		Zhang et al. (2010)	Q	287, 291
perfluorooctane sulfonamide	5.5×10^{-6}		HSDB (2015)	Q	99
$C_8H_2F_{17}NO_2S$	3.4		Arp et al. (2006)	Q	633
(PFOSA)	7.9×10^{-6}		Arp et al. (2006)	Q	634
[754-91-6]					
RRRXPPIDPYTNJG-UHFFFAOYSA-N					
emtricitabine	9.0×10^{11}		HSDB (2015)	Q	99
$C_8H_{10}FN_3O_3S$					
[143491-57-0]					
XQSPYNMVSIKCOC-NTSWFWBYSA-N					
N-ethyl-1,1,2,2,3,3,4,4,4-nonafluoro-N-(2-hydroxyethyl)butane-1-sulfonamide	1.3×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_8H_{10}F_9NO_3S$	8.8		Zhang et al. (2010)	Q	287, 289
[34449-89-3]	1.4×10^{-1}		Zhang et al. (2010)	Q	287, 290
ZSBOIPHQFKYRMG-UHFFFAOYSA-N	2.1×10^{2}		Zhang et al. (2010)	Q	287, 291
1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-N-methylheptane-1-sulphonamide	1.3×10^{-5}		Zhang et al. (2010)	Q	287, 288
$C_8H_4NO_2F_{15}S$	1.6×10^{-3}		Zhang et al. (2010)	Q	287, 289
[68259-14-3]	1.2×10^{-4}		Zhang et al. (2010)	Q	287, 290
KDHCALLFPWZTPN-UHFFFAOYSA-N	2.4×10^{-2}		Zhang et al. (2010)	Q	287, 291
1,1,2,2,3,3,4,4,5,5,5-undecafluoro-N-(2-hydroxyethyl)-N-methylpentane-1-sulphonamide	3.4		Zhang et al. (2010)	Q	287, 288
$C_8H_8NO_3F_{11}S$	2.9		Zhang et al. (2010)	Q	287, 289
[68555-74-8]	2.1×10^{-1}		Zhang et al. (2010)	Q	287, 290
BRBCKWCOTRPYGH-UHFFFAOYSA-N	5.6×10^{1}		Zhang et al. (2010)	Q	287, 291

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-(3-(dimethylamino)propyl)- nonafluoro-1-butanesulfonamide	2.1		Zhang et al. (2010)	Q	287, 288
$C_9H_{13}F_9N_2O_2S$	3.1×10^{1}		Zhang et al. (2010)	Q	287, 289
[68555-77-1]	1.1		Zhang et al. (2010)	Q	287, 290
XMRMVBVJGSKMEN-UHFFFAOYSA-N	6.0×10^{2}		Zhang et al. (2010)	Q	287, 291
N- methylperfluorooctanesulphonamide	4.4×10^{-4}		Abusallout et al. (2022)	M	
$C_9H_4F_{17}NO_2S$	2.4×10^{-6}		Zhang et al. (2010)	Q	287, 288
(N-MeFOSA)	2.1×10^{-4}		Zhang et al. (2010)	Q	287, 289
[31506-32-8]	5.2×10^{-5}		Zhang et al. (2010)	Q	287, 290
SRMWNTGHXHOWBT-UHFFFAOYSA-N	5.0×10^{-3}		Zhang et al. (2010)	Q	287, 291
N-ethyl-1,1,2,2,3,3,4,4,5,5,5- undecafluoro-N-(2-hydroxyethyl)- 1-pentanesulfonamide	2.5		Zhang et al. (2010)	Q	287, 288
$C_9H_{10}NO_3F_{11}S$	2.3		Zhang et al. (2010)	Q	287, 289
[68555-72-6]	6.0×10^{-2}		Zhang et al. (2010)	Q	287, 290
GBPAQIZWHVCENQ-UHFFFAOYSA-N	4.1×10^{1}		Zhang et al. (2010)	Q	287, 291
1,1,2,2,3,3,4,4,5,5,6,6,6- tridecafluoro-N-(2-hydroxyethyl)- N-methyl-1-hexanesulfonamide	6.4×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_9H_8NO_3F_{13}S$	6.0×10^{-1}		Zhang et al. (2010)	Q	287, 289
[68555-75-9]	9.2×10^{-2}		Zhang et al. (2010)	Q	287, 290
UYIBZOUSVFOPJK-UHFFFAOYSA-N	9.9		Zhang et al. (2010)	Q	287, 291
N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,6- tridecafluoro-N-(2- hydroxyethyl)hexane-1- sulfonamide	4.7×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_{10}H_{10}F_{13}NO_3S$	4.6×10^{-1}		Zhang et al. (2010)	Q	287, 289
[34455-03-3]	3.1×10^{-2}		Zhang et al. (2010)	Q	287, 290
SSGYCIQAXNQIBC-UHFFFAOYSA-N	8.8		Zhang et al. (2010)	Q	287, 291
2- methyl[(nonafluorobutyl)sulfonyl] aminoethyl acrylate	5.1×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_{10}H_{10}F_9NO_4S$	5.3×10^{-1}		Zhang et al. (2010)	Q	287, 289
[67584-55-8]	8.2×10^{1}		Zhang et al. (2010)	Q	287, 290
KEMCLRGAIUJRAN-UHFFFAOYSA-N	4.8×10^{1}		Zhang et al. (2010)	Q	287, 291

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-ethylperfluorooctanesulfonamide	9.4×10^{-4}		Abusallout et al. (2022)	M	
$C_{10}H_6F_{17}NO_2S$	1.8×10^{-6}		HSDB (2015)	Q	99
(N-EtFOSA)	1.8×10^{-6}		Zhang et al. (2010)	Q	287, 288
[4151-50-2]	1.4×10^{-4}		Zhang et al. (2010)	Q	287, 289
CCEKAJIANROZEO-UHFFFAOYSA-N	9.5×10^{-6}		Zhang et al. (2010)	Q	287, 290
	3.8×10^{-3}		Zhang et al. (2010)	Q	287, 291
	6.4×10^{-3}		Arp et al. (2006)	Q	633
	7.5×10^{-3}		Arp et al. (2006)	Q	634
1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-N-(2-hydroxyethyl)-N-methylheptane-1-sulphonamide	1.2×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_{10}H_8NO_3F_{15}S$	9.5×10^{-2}		Zhang et al. (2010)	Q	287, 289
[68555-76-0]	4.5×10^{-2}		Zhang et al. (2010)	Q	287, 290
UIZUTEDYGNRNSW-UHFFFAOYSA-N	2.1		Zhang et al. (2010)	Q	287, 291
N-methyl perfluorooctane sulfonamidoethanol	2.3×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{11}H_8F_{17}NO_3S$	1.2×10^{-2}		Zhang et al. (2010)	Q	287, 289
(MeFOSE)	1.9×10^{-2}		Zhang et al. (2010)	Q	287, 290
[24448-09-7]	4.3×10^{-1}		Zhang et al. (2010)	Q	287, 291
PLGACQRCZCVKGK-UHFFFAOYSA-N	4.8×10^{-1}		Arp et al. (2006)	Q	633
	2.1×10^{-3}		Arp et al. (2006)	Q	634
N-ethyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-pentadecafluoro-N-(2-hydroxyethyl)-1-heptanesulfonamide	9.0×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{11}H_{10}NO_3F_{15}S$	7.2×10^{-2}		Zhang et al. (2010)	Q	287, 289
[68555-73-7]	1.5×10^{-2}		Zhang et al. (2010)	Q	287, 290
HINASMOVWHGCAK-UHFFFAOYSA-N	1.8		Zhang et al. (2010)	Q	287, 291
mefluidide $C_{11}H_{13}F_3N_2O_3S$ [53780-34-0] OKIBNKKYNPBDRS-UHFFFAOYSA-N	7.6×10^{5}		HSDB (2015)	Q	99
N-(3-(dimethylamino)propyl)-1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-hexanesulfonamide	7.7×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{11}H_{13}N_2O_2F_{13}S$	1.5		Zhang et al. (2010)	Q	287, 289
[50598-28-2]	2.2×10^{-1}		Zhang et al. (2010)	Q	287, 290
INDOGKYZYLAGEM-UHFFFAOYSA-N	2.5×10^{1}		Zhang et al. (2010)	Q	287, 291

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-(methyl((undecafluoropentyl) sulfonyl)amino)ethyl prop-2-enoate	9.7×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{11}H_{10}F_{11}NO_4S$	2.0×10^{-1}		Zhang et al. (2010)	Q	287, 289
[67584-56-9]	7.5×10^{1}		Zhang et al. (2010)	Q	287, 290
FZWFDJBZTLTRGH-UHFFFAOYSA-N	9.7		Zhang et al. (2010)	Q	287, 291
2-(methyl((nonafluorobutyl) sulphonyl)amino)ethyl methacrylate	3.3×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_{11}H_{12}F_9NO_4S$	5.0×10^{-1}		Zhang et al. (2010)	Q	287, 289
[67584-59-2]	1.9×10^{-1}		Zhang et al. (2010)	Q	287, 290
BEIWUHUHJDEMQO-UHFFFAOYSA-N	2.9×10^{1}		Zhang et al. (2010)	Q	287, 291
N-(3-(dimethylamino)propyl) pentadecafluoro-1-heptanesulfonamide	1.5×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{12}H_{13}F_{15}N_2O_2S$	2.3×10^{-1}		Zhang et al. (2010)	Q	287, 289
[67584-54-7]	1.8×10^{-2}		Zhang et al. (2010)	Q	287, 290
RFJQYRXZGNILIY-UHFFFAOYSA-N	5.2		Zhang et al. (2010)	Q	287, 291
acrylic acid 2-[methyl[(tridecafluorohexyl)sulfonyl] amino]ethyl ester	1.8×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{12}H_{10}F_{13}NO_4S$	6.0×10^{-2}		Zhang et al. (2010)	Q	287, 289
[67584-57-0]	3.4×10^{1}		Zhang et al. (2010)	Q	287, 290
HLKZFXXWGVPYAY-UHFFFAOYSA-N	2.0		Zhang et al. (2010)	Q	287, 291
N-ethyl perfluorooctane sulfonamidoethanol	1.7×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{12}H_{10}F_{17}NO_3S$	8.6×10^{-3}		Zhang et al. (2010)	Q	287, 289
(EtFOSE)	6.2×10^{-3}		Zhang et al. (2010)	Q	287, 290
[1691-99-2]	3.3×10^{-1}		Zhang et al. (2010)	Q	287, 291
HUFHNYZNTFSKCT-UHFFFAOYSA-N	5.7×10^{-2}		Arp et al. (2006)	Q	633
	1.2×10^{-3}		Arp et al. (2006)	Q	634
flumetsulam $C_{12}H_9F_2N_5O_2S$ [98967-40-9] RXCPQSJAVKGONC-UHFFFAOYSA-N	1.5×10^{11}		Ebert et al. (2023)	?	316
florasulam	1.7×10^{6}		HSDB (2015)	V	
$C_{12}H_8F_3N_5O_3S$	2.3×10^{6}		Maniere et al. (2011)	?	12, 493, 165
[145701-23-1]	3.4×10^{7}		Maniere et al. (2011)	?	12, 573, 165
QZXATCCPQKOEIH-UHFFFAOYSA-N	3.0×10^{4}		Maniere et al. (2011)	?	12, 570, 165

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-(methyl((pentadecafluoroheptyl) sulphonyl)amino)ethyl acrylate	3.5×10^{-3}		Zhang et al. (2010)	Q	287, 288
$C_{13}H_{10}F_{15}NO_4S$	1.5×10^{-2}		Zhang et al. (2010)	Q	287, 289
[68084-62-8]	9.9		Zhang et al. (2010)	Q	287, 290
BEYGZFVOTUDDJK-UHFFFAOYSA-N	4.2×10^{-1}		Zhang et al. (2010)	Q	287, 291
flazasulfuron	1.6×10^{6}		HSDB (2015)	Q	99
$C_{13}H_{12}F_3N_5O_5S$	$>3.9\times10^{5}$		Maniere et al. (2011)	?	165
[104040-78-0]					
HWATZEJQIXKWQS-UHFFFAOYSA-N					
tritosulfuron	$>1.0\times10^{4}$		Maniere et al. (2011)	?	12, 165
$C_{13}H_9F_6N_5O_4S$					
[142469-14-5]					
KVEQCVKVIFQSGC-UHFFFAOYSA-N					
pyroxsulam	1.4×10^{6}		Maniere et al. (2011)	?	241, 165
$C_{14}H_{13}F_3N_6O_5S$					
[422556-08-9]					
GLBLPMUBLHYFCW-UHFFFAOYSA-N					
N-methyl perfluorooctane sulfonamidoethylacrylate	4.4×10^{-2}		Arp et al. (2006)	Q	633
$C_{14}H_{10}F_{17}NO_4S$	2.2×10^{-3}		Arp et al. (2006)	Q	634
(MeFOSEA)					
[25268-77-3]					
RTJZWOGSCLVJLD-UHFFFAOYSA-N					
pyrasulfotole	7.0×10^{8}		HSDB (2015)	V	
$C_{14}H_{13}F_3N_2O_4S$					
[365400-11-9]					
CZRVDACSCJKRFL-UHFFFAOYSA-N					
triafamone	8.2×10^{3}		Ebert et al. (2023)	?	318
$C_{14}H_{13}F_3N_4O_5S$					
[874195-61-6]					
GBHVIWKSEHWFDD-UHFFFAOYSA-N					
flufenacet	1.7×10^{3}		HSDB (2015)	V	
$C_{14}H_{13}F_4N_3O_2S$	1.1×10^{3}		Maniere et al. (2011)	?	12, 165
[142459-58-3]					
IANUJLZYFUDJIH-UHFFFAOYSA-N					

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
N-butyl-1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-N-(2-hydroxyethyl)-1-octanesulfonamide	9.7×10^{-3}		Zhang et al. (2010)	Q	287, 288
$C_{14}H_{14}F_{17}NO_3S$	4.1×10^{-3}		Zhang et al. (2010)	Q	287, 289
[2263-09-4]	3.8×10^{-2}		Zhang et al. (2010)	Q	287, 290
AQWROZBAYZBWIH-UHFFFAOYSA-N	2.2×10^{-1}		Zhang et al. (2010)	Q	287, 291
ethyl N-ethyl-N-[(heptadecafluorooctyl) sulphonyl]glycinate	1.3×10^{-5}		Zhang et al. (2010)	Q	287, 288
$C_{14}H_{12}NO_4F_{17}S$	1.8×10^{-3}		Zhang et al. (2010)	Q	287, 289
[1869-77-8]	4.3		Zhang et al. (2010)	Q	287, 290
LMUUXHHNCDERBQ-UHFFFAOYSA-N	3.0×10^{-2}		Zhang et al. (2010)	Q	287, 291
perfluidone	1.3×10^{2}		Duchowicz et al. (2020)	V	186
$C_{14}H_{12}F_3NO_4S_2$	1.6×10^{8}		Duchowicz et al. (2020)	Q	
[37924-13-3]					
WHTBVLXUSXVMEV-UHFFFAOYSA-N					
2-(((heptadecafluorooctyl)sulfonyl) methylamino)ethyl methacrylate	4.2×10^{-4}		Zhang et al. (2010)	Q	287, 288
$C_{15}H_{12}F_{17}NO_4S$	3.3×10^{-3}		Zhang et al. (2010)	Q	287, 289
[14650-24-9]	2.5		Zhang et al. (2010)	Q	287, 290
UZMOXNBUTMPDCX-UHFFFAOYSA-N	5.4×10^{-2}		Zhang et al. (2010)	Q	287, 291
2-(N-ethylperfluorooctane-sulfonamido)ethyl acrylate	1.1		Ebert et al. (2023)	?	371
$C_{15}H_{12}F_{17}NO_4S$					
[423-82-5]					
ZAZJGBCGMUKZEL-UHFFFAOYSA-N					
isoxaflutole	5.3×10^{4}		MacBean (2012b)	X	350
$C_{15}H_{12}F_3NO_4S$	5.3×10^{4}		Maniere et al. (2011)	?	12, 165
[141112-29-0]					
OYIKARCXOQLFHF-UHFFFAOYSA-N					
primisulfuron-methyl	7.0×10^{6}		HSDB (2015)	Q	99
$C_{15}H_{12}F_4N_4O_7S$					
[86209-51-0]					
ZTYVMAQSHCZXLF-UHFFFAOYSA-N					
dithiopyr	6.5		Ebert et al. (2023)	?	739
$C_{15}H_{16}F_5NO_2S_2$					
[97886-45-8]					
YUBJPYNSGLJZPQ-UHFFFAOYSA-N					

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
penoxsulam	9.0×10^{12}		HSDB (2015)	V	
$C_{16}H_{14}F_5N_5O_5S$	1.2×10^{14}		Maniere et al. (2011)	?	241, 573, 165
[219714-96-2]	4.7×10^{11}		Maniere et al. (2011)	?	241, 570, 165
SYJGKVOENHZYMQ-UHFFFAOYSA-N	3.4×10^{13}		Maniere et al. (2011)	?	241, 493, 165
pantoprazole $C_{16}H_{15}F_2N_3O_4S$ [102625-70-7] IQPSEEYGBUAQFF-UHFFFAOYSA-N	1.7×10^{14}		HSDB (2015)	Q	99
2-(N-ethylperfluorooctanesulfamido)ethyl methacrylate	3.2×10^{-4}		Zhang et al. (2010)	Q	287, 288
$C_{16}H_{14}F_{17}NO_4S$	3.9×10^{-3}		Zhang et al. (2010)	Q	287, 289
[376-14-7]	1.5		Zhang et al. (2010)	Q	287, 290
DBCGADAHIXJHCE-UHFFFAOYSA-N	4.1×10^{-2}		Zhang et al. (2010)	Q	287, 291
thiazopyr	2.1×10^{1}		Duchowicz et al. (2020)	V	186
$C_{16}H_{17}F_5N_2O_2S$	2.1×10^{1}		HSDB (2015)	V	
[117718-60-2]	8.7×10^{3}		Duchowicz et al. (2020)	Q	
YIJZJEYQBAAWRJ-UHFFFAOYSA-N					
penthiopyrad	7.1×10^{3}		Maniere et al. (2011)	?	12, 570, 165
$C_{16}H_{20}F_3N_3OS$	1.3×10^{2}		Maniere et al. (2011)	?	12, 493, 165
[183675-82-3]	2.4×10^{3}		Maniere et al. (2011)	?	12, 577, 165
PFFIDZXUXFLSSR-UHFFFAOYSA-N	1.6×10^{2}		Maniere et al. (2011)	?	12, 572, 165
triflusulfuron-methyl	$>4.2\times10^{2}$		Maniere et al. (2011)	?	241, 577, 165
$C_{17}H_{19}F_3N_6O_6S$ [126535-15-7] IMEVJVISCHQJRM-UHFFFAOYSA-N					
celecoxib $C_{17}H_{14}F_3N_3O_2S$ [169590-42-5] RZEKVGVHFLEQIL-UHFFFAOYSA-N	1.3×10^{7}		HSDB (2015)	Q	99

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
2-(butyl((heptadecafluorooctyl) sulfonyl)amino)ethyl acrylate	2.9×10^{-4}		Zhang et al. (2010)	Q	287, 288
$C_{17}H_{16}F_{17}NO_4S$	4.1×10^{-3}		Zhang et al. (2010)	Q	287, 289
[383-07-3]	1.8		Zhang et al. (2010)	Q	287, 290
AQQNNAXBGPWALO-UHFFFAOYSA-N	4.3×10^{-2}		Zhang et al. (2010)	Q	287, 291
thidiazimin	3.5×10^{8}		MacBean (2012a)	?	
$C_{18}H_{17}N_4O_2FS$					
[123249-43-4]					
HZKBYBNLTLVSPX-JZJYNLBNSA-N					
benthiavalicarb isopropyl	1.1×10^{2}		MacBean (2012b)	X	350
$C_{18}H_{24}FN_3O_3S$	$>1.1\times10^{2}$		Maniere et al. (2011)	?	12, 165
[177406-68-7]					
USRKFGIXLGKMKU-IAQYHMDHSA-N					
flutianil	7.2×10^{1}		Ebert et al. (2023)	?	318
$C_{19}H_{14}F_4N_2OS_2$					
[958647-10-4]					
KGXUEPOHGFWQKF-ZCXUNETKSA-N					
rosuvastatin	2.9×10^{14}		HSDB (2015)	Q	99
$C_{22}H_{28}N_3O_6FS$					
[287714-41-4]					
BPRHUIZQVSMCRT-YXWZHEERSA-N					
oxathiapiprolin	2.8×10^{2}		Maniere et al. (2011)	?	12, 165
$C_{24}H_{22}F_5N_5O_2S$					
[1003318-67-9]					
IAQLCKZJGNTRDO-UHFFFAOYSA-N					
trichloromethanesulfenyl chloride	4.1×10^{-2}		Zhang et al. (2010)	Q	287, 288
CCl_4S	6.9×10^{-4}		Zhang et al. (2010)	Q	287, 289
[594-42-3]	9.5×10^{-4}		Zhang et al. (2010)	Q	287, 290
RYFZYYUIAZYQLC-UHFFFAOYSA-N	5.3×10^{-3}		Zhang et al. (2010)	Q	287, 291
1,1,2,2-tetrachloroethanesulfenyl chloride	8.8×10^{-2}		Zhang et al. (2010)	Q	287, 288
C_2HCl_5S	3.7×10^{-3}		Zhang et al. (2010)	Q	287, 289
[1185-09-7]	1.9×10^{-2}		Zhang et al. (2010)	Q	287, 290
LCVOCDOSGJHZFH-UHFFFAOYSA-N	6.7×10^{-2}		Zhang et al. (2010)	Q	287, 291
2-chloroethyl methyl sulfide	5.3×10^{-2}		Bartelt-Hunt et al. (2008)	?	21
C_3H_7ClS					
[542-81-4]					
MYFKLQFBFSHBPA-UHFFFAOYSA-N					

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
2-chloroethyl ethyl sulfide C_4H_9ClS [693-07-2] GBNVXYXIRHSYEG-UHFFFAOYSA-N	2.0×10^{-2} 2.7×10^{-2}		HSDB (2015) Bartelt-Hunt et al. (2008)	Q ?	99 21
2,2'-dichlorodiethylsulfide $(ClCH_2CH_2)_2S$ (mustard gas) [505-60-2] QKSKPIVNLNLAAV-UHFFFAOYSA-N	3.0×10^{-1} 2.2×10^{-2} 1.5×10^{-1} 1.6×10^{-1} 4.0×10^{-1} 4.1×10^{-1} 4.1×10^{-1}		Hine and Mookerjee (1975) Keshavarz et al. (2022) Duchowicz et al. (2020) Modarresi et al. (2007) Duchowicz et al. (2020) Bartelt-Hunt et al. (2008) Opresko et al. (1998)	V Q Q Q ? ? ?	 299 67 185, 21 21
1,2-bis(2-chloroethylthio)ethane $C_6H_{12}Cl_2S_2$ (sesquimustard) [3563-36-8] AMGNHZVUZWILSB-UHFFFAOYSA-N	8.8×10^{1}		Ebert et al. (2023)	?	318
pentachlorobenzenethiol C_6HCl_5S [133-49-3] LLMLGZUZTFMXSA-UHFFFAOYSA-N	6.6×10^{-2} 8.4×10^{-2} 2.7×10^{-2} 1.3 2.2×10^{-2}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	99 287, 288 287, 289 287, 290 287, 291
chloroethyl phenyl sulfide C_8H_9ClS [5535-49-9] QDXIHHOPZFCEAP-UHFFFAOYSA-N	1.3×10^{-1}		Bartelt-Hunt et al. (2008)	?	21
tetrasul $C_{12}H_6Cl_4S$ [2227-13-6] QUWSDLYBOVGOCW-UHFFFAOYSA-N	9.3×10^{-1}		MacBean (2012a)	?	
methanesulfonyl chloride CH_3ClO_2S [124-63-0] QARBMVPHQWIHKH-UHFFFAOYSA-N	2.2×10^{-1}		HSDB (2015)	Q	99
bis(trichloromethyl)sulfone $C_2Cl_6O_2S$ [3064-70-8] YBNLWIZAWPBUKQ-UHFFFAOYSA-N	8.2×10^{2} 8.2×10^{2} 1.2×10^{-2} 3.1×10^{3} 1.0×10^{1}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	99 287, 288 287, 289 287, 290 287, 291
benzenesulfonyl chloride $C_6H_5ClO_2S$ [98-09-9] CSKNSYBAZOQPLR-UHFFFAOYSA-N	1.1 1.7×10^{1} 6.7 1.6×10^{2}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
4-methylbenzenesulfonyl chloride	1.0		Zhang et al. (2010)	Q	287, 288
$C_7H_7ClO_2S$	1.8×10^{1}		Zhang et al. (2010)	Q	287, 289
[98-59-9]	1.2×10^{1}		Zhang et al. (2010)	Q	287, 290
YYROPELSRYBVMQ-UHFFFAOYSA-N	9.2×10^{1}		Zhang et al. (2010)	Q	287, 291
endosulfan	9.4×10^{-1}		Mackay et al. (2006d)	V	
$C_9H_6Cl_6O_3S$	1.1×10^{2}		Zhang et al. (2010)	Q	287, 288
[115-29-7]	2.4×10^{1}		Zhang et al. (2010)	Q	287, 289
RDYMFSUJUZBWLH-UHFFFAOYSA-N	1.1×10^{2}		Zhang et al. (2010)	Q	287, 290
	2.3×10^{8}		Zhang et al. (2010)	Q	287, 291
	3.1×10^{1}		Hilal et al. (2008)	Q	
	7.8×10^{-1}		Modarresi et al. (2007)	Q	67
α-endosulfan	1.4		Shen and Wania (2005)	L	366
$C_9H_6Cl_6O_3S$	1.4		Shen and Wania (2005)	L	367
(endosulfan I)	1.4		Muir et al. (2004)	L	367
[959-98-8]	1.4		Muir et al. (2004)	L	366
RDYMFSUJUZBWLH-AMHWMVONSA-N	1.2		Chao et al. (2017)	M	
	1.3	4200	Cetin et al. (2006)	M	
	1.4		Altschuh et al. (1999)	M	
	1.5×10^{-1}		Rice et al. (1997b)	M	12
	1.3×10^{-1}	2300	Rice et al. (1997a)	M	
	1.5		Cotham and Bidleman (1989)	V	
	3.4×10^{-1}		Suntio et al. (1988)	V	12
	9.2×10^{-1}		Suntio et al. (1988)	C	
	9.6×10^{-2}		Keshavarz et al. (2022)	Q	
	5.2×10^{1}		Duchowicz et al. (2020)	Q	
	8.0×10^{-1}		Modarresi et al. (2007)	Q	67
		3200	Kühne et al. (2005)	Q	
	1.4		Duchowicz et al. (2020)	?	185, 21
		2300	Kühne et al. (2005)	?	
β-endosulfan	2.5×10^{1}		Shen and Wania (2005)	L	366
$C_9H_6Cl_6O_3S$	2.2×10^{1}		Shen and Wania (2005)	L	367
(endosulfan II)	6.4		Chao et al. (2017)	M	
[33213-65-9]	1.9×10^{1}	3700	Cetin et al. (2006)	M	
RDYMFSUJUZBWLH-MDBBVBRHSA-N	2.5		Altschuh et al. (1999)	M	
	1.1		Rice et al. (1997b)	M	12
	1.1		Rice et al. (1997a)	M	12
	1.6×10^{1}		Cotham and Bidleman (1989)	V	
	1.6×10^{3}		Keshavarz et al. (2022)	Q	
	5.2×10^{1}		Duchowicz et al. (2020)	Q	184
	3.1×10^{1}		Hilal et al. (2008)	Q	
	8.0×10^{-1}		Modarresi et al. (2007)	Q	67
	2.5×10^{1}		Duchowicz et al. (2020)	?	185, 21

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
endosulfan sulfate $C_9H_6Cl_6O_4S$ [1031-07-8] AAPVQEMYVNZIOO-UHFFFAOYSA-N	8.2×10^{5}		HSDB (2015)	V	
mcpa-thioethyl $C_{11}H_{13}ClO_2S$ [25319-90-8] AZFKQCNGMSSWDS-UHFFFAOYSA-N	4.5×10^{-1}		Mackay et al. (2006d)	V	
1,1'-sulfonylbis(4-chlorobenzene) $C_{12}H_8Cl_2O_2S$ [80-07-9] GPAPPPVRLPGFEQ-UHFFFAOYSA-N	7.0×10^{1} 7.2×10^{1} 6.5×10^{3} 5.0×10^{4} 3.1×10^{3}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	99 287, 288 287, 289 287, 290 287, 291
2,2'-thiobis-4,6-dichlorophenol $C_{12}H_6Cl_4O_2S$ (bithionol) [97-18-7] JFIOVJDNOJYLKP-UHFFFAOYSA-N	1.1×10^{5}		Ebert et al. (2023)	?	318
1,2,4-trichloro-5-[(4-chlorophenyl)sulfonyl]benzene $C_{12}H_6Cl_4O_2S$ (tetradifon) [116-29-0] MLGCXEBRWGEOQX-UHFFFAOYSA-N	6.9×10^{3} 6.9×10^{3} 1.0×10^{3}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
ovex $C_{12}H_8Cl_2O_3S$ (chlorfenson) [80-33-1] RZXLPPRPEOUENN-UHFFFAOYSA-N	6.2×10^{1}		HSDB (2015)	Q	99
sulphenone $C_{12}H_9ClO_2S$ [80-00-2] OFCFYWOKHPOXKF-UHFFFAOYSA-N	5.2×10^{1}		HSDB (2015)	Q	99
sulcotrione $C_{14}H_{13}ClO_5S$ [99105-77-8] PQTBTIFWAXVEPB-UHFFFAOYSA-N	1.7×10^{6}		Maniere et al. (2011)	?	12, 816, 165
aramite $C_{15}H_{23}ClO_4S$ [140-57-8] YKFRAOGHWKADFJ-UHFFFAOYSA-N	5.2×10^{1}		HSDB (2015)	Q	99

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
6-chloro-2-(6-chloro-4-methyl-3-oxobenzo[b]thien-2(3H)-ylidene)-4-methylbenzo[b]thiophene-3(2H)-one	3.2×10^{7}		Zhang et al. (2010)	Q	287, 288
$C_{18}H_{10}Cl_2O_2S_2$	1.2×10^{7}		Zhang et al. (2010)	Q	287, 289
[2379-74-0]	5.4×10^{4}		Zhang et al. (2010)	Q	287, 290
NDDLLTAIKYHPOD-ISLYRVAYSA-N	2.4×10^{6}		Zhang et al. (2010)	Q	287, 291
5-chloro-3-(trichloromethyl)-1,2,4-thiadiazole	1.6×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_3Cl_4N_2S$	1.9×10^{1}		Zhang et al. (2010)	Q	287, 289
[5848-93-1]	7.3×10^{-1}		Zhang et al. (2010)	Q	287, 290
MARKPJMFLDWCID-UHFFFAOYSA-N	4.2×10^{-1}		Zhang et al. (2010)	Q	287, 291
2,4-dichloro-6-(methylthio)-1,3,5-triazine	1.3×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_4H_3Cl_2N_3S$	1.3×10^{1}		Zhang et al. (2010)	Q	287, 289
[13705-05-0]	9.7×10^{-1}		Zhang et al. (2010)	Q	287, 290
MWPZLWRHHPWTFS-UHFFFAOYSA-N	1.7×10^{1}		Zhang et al. (2010)	Q	287, 291
chlorthiamid $C_7H_5Cl_2NS$ [1918-13-4] KGKGSIUWJCAFPX-UHFFFAOYSA-N	3.5×10^{4}		MacBean (2012a)	?	
(2-chlorophenyl)thiourea $C_7H_7ClN_2S$ [5344-82-1] YZUKKTCDYSIWKJ-UHFFFAOYSA-N	$>9.9\times10^{1}$		HSDB (2015)	Q	545
2-chloroallyl-N,N-diethyldithiocarbamate	1.5		Duchowicz et al. (2020)	V	186
$C_8H_{14}ClNS_2$	1.5		HSDB (2015)	V	
[95-06-7]	2.1×10^{2}		Duchowicz et al. (2020)	Q	
XJCLWVXTCRQIDI-UHFFFAOYSA-N	2.1×10^{1}		Hilal et al. (2008)	Q	
	4.1		Modarresi et al. (2007)	Q	67
thiacloprid	9.0×10^{8}		HSDB (2015)	V	
$C_{10}H_9ClN_4S$	2.1×10^{9}		Maniere et al. (2011)	?	241, 165
[111988-49-9]					
HOKKPVIRMVDYPB-UHFFFAOYSA-N					
chloromethiuron $C_{10}H_{13}N_2ClS$ [28217-97-2] IBZZDPVVVSNQOY-UHFFFAOYSA-N	2.0×10^{5}		MacBean (2012a)	?	
imibenconazole	4.9×10^{4}		Duchowicz et al. (2020)	V	186
$C_{17}H_{13}Cl_3N_4S$	6.8×10^{3}		Duchowicz et al. (2020)	Q	
[86598-92-7]					
AGKSTYPVMZODRV-UHFFFAOYSA-N					

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
etridiazole	3.6×10^{1}		Duchowicz et al. (2020)	V	186
$C_5H_5Cl_3N_2OS$	3.3×10^{-1}		HSDB (2015)	V	
[2593-15-9]	1.6×10^{1}		Mackay et al. (2006d)	V	
KQTVWCSONPJJPE-UHFFFAOYSA-N	5.3×10^{1}		Duchowicz et al. (2020)	Q	
4-chloro-3-nitrobenzenesulfonamide	8.2×10^{3}		HSDB (2015)	Q	99
$C_6H_5ClN_2O_4S$					
[97-09-6]					
SPZGXONNVLTQDE-UHFFFAOYSA-N					
clothianidin	3.4×10^{10}		MacBean (2012b)	X	350
$C_6H_8ClN_5O_2S$	3.4×10^{10}		Maniere et al. (2011)	?	12, 165
[210880-92-5]					
PGOOBECODWQEAB-UHFFFAOYSA-N					
chlobenthiazone	1.3		MacBean (2012a)	?	
C_8H_6NOClS					
[63755-05-5]					
QCPASDYEQAVIJF-UHFFFAOYSA-N					
prothiocarb hydrochloride	2.5×10^{9}		MacBean (2012a)	?	
$C_8H_{19}ClN_2OS$					
[19622-19-6]					
NMFAMPYSJHIYMR-UHFFFAOYSA-N					
thicyofen	$>2.3\times10^{10}$		MacBean (2012a)	?	
$C_8H_5N_2OClS_2$					
[116170-30-0]					
GNOOAFGERMHQJE-UHFFFAOYSA-N					
thiamethoxam	2.1×10^{9}		HSDB (2015)	V	
$C_8H_{10}ClN_5O_3S$	2.1×10^{9}		Maniere et al. (2011)	?	165
[153719-23-4]					
NWWZPOKUUAIXIW-DHZHZOJOSA-N					
4-amino-3,5-dichloro-N-ethyl-2-methylbenzenesulfonamide	3.8×10^{4}		Zhang et al. (2010)	Q	287, 288
$C_9H_{12}Cl_2N_2O_2S$	1.1×10^{4}		Zhang et al. (2010)	Q	287, 289
[151574-12-8]	1.2×10^{6}		Zhang et al. (2010)	Q	287, 290
SBBHTEMLRJJIGK-UHFFFAOYSA-N	1.5×10^{7}		Zhang et al. (2010)	Q	287, 291
dichlofluanid	2.6×10^{2}		Duchowicz et al. (2020)	V	186
$C_9H_{11}Cl_2FN_2O_2S_2$	1.9×10^{2}		Mackay et al. (2006d)	V	
[1085-98-9]	2.5×10^{4}		Siebers and Mattusch (1996)	V	12
WURGXGVFSMYFCG-UHFFFAOYSA-N	5.7×10^{2}		Duchowicz et al. (2020)	Q	
	1.5×10^{1}		HSDB (2015)	Q	99

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
captan	1.4×10^{3}		HSDB (2015)	V	
$C_9H_8Cl_3NO_2S$	1.5×10^{3}		Mackay et al. (2006d)	V	
[133-06-2]	1.7		Suntio et al. (1988)	V	12
LDVVMCZRFWMZSG-UHFFFAOYSA-N	1.6×10^{-2}		Barcelo and Hennion (1997)	X	567
	2.1×10^{-3}		Goodarzi et al. (2010)	Q	568, 571
	3.3×10^{3}		Maniere et al. (2011)	?	12, 570, 165
	5.0×10^{3}		Maniere et al. (2011)	?	12, 493, 165
benazolin	4.2×10^{6}		Ebert et al. (2023)	?	316
$C_9H_6ClNO_3S$					
[3813-05-6]					
HYJSGOXICXYZGS-UHFFFAOYSA-N					
folpet	1.3×10^{2}		Duchowicz et al. (2020)	V	186
$C_9H_4Cl_3NO_2S$	1.3×10^{2}		HSDB (2015)	V	
[133-07-3]	2.6		Mackay et al. (2006d)	V	
HKIOYBQGHSTUDB-UHFFFAOYSA-N	2.6×10^{-2}		Barcelo and Hennion (1997)	X	567
	1.9×10^{1}		Duchowicz et al. (2020)	Q	
	1.2×10^{-1}		Goodarzi et al. (2010)	Q	568
	1.2×10^{2}		Maniere et al. (2011)	?	165
captafol	2.0×10^{3}		Duchowicz et al. (2020)	V	186
$C_{10}H_9Cl_4NO_2S$	3.7×10^{3}		HSDB (2015)	V	
(difolatan)	3.7×10^{1}		Duchowicz et al. (2020)	Q	
[2425-06-1]					
JHRWWRDRBPCWTF-UHFFFAOYSA-N					
diallate	2.6		HSDB (2015)	V	
$C_{10}H_{17}Cl_2NOS$	9.3		Mackay et al. (2006d)	V	
(avadex)	4.0		Suntio et al. (1988)	V	12
[2303-16-4]	2.6		MacBean (2012a)	?	
SPANOECCGNXGNR-UITAMQMPSA-N					
triallate	8.2×10^{-1}		HSDB (2015)	V	
$C_{10}H_{16}Cl_3NOS$	8.8×10^{-1}		Mackay et al. (2006d)	V	
[2303-17-5]	9.8×10^{-1}		Suntio et al. (1988)	V	12
MWBPRDONLNQCFV-UHFFFAOYSA-N	1.0×10^{-2}		Barcelo and Hennion (1997)	X	567
	1.6×10^{-2}		Goodarzi et al. (2010)	Q	568
	1.1		Maniere et al. (2011)	?	12, 165
tolylfluanid	1.3×10^{1}		Duchowicz et al. (2020)	V	186
$C_{10}H_{13}Cl_2FN_2O_2S_2$	1.3×10^{1}		HSDB (2015)	V	
[731-27-1]	1.6×10^{2}		Mackay et al. (2006d)	V	
HYVWIQDYBVKITD-UHFFFAOYSA-N	3.7×10^{2}		Duchowicz et al. (2020)	Q	

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tiadinil $C_{11}H_{10}ClN_3OS$ [223580-51-6] VJQYLJSMBWXGDV-UHFFFAOYSA-N	5.3×10^{4}		Ebert et al. (2023)	?	318
benazolin-ethyl $C_{11}H_{10}NO_3ClS$ [25059-80-7] WQRCEBAZAUAUQC-UHFFFAOYSA-N	4.7×10^{2} 5.2×10^{3}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
orbencarb $C_{12}H_{16}ClNOS$ [34622-58-7] LLLFASISUZUJEQ-UHFFFAOYSA-N	2.0×10^{1}		Ebert et al. (2023)	?	318
S-(4-chlorobenzyl) diethylthiocarbamate $C_{12}H_{16}ClNOS$ (thiobencarb) [28249-77-6] QHTQREMOGMZHJV-UHFFFAOYSA-N	1.9×10^{1} 4.9 3.7×10^{1} 5.8×10^{1} 3.7×10^{1}		Watanabe (1993) Kawamoto and Urano (1989) HSDB (2015) Woodrow et al. (1990) Armbrust (2000) Mackay et al. (2006d)	M M V V C W	 12 817
furosemide $C_{12}H_{11}ClN_2O_5S$ [54-31-9] ZZUFCTLCJUWOSV-UHFFFAOYSA-N	2.5×10^{10}		HSDB (2015)	Q	99
chlorsulfuron $C_{12}H_{12}ClN_5O_4S$ [64902-72-3] VJYIFXVZLXQVHO-UHFFFAOYSA-N	3.2×10^{4} 1.5×10^{5} 2.9×10^{10}		Mackay et al. (2006d) Armbrust (2000) Maniere et al. (2011)	V C ?	 241, 165
phosalone $C_{12}H_{15}ClNO_4S_2$ [2310-17-0] IOUNQDKNJZEDEP-UHFFFAOYSA-N	2.5×10^{1}		HSDB (2015)	Q	99
dimethenamid $C_{12}H_{18}ClNO_2S$ [87674-68-8] JLYFCTQDENRSOL-UHFFFAOYSA-N	8.9×10^{2} 4.7 4.5×10^{2} 2.3×10^{2} 1.2×10^{2}		Keshavarz et al. (2022) Duchowicz et al. (2020) Hilal et al. (2008) Modarresi et al. (2007) Duchowicz et al. (2020)	Q Q Q Q ?	 67 185, 21
dimethenamid-p $C_{12}H_{18}ClNO_2S$ [163515-14-8] JLYFCTQDENRSOL-VIFPVBQESA-N	2.1×10^{3} 2.1×10^{3}		MacBean (2012b) Maniere et al. (2011)	X ?	350 165

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

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cyazofamid $C_{13}H_{13}ClN_4O_2S$ [120116-88-3] YXKMMRDKEKCERS-UHFFFAOYSA-N	2.5×10^{1} $>2.5\times10^{1}$		HSDB (2015) Maniere et al. (2011)	V ?	 241, 165
metosulam $C_{14}H_{13}Cl_2N_5O_4S$ [139528-85-1] VGHPMIFEKOFHHQ-UHFFFAOYSA-N	1.2×10^{12}		Maniere et al. (2011)	?	12, 165
prothioconazole $C_{14}H_{15}Cl_2N_3OS$ [178928-70-6] MNHVNIJQQRJYDH-UHFFFAOYSA-N	2.2×10^{4} $>3.3\times10^{4}$		HSDB (2015) Maniere et al. (2011)	V ?	 12, 165
triasulfuron $C_{14}H_{16}ClN_5O_5S$ [82097-50-5] XOPFESVZMSQIKC-UHFFFAOYSA-N	8.0×10^{8}		Ebert et al. (2023)	?	316
chlorimuron-ethyl $C_{15}H_{15}ClN_4O_6S$ [90982-32-4] NSWAMPCUPHPTTC-UHFFFAOYSA-N	5.5×10^{9}		HSDB (2015)	V	
clopidogrel $C_{16}H_{16}ClNO_2S$ [113665-84-2] GKTWGGQPFAXNFI-HNNXBMFYSA-N	4.5×10^{3}		HSDB (2015)	Q	99
thenylchlor $C_{16}H_{18}ClNO_2S$ [96491-05-3] KDWQYMVPYJGPHS-UHFFFAOYSA-N	1.2×10^{3} 6.3×10^{1}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
chlorpromazine $C_{17}H_{19}ClN_2S$ [50-53-3] ZPEIMTDSQAKGNT-UHFFFAOYSA-N	6.5×10^{4}		Ebert et al. (2023)	?	316
hexythiazox $C_{17}H_{21}N_2O_2ClS$ [78587-05-0] XGWIJUOSCAQSSV-XHDPSFHLSA-N	4.2×10^{2} 8.4×10^{1}		HSDB (2015) Maniere et al. (2011)	V ?	 12, 165
clethodim $C_{17}H_{26}ClNO_3S$ [99129-21-2] INNPZTGYZSAJFN-ZTVUPKSFSA-N	8.2×10^{5} 7.1×10^{6}		HSDB (2015) Maniere et al. (2011)	Q ?	99 12, 165

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
clindamycin $C_{18}H_{33}N_2O_5ClS$ [18323-44-9] KDLRVYVGXIQJDK-AWPVFWJPSA-N	3.4×10^{16}		HSDB (2015)	Q	99
pyridate $C_{19}H_{23}ClN_2O_2S$ [55512-33-9] JTZCTMAVMHRNTR-UHFFFAOYSA-N	3.0×10^{2} 4.9 8.3×10^{3}		Barcelo and Hennion (1997) Goodarzi et al. (2010) Maniere et al. (2011)	X Q ?	567 568 12, 165
vismodegib $C_{19}H_{14}Cl_2N_2O_3S$ [879085-55-9] BPQMGSKTAYIVFO-UHFFFAOYSA-N	6.2×10^{11}		HSDB (2015)	Q	99
pyridaben $C_{19}H_{25}ClN_2OS$ [96489-71-3] DWFZBUWUXWZWKD-UHFFFAOYSA-N	2.1×10^{-1}		HSDB (2015)	V	
tembotrione $C_{17}H_{16}ClF_3O_6S$ [335104-84-2] IUQAXCIUEPFPSF-UHFFFAOYSA-N	5.8×10^{9} 5.8×10^{9}		HSDB (2015) Maniere et al. (2011)	V ?	 12, 165
fluensulfone $C_7H_5ClF_3NO_2S_2$ [318290-98-1] XSNMWAPKHUGZGQ-UHFFFAOYSA-N	6.1×10^{1}		Ebert et al. (2023)	?	318
fluothiuron $C_{10}H_{10}Cl_2F_2N_2OS$ [33439-45-1] YFEUKKUPOVGUIW-UHFFFAOYSA-N	$>2.3\times10^{10}$		MacBean (2012a)	?	
sulfentrazone $C_{11}H_{10}Cl_2F_2N_4O_3S$ [122836-35-5] OORLZFUTLGXMEF-UHFFFAOYSA-N	1.5×10^{7} 1.5×10^{7} 3.7×10^{8}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
flurazole $C_{12}H_7NO_2ClF_3S$ [72850-64-7] MKQSWTQPLLCSOB-UHFFFAOYSA-N	4.0×10^{1} 1.2×10^{2} 4.0×10^{1}		Duchowicz et al. (2020) Duchowicz et al. (2020) MacBean (2012a)	V Q ?	186
fipronil $C_{12}H_4Cl_2F_6N_4OS$ [120068-37-3] ZOCSXAVNDGMNBV-UHFFFAOYSA-N	1.2×10^{4} 1.2×10^{4} 4.4×10^{7}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
flusulfamide $C_{13}H_7Cl_2F_3N_2O_4S$ [106917-52-6] GNVDAZSPJWCIQZ-UHFFFAOYSA-N	4.0×10^{3}		Ebert et al. (2023)	?	318
ethiprole $C_{13}H_9Cl_2F_3N_4OS$ [181587-01-9] FNELVJVBIYMIMC-UHFFFAOYSA-N	2.5×10^{5}		Ebert et al. (2023)	?	318
diclosulam $C_{13}H_{10}Cl_2FN_5O_3S$ [145701-21-9] QNXAVFXEJCPCJO-UHFFFAOYSA-N	2.5×10^{10}		Ebert et al. (2023)	?	318
cloransulam-methyl $C_{15}H_{13}ClFN_5O_5S$ [147150-35-4] BIKACRYIQSLICJ-UHFFFAOYSA-N	1.6×10^{11}		Ebert et al. (2023)	?	318
fluthiacet-methyl $C_{15}H_{15}ClFN_3O_3S_2$ [117337-19-6] ZCNQYNHDVRPZIH-UHFFFAOYSA-N	4.8×10^{3} 4.7×10^{3} 4.2×10^{5} 6.6×10^{5}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Modarresi et al. (2007)	V V Q Q	186 67
vemurafenib $C_{23}H_{18}ClF_2N_3O_3S$ [918504-65-1] GPXBXXGIAQBQNI-UHFFFAOYSA-N	8.2×10^{11}		HSDB (2015)	Q	99
tetrabromobisphenol S $C_{12}H_6Br_4O_4S$ [39635-79-5] JHJUYGMZIWDHMO-UHFFFAOYSA-N	1.5×10^{11} 9.7×10^{5} 5.8×10^{6} 1.2×10^{7}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
1,3-dibromo-5-[3,5-dibromo-4-(2,3-dibromopropoxy)benzenesulfonyl]-2-(2,3-dibromopropoxy)benzene $C_{18}H_{14}Br_8O_4S$ [42757-55-1] CWZVMVIHYSYLSI-UHFFFAOYSA-N	8.2×10^{8} 5.2×10^{8} 1.8×10^{11} 6.4×10^{8}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
bromphenol blue $C_{19}H_{10}Br_4O_5S$ [115-39-9] UDSAIICHUKSCKT-UHFFFAOYSA-N	1.9×10^{13} 5.1×10^{5} 9.2×10^{9} 5.3×10^{10}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291

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Table A9.1: Sulfur (C, H, O, N, Cl, S) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bromcresol green $C_{21}H_{14}Br_4O_5S$ [76-60-8] FRPHFZCDPYBUAU-UHFFFAOYSA-N	1.5×10^{13} 1.0×10^{6} 1.8×10^{9} 1.6×10^{10}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
bromocresol purple $C_{21}H_{16}Br_2O_5S$ [115-40-2] ABIUHPWEYMSGSR-UHFFFAOYSA-N	9.9×10^{12}		HSDB (2015)	Q	99
difethialone $C_{31}H_{23}BrO_2S$ [104653-34-1] VSVAQRUUFVBBFS-UHFFFAOYSA-N	9.9 9.9 5.4×10^{6}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
amisulbrom $C_{13}H_{13}BrFN_5O_4S_2$ [348635-87-0] BREATYVWRHIPIY-UHFFFAOYSA-N	4.7×10^{1} 3.6×10^{4}		MacBean (2012b) Maniere et al. (2011)	X ?	350 241, 165
thifluzamide $C_{13}H_6Br_2F_6N_2O_2S$ [130000-40-7] WOSNCVAPUOFXEH-UHFFFAOYSA-N	1.2×10^{6}		Ebert et al. (2023)	?	318
amical 48 $C_8H_8I_2O_2S$ (diiodomethyl *p*-tolyl sulfone) [20018-09-1] XOILGBPDXMVFIP-UHFFFAOYSA-N	1.3×10^{3}		HSDB (2015)	Q	99
flubendiamide $C_{23}H_{22}F_7IN_2O_4S$ [272451-65-7] ZGNITFSDLCMLGI-UHFFFAOYSA-N	4.5×10^{-2}		HSDB (2015)	V	

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A10 Organic species with phosphorus (P)

A10.1 Phosphorus (C, H, O, N, Cl, Br, S, P)

Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
9-icosyl-9-phosphabicyclo[4.2.1]nonane	3.1×10^{-5}		Zhang et al. (2010)	Q	287, 288
$C_{28}H_{55}P$	3.1×10^{-3}		Zhang et al. (2010)	Q	287, 289
[13886-99-2]	2.2×10^{-2}		Zhang et al. (2010)	Q	287, 290
UNOOEFGBOLKBFW-UHFFFAOYSA-N	8.0×10^{-6}		Zhang et al. (2010)	Q	287, 291
triphenylphosphine	4.3×10^{2}		Zhang et al. (2010)	Q	287, 288
$C_{18}H_{15}P$	9.5×10^{-3}		Zhang et al. (2010)	Q	287, 289
[603-35-0]	1.3×10^{1}		Zhang et al. (2010)	Q	287, 290
RIOQSEWOXXDEQQ-UHFFFAOYSA-N	4.8		Zhang et al. (2010)	Q	287, 291
phosphoric acid, trimethyl ester	1.4×10^{3}		Wolfenden and Williams (1983)	M	12
$C_3H_9O_4P$	6.3×10^{1}		Yaws (2003)	X	237
(trimethyl phosphate)	6.1×10^{1}		Gharagheizi et al. (2010)	Q	246
[512-56-1]	1.4×10^{3}		Bartelt-Hunt et al. (2008)	?	21
WVLBCYQITXONBZ-UHFFFAOYSA-N	5.2×10^{1}		Yaws (1999)	?	21
trimethyl phosphite	9.0×10^{-1}		HSDB (2015)	Q	99
$C_3H_9O_3P$					
[121-45-9]					
CYTQBVOFDCPGCX-UHFFFAOYSA-N					
dimethyl methylphosphonate	7.6		HSDB (2015)	Q	99
$C_3H_9O_3P$	7.6		Bartelt-Hunt et al. (2008)	?	21
[756-79-6]					
VONWDASPFIQPDY-UHFFFAOYSA-N					
diethyl hydrogen phosphite	1.7		HSDB (2015)	Q	99
$C_4H_{11}O_3P$	5.5×10^{-3}		Bartelt-Hunt et al. (2008)	?	21
[762-04-9]					
MJUJXFBTEFXVKU-UHFFFAOYSA-N					
triethylphosphate	2.7×10^{2}		Wolfenden and Williams (1983)	M	12
$C_6H_{15}O_4P$	1.4×10^{2}		Abraham et al. (1994a)	R	
[78-40-0]	6.7×10^{1}		Yaws (2003)	X	258
DQWPFSLDHJDLRL-UHFFFAOYSA-N	6.6×10^{1}		Yaws (2003)	X	237
	5.2×10^{1}		Dupeux et al. (2022)	Q	259
	6.7×10^{1}		Gharagheizi et al. (2010)	Q	246
	6.6		Bartelt-Hunt et al. (2008)	?	21
	9.6×10^{1}		Yaws (1999)	?	21
diethyl ethyl phosphonate	3.4		Bartelt-Hunt et al. (2008)	?	21
$C_6H_{15}O_3P$					
[78-38-6]					
AATNZNJRDOVKDD-UHFFFAOYSA-N					

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
mevinphos			Mackay et al. (2006d)	V	558
$C_7H_{13}O_6P$	2.4×10^{5}		Sanders and Seiber (1983)	V	87
[7786-34-7]	2.5×10^{3}		HSDB (2015)	Q	99
GEPDYQSQVLXLEU-AATRIKPKSA-N					
diisopropyl methanephosphonate	2.2×10^{-1}		HSDB (2015)	V	
$C_7H_{17}O_3P$	2.2×10^{-1}		Bartelt-Hunt et al. (2008)	?	21
[1445-75-6]					
WOAFDHWYKSOANX-UHFFFAOYSA-N					
dibutyl hydrogen phosphite	5.5×10^{-1}		HSDB (2015)	Q	99
$C_8H_{19}O_3P$					
[1809-19-4]					
NFJPGAKRJKLOJK-UHFFFAOYSA-N					
dibutyl phosphate	2.3×10^{3}		HSDB (2015)	Q	99
$C_8H_{19}O_4P$					
[107-66-4]					
JYFHYPJRHGVZDY-UHFFFAOYSA-N					
tetraethyl pyrophosphate	4.5×10^{4}		HSDB (2015)	V	
$C_8H_{20}O_7P_2$					
[107-49-3]					
IDCBOTIENDVCBQ-UHFFFAOYSA-N					
tripropyl phosphate	1.5×10^{1}		Wolfenden and Williams (1983)	M	12
$C_9H_{21}O_4P$					
[513-08-6]					
RXPQRKFMDQNODS-UHFFFAOYSA-N					
triallyl phosphate	1.8×10^{1}		HSDB (2015)	Q	99
$C_9H_{15}O_4P$					
[1623-19-4]					
XHGIFBQQEGRTPB-UHFFFAOYSA-N					
tributylphosphate	7.0		HSDB (2015)	V	
$C_{12}H_{27}O_4P$	1.6×10^{1}		Glotfelty et al. (1987)	V	
[126-73-8]	4.8		Yoshida et al. (1983)	V	
STCOOQWBFONSKY-UHFFFAOYSA-N					
hexaethyl tetraphosphate	3.0×10^{11}		HSDB (2015)	Q	99
$C_{12}H_{30}O_{13}P_4$					
[757-58-4]					
DAJYZXUXDOSMCG-UHFFFAOYSA-N					
crotoxyphos	1.7×10^{3}		HSDB (2015)	V	
$C_{14}H_{19}O_6P$	1.7×10^{3}		Mackay et al. (2006d)	V	
[7700-17-6]	1.7×10^{3}		MacBean (2012a)	?	
XXXSILNSXNPGKG-ZHACJKMWSA-N					

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
phosphoric acid, dibutyl phenyl ester $C_{14}H_{23}O_4P$ [2528-36-1] YICSVBJRVMLQNS-UHFFFAOYSA-N	2.0×10^{1}		HSDB (2015)	Q	99
bis(2-ethylhexyl) hydrogen phosphite $C_{16}H_{35}O_3P$ [3658-48-8] HZIUHEQKVCPTAJ-UHFFFAOYSA-N	5.8×10^{-2} 6.6×10^{-4}		HSDB (2015) Bartelt-Hunt et al. (2008)	Q ?	99 21
bis(2-ethylhexyl)hydrogen phosphate $C_{16}H_{35}O_4P$ (bis(2-ethylhexyl) phosphate) [298-07-7] SEGLCEQVOFDUPX-UHFFFAOYSA-N	2.4×10^{2}		HSDB (2015)	Q	99
triphenyl phosphate $C_{18}H_{15}O_4P$ [115-86-6] XZZNDPSIHUTMOC-UHFFFAOYSA-N	3.0		HSDB (2015)	V	
tris(2-butoxyethyl) phosphate $C_{18}H_{39}O_7P$ [78-51-3] WTLBZVNBAKMVDP-UHFFFAOYSA-N	8.2×10^{5}		HSDB (2015)	Q	99
p-cresyl diphenyl phosphate $C_{19}H_{17}O_4P$ [78-31-9] OJUZRFGUKHQNJX-UHFFFAOYSA-N	9.9×10^{1}		HSDB (2015)	Q	447
triphenylphosphine oxide $C_{18}H_{15}OP$ [791-28-6] FIQMHBFVRAXMOP-UHFFFAOYSA-N	1.9×10^{4} 4.6×10^{4} 1.1×10^{7} 2.5×10^{-1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
phosphorous acid, triphenyl ester $C_{18}H_{15}O_3P$ [101-02-0] HVLLSGMXQDNUAL-UHFFFAOYSA-N	1.8×10^{1} 4.4×10^{-2} 1.5×10^{2} 7.0×10^{4}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
trihexylphosphine oxide $C_{18}H_{39}OP$ [3084-48-8] PPDZLUVUQQGIOJ-UHFFFAOYSA-N	4.5×10^{-3} 2.9×10^{-3} 5.8×10^{4} 3.5×10^{-7}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
phosphoric acid, octyl diphenyl ester $C_{20}H_{27}O_4P$ [115-88-8] YAFOVCNAQTZDQB-UHFFFAOYSA-N	3.9×10^{1}		HSDB (2015)	Q	99
octyldihexylphosphine oxide $C_{20}H_{43}OP$ [31160-64-2] XHRRUIJGMKIISX-UHFFFAOYSA-N	2.5×10^{-3} 3.1×10^{-3} 5.3×10^{4} 2.3×10^{-7}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
octicizer $C_{20}H_{27}O_4P$ [1241-94-7] CGSLYBDCEGBZCG-UHFFFAOYSA-N	1.0×10^{-1} 2.7 1.8×10^{-1}		Keshavarz et al. (2022) Duchowicz et al. (2020) Duchowicz et al. (2020)	Q Q ?	 185, 21
tris(methylphenyl) phosphate $C_{21}H_{21}O_4P$ (tricresyl phosphate) [1330-78-5] IUJIYUAKFBGBCG-UHFFFAOYSA-N	1.2×10^{1}		HSDB (2015)	V	
phosphoric acid, (1-methylethyl)phenyl diphenyl ester $C_{21}H_{21}O_4P$ [28108-99-8] JJXNVYMIYBNZQX-UHFFFAOYSA-N	1.3×10^{2}		HSDB (2015)	Q	99
phosphoric acid, tris(2-methylphenyl) ester $C_{21}H_{21}O_4P$ (tri-*o*-cresyl phosphate) [78-30-8] YSMRWXYRXBRSND-UHFFFAOYSA-N	5.2		HSDB (2015)	Q	447
phosphoric acid, tris(3-methylphenyl) ester $C_{21}H_{21}O_4P$ (tri-*m*-cresyl phosphate) [563-04-2] RMLPZKRPSQVRAB-UHFFFAOYSA-N	1.4×10^{-1} 5.1 9.9 1.2×10^{-1}		Keshavarz et al. (2022) Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	Q Q Q ?	 447 185, 21
phosphoric acid, tris(4-methylphenyl) ester $C_{21}H_{21}O_4P$ (tri-*p*-cresyl phosphate) [78-32-0] BOSMZFBHAYFUBJ-UHFFFAOYSA-N	1.8×10^{2}		HSDB (2015)	Q	447

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
(3-*tert*-butylphenyl) diphenyl phosphate $C_{22}H_{23}O_4P$ NIAVXHWAURFNOW-UHFFFAOYSA-N	1.1×10^{1}		Ebert et al. (2023)	?	365
(4-*tert*-butylphenyl) diphenyl phosphate	4.5×10^{1}		HSDB (2015)	V	
$C_{22}H_{23}O_4P$	1.8×10^{2}		Keshavarz et al. (2022)	Q	
[981-40-8]	3.6		Duchowicz et al. (2020)	Q	
ULGAVXUJJBOWOD-UHFFFAOYSA-N	1.1×10^{1}		Duchowicz et al. (2020)	?	185, 21
isodecyl diphenyl phosphate $C_{22}H_{31}O_4P$ [29761-21-5] RYUJRXVZSJCHDZ-UHFFFAOYSA-N	2.3×10^{1}		HSDB (2015)	Q	99
dioctylhexylphosphine oxide	1.4×10^{-3}		Zhang et al. (2010)	Q	287, 288
$C_{22}H_{47}OP$	3.4×10^{-3}		Zhang et al. (2010)	Q	287, 289
[31160-66-4]	4.0×10^{4}		Zhang et al. (2010)	Q	287, 290
MKEFGIKZZDCMQC-UHFFFAOYSA-N	1.4×10^{-7}		Zhang et al. (2010)	Q	287, 291
tris(2,4-dimethylphenyl)phosphate $C_{24}H_{27}O_4P$ [3862-12-2] KOWVWXQNQNCRRS-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	99
tris(2,5-dimethylphenyl)phosphate $C_{24}H_{27}O_4P$ [19074-59-0] MDHAARLWBHZGIP-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	99
tris(2,6-dimethylphenyl)phosphate $C_{24}H_{27}O_4P$ [121-06-2] QLORRTLBSJTMSN-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	99
tris(3,4-dimethylphenyl)phosphate $C_{24}H_{27}O_4P$ [3862-11-1] BCTKCHOESSAGCN-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	99
tris(3,5-dimethylphenyl)phosphate $C_{24}H_{27}O_4P$ [25653-16-1] LLPMAOBOEQFPRE-UHFFFAOYSA-N	1.4×10^{2}		HSDB (2015)	Q	99
tris(4-isopropylphenyl) phosphate $C_{27}H_{33}O_4P$ [26967-76-0] ANVREEJNGJMLOV-UHFFFAOYSA-N	3.4×10^{1}		HSDB (2015)	Q	99

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
trioctylphosphine oxide	8.2×10^{-4}		Zhang et al. (2010)	Q	287, 288
$C_{24}H_{51}OP$	3.7×10^{-3}		Zhang et al. (2010)	Q	287, 289
[78-50-2]	3.4×10^{4}		Zhang et al. (2010)	Q	287, 290
ZMBHCYHQLYEYDV-UHFFFAOYSA-N	9.2×10^{-8}		Zhang et al. (2010)	Q	287, 291
bis(2-ethylhexyl)-2-ethylhexyl phosphonate	2.1×10^{-2}		Zhang et al. (2010)	Q	287, 288
$C_{24}H_{51}O_3P$	6.2×10^{-6}		Zhang et al. (2010)	Q	287, 289
[126-63-6]	5.4×10^{4}		Zhang et al. (2010)	Q	287, 290
GOCVCBDBQYEFQD-UHFFFAOYSA-N	7.7×10^{-5}		Zhang et al. (2010)	Q	287, 291
	1.3×10^{-3}		Bartelt-Hunt et al. (2008)	?	21
didodecyl hydrogen phosphate $C_{24}H_{51}O_4P$ [7057-92-3] JTXUVYOABGUBMX-UHFFFAOYSA-N	2.5×10^{1}		HSDB (2015)	Q	99
phosphoric acid, tris(2-ethylhexyl) ester $C_{24}H_{51}O_4P$ (trioctyl phosphate) [78-42-2] GTVWRXDRKAHEAD-UHFFFAOYSA-N	1.2×10^{2}		HSDB (2015)	V	
diisodecylphenyl phosphite	1.9		Zhang et al. (2010)	Q	287, 288
$C_{26}H_{47}O_3P$	2.5		Zhang et al. (2010)	Q	287, 289
[25550-98-5]	1.6×10^{3}		Zhang et al. (2010)	Q	287, 290
SXXILWLQSQDLDL-UHFFFAOYSA-N	3.9×10^{-3}		Zhang et al. (2010)	Q	287, 291
4-nonylphenyl diphenyl phosphate	8.1×10^{2}		Keshavarz et al. (2022)	Q	
$C_{27}H_{33}O_4P$	2.5×10^{1}		Duchowicz et al. (2020)	Q	184
[64532-97-4]	7.0×10^{2}		Duchowicz et al. (2020)	?	185, 21
LMCLPMXCYFSRNG-UHFFFAOYSA-N					
resorcinol bis(diphenyl phosphate)	3.4×10^{7}		Zhang et al. (2010)	Q	287, 288
$C_{30}H_{24}O_8P_2$	1.4×10^{-2}		Zhang et al. (2010)	Q	287, 289
[57583-54-7]	2.6×10^{8}		Zhang et al. (2010)	Q	287, 290
OWICEWMBIBPFAH-UHFFFAOYSA-N	3.9×10^{16}		Zhang et al. (2010)	Q	287, 291
hydroquinone bis(diphenyl phosphate) $C_{30}H_{24}O_8P_2$ [51732-57-1] RECLNCPBBUHRDY-UHFFFAOYSA-N	3.4×10^{12}		Abraham et al. (2019)	Q	
tris(4-*tert*-butylphenyl) phosphate	1.4×10^{1}		Zhang et al. (2010)	Q	287, 288
$C_{30}H_{39}O_4P$	8.4×10^{-4}		Zhang et al. (2010)	Q	287, 289
[78-33-1]	1.6×10^{3}		Zhang et al. (2010)	Q	287, 290
LORSVOJSXMHDHF-UHFFFAOYSA-N	3.5×10^{1}		Zhang et al. (2010)	Q	287, 291

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tris-(2,4-di-*tert*-butylphenyl) phosphite $C_{42}H_{63}O_3P$ [31570-04-4] JKIJEFPNVSHHEI-UHFFFAOYSA-N	6.1×10^{-2}		Zhang et al. (2010)	Q	287, 288
	6.5×10^{-5}		Zhang et al. (2010)	Q	287, 289
	1.5×10^{2}		Zhang et al. (2010)	Q	287, 290
	5.8		Zhang et al. (2010)	Q	287, 291
glyphosate $C_3H_8NO_5P$ [1071-83-6] XDDAORKBJWWYJS-UHFFFAOYSA-N	1.8×10^{6}		Mackay et al. (2006d)	V	
	4.8×10^{6}		Maniere et al. (2011)	?	165
krenite $C_3H_{11}N_2O_4P$ (fosamine-ammonium) [25954-13-6] OTSAMNSACVKIOJ-UHFFFAOYSA-N	2.0×10^{7}		HSDB (2015)	V	
tabun $C_5H_{11}N_2O_2P$ [77-81-6] PJVJTCIRVMBVIA-UHFFFAOYSA-N	6.6×10^{1}		HSDB (2015)	V	
	6.2×10^{2}		Bartelt-Hunt et al. (2008)	?	21
	6.5×10^{1}		Opresko et al. (1998)	?	
glufosinate-ammonium $C_5H_{15}N_2O_4P$ [77182-82-2] ZBMRKNMTMPPMMK-UHFFFAOYSA-N	2.2×10^{8}		MacBean (2012b)	X	350
hexamethylphosphoramide $C_6H_{18}N_3OP$ [680-31-9] GNOIPBMMFNIUFM-UHFFFAOYSA-N	4.9×10^{2}		Duchowicz et al. (2020)	V	186
	5.3×10^{-4}		Duchowicz et al. (2020)	Q	
monocrotophos $C_7H_{14}NO_5P$ [6923-22-4] KRTSDMXIXPKRQR-AATRIKPKSA-N	1.5×10^{7}		HSDB (2015)	V	
			Mackay et al. (2006d)	V	558
dicrotophos $C_8H_{16}NO_5P$ [141-66-2] VEENJGZXVHKXNB-VOTSOKGWSA-N	2.0×10^{5}		Mackay et al. (2006d)	V	
	7.8×10^{4}		Keshavarz et al. (2022)	Q	
	1.0×10^{3}		Duchowicz et al. (2020)	Q	
	2.0×10^{5}		Duchowicz et al. (2020)	?	185, 21
octamethyldiphosphoramide $C_8H_{24}N_4O_3P_2$ (schradan) [152-16-9] SZKKRCSOSQAJDE-UHFFFAOYSA-N	1.6×10^{11}		HSDB (2015)	Q	99

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
fyrol 6 $C_9H_{22}NO_5P$ (diethyl ((diethanolamino)methyl) phosphonate) [2781-11-5] CCJKFLLIJCGHMO-UHFFFAOYSA-N	6.2×10^{1}		HSDB (2015)	V	
diethyl 4-nitrophenyl phosphate $C_{10}H_{14}NO_6P$ (paraoxon) [311-45-5] WYMSBXTXOHUIGT-UHFFFAOYSA-N	9.1×10^{4} 1.6×10^{3} 9.0×10^{1} 1.5×10^{4} 2.7×10^{-1}		Duchowicz et al. (2020) Glotfelty et al. (1987) Duchowicz et al. (2020) HSDB (2015) Bartelt-Hunt et al. (2008)	V V Q Q ?	186 99 21
dimethyl 4-nitrophenyl phosphate $C_8H_{10}NO_6P$ (methyl paraoxon) [950-35-6] BAFQDKPJKOLXFZ-UHFFFAOYSA-N	$>1.1\times10^{4}$		Woodrow et al. (1990)	V	
buminafos $C_{18}H_{38}NO_3P$ [51249-05-9] NMBXMBCZBXUXAM-UHFFFAOYSA-N	5.0		MacBean (2012a)	?	12
methylphosphonyldifluoride CH_3F_2OP [676-99-3] PQIOSYKVBBWRRI-UHFFFAOYSA-N	4.5×10^{-1}		HSDB (2015)	Q	99
sarin $C_4H_{10}FO_2P$ [107-44-8] DYAHQFWOVKZOOW-UHFFFAOYSA-N	1.7×10^{1} 1.1 1.8×10^{1}		HSDB (2015) Bartelt-Hunt et al. (2008) Opresko et al. (1998)	V ? ?	 21
dimefox $C_4H_{12}FN_2OP$ [115-26-4] PGJBQBDNXAZHBP-UHFFFAOYSA-N	4.5×10^{2}		HSDB (2015)	V	
isoflurophate $C_6H_{14}FO_3P$ (diisopropyl fluorophosphate) [55-91-4] MUCZHBLJLSDCSD-UHFFFAOYSA-N	3.1 7.6×10^{-5}		HSDB (2015) Bartelt-Hunt et al. (2008)	Q ?	99 21
cyclohexyl methylphosphonofluoridate $C_7H_{14}FO_2P$ (cyclosarin) [329-99-7] SNTRKUOVAPUGAY-UHFFFAOYSA-N	3.5 3.5 4.3×10^{3}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
soman	2.1		HSDB (2015)	V	
$C_7H_{16}FO_2P$	2.1		Bartelt-Hunt et al. (2008)	?	21
[96-64-0]	2.2		Opresko et al. (1998)	?	
GRXKLBBBQUKJJZ-UHFFFAOYSA-N					
mipafox	3.3×10^{3}		HSDB (2015)	V	
$C_6H_{16}FN_2OP$					
[371-86-8]					
UOSHUBFBCPGQAY-UHFFFAOYSA-N					
phenylphosphonous dichloride	6.5×10^{-1}		Zhang et al. (2010)	Q	287, 288
$C_6H_5Cl_2P$	2.5×10^{-3}		Zhang et al. (2010)	Q	287, 289
[644-97-3]	6.2×10^{-2}		Zhang et al. (2010)	Q	287, 290
IMDXZWRLUZPMDH-UHFFFAOYSA-N	3.3×10^{-2}		Zhang et al. (2010)	Q	287, 291
chlorphonium chloride	2.8×10^{7}		MacBean (2012a)	?	12
$C_{19}H_{32}Cl_3P$					
[115-78-6]					
IVHVNMLJNASKHW-UHFFFAOYSA-M					
triclofos	7.0×10^{7}		HSDB (2015)	Q	99
$C_2H_4Cl_3O_4P$					
[306-52-5]					
YYQRGCZGSFRBAM-UHFFFAOYSA-N					
(2-chloroethyl)-phosphonic acid	6.9×10^{7}		HSDB (2015)	V	
$C_2H_6ClO_3P$	$>6.9\times10^{6}$		Maniere et al. (2011)	?	241, 165
(ethephon)					
[16672-87-0]					
UDPGUMQDCGORJQ-UHFFFAOYSA-N					
1-hydroxy-2,2,2-trichloroethylphosphonic acid, dimethyl ester	5.5×10^{1}		Chao et al. (2017)	M	
$C_4H_8Cl_3O_4P$	$>8.1\times10^{2}$		Kawamoto and Urano (1989)	M	
(trichlorfon)	5.8×10^{5}		HSDB (2015)	V	
[52-68-6]	6.0×10^{5}		Mackay et al. (2006d)	V	
NFACJZMKEDPNKN-UHFFFAOYSA-N	5.9×10^{5}		Suntio et al. (1988)	V	12
	5.8×10^{3}		Barcelo and Hennion (1997)	X	567
	3.8×10^{1}		Goodarzi et al. (2010)	Q	568
dimethyl-2,2-dichlorovinyl phosphate	3.9×10^{1}	11000	Gautier et al. (2003)	M	
$C_4H_7Cl_2O_4P$	8.1×10^{-2}		Kawamoto and Urano (1989)	M	
(dichlorvos)	1.7×10^{1}		HSDB (2015)	V	
[62-73-7]	5.2		Mackay et al. (2006d)	V	
OEBRKCOSUFCWJD-UHFFFAOYSA-N	5.3		Suntio et al. (1988)	V	12
	5.2×10^{-2}		Barcelo and Hennion (1997)	X	567
	9.7×10^{-1}		Goodarzi et al. (2010)	Q	568, 571

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tris(2-chloroethyl) phosphate $C_6H_{12}Cl_3O_4P$ [115-96-8] HQUQLFOMPYWACS-UHFFFAOYSA-N	3.0		HSDB (2015)	V	
cyclophosphamide $C_7H_{15}Cl_2N_2O_2P$ [50-18-0] CMSMOCZEIVJLDB-UHFFFAOYSA-N	7.0×10^{5}		HSDB (2015)	Q	99
ifosfamide $C_7H_{15}Cl_2N_2O_2P$ [3778-73-2] HOMGKSMUEGBAAB-UHFFFAOYSA-N	7.0×10^{5}		HSDB (2015)	Q	99
butonate $C_8H_{14}Cl_3O_5P$ [126-22-7] BKAQXYNWONVOAX-UHFFFAOYSA-N	3.3×10^{4}		HSDB (2015)	Q	99
phosphoric acid, 7-chlorobicyclo[3.2.0]hepta-2,6-dien-6-yl dimethyl ester $C_9H_{12}ClO_4P$ (heptenophos) [23560-59-0] GBAWQJNHVWMTLU-UHFFFAOYSA-N	5.8×10^{1} 4.3×10^{3}		HSDB (2015) MacBean (2012a)	V ?	
tris(2,3-dichloropropyl) phosphate $C_9H_{15}Cl_6O_4P$ [78-43-3] JZZBTMVTLBHJHL-UHFFFAOYSA-N	3.8×10^{3}		HSDB (2015)	Q	99
tris(1,3-dichloroisopropyl)phosphate $C_9H_{15}Cl_6O_4P$ [13674-87-8] ASLWPAWFJZFCKF-UHFFFAOYSA-N	3.8×10^{3} 3.8×10^{3} 4.1×10^{-2} 1.3×10^{7} 3.0		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	99 287, 288 287, 289 287, 290 287, 291
tris(2-chloropropyl) phosphate $C_9H_{18}Cl_3O_4P$ [6145-73-9] GTRSAMFYSUBAGN-UHFFFAOYSA-N	1.6×10^{2} 1.4×10^{-3} 6.7×10^{2} 3.8×10^{-1}		Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q	287, 288 287, 289 287, 290 287, 291
tri-(2-chloroisopropyl)phosphate $C_9H_{18}Cl_3O_4P$ [13674-84-5] KVMPUXDNESXNOH-UHFFFAOYSA-N	1.6×10^{2} 1.6×10^{2} 1.9×10^{-4} 3.6×10^{4} 3.8×10^{-1}		HSDB (2015) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010) Zhang et al. (2010)	Q Q Q Q Q	99 287, 288 287, 289 287, 290 287, 291

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bis(2-chloropropyl) 2-chloro-1-methylethyl phosphate	1.6×10^{2}		Zhang et al. (2010)	Q	287, 288
$C_9H_{18}Cl_3O_4P$	7.2×10^{-4}		Zhang et al. (2010)	Q	287, 289
[76649-15-5]	5.6×10^{3}		Zhang et al. (2010)	Q	287, 290
WDLBXPUJJVVRGX-UHFFFAOYSA-N	3.8×10^{-1}		Zhang et al. (2010)	Q	287, 291
tetrachlorvinphos	5.5×10^{3}		HSDB (2015)	V	
$C_{10}H_9Cl_4O_4P$	2.4×10^{3}		Ebert et al. (2023)	?	316
[22248-79-9]	5.4×10^{3}		MacBean (2012a)	?	
UBCKGWBNUIFUST-YHYXMXQVSA-N					
dimethylvinphos	3.0×10^{2}		Ebert et al. (2023)	?	318
$C_{10}H_{10}Cl_3O_4P$					
[2274-67-1]					
QSGNQELHULIMSJ-UHFFFAOYSA-N					
diphenyl chlorophosphate	3.7×10^{-2}		Bartelt-Hunt et al. (2008)	?	21
$C_{12}H_{10}ClO_3P$					
[2524-64-3]					
BHIIGRBMZRSDRI-UHFFFAOYSA-N					
chlorfenvinphos	3.4×10^{2}		HSDB (2015)	V	
$C_{12}H_{14}Cl_3O_4P$	3.4×10^{3}		Mackay et al. (2006d)	V	
(clofenvinfos)	3.6×10^{3}		Suntio et al. (1988)	V	12
[470-90-6]	3.5×10^{1}		Barcelo and Hennion (1997)	X	567
FSAVDKDHPDSCTO-XYOKQWHBSA-N	4.1		Goodarzi et al. (2010)	Q	568
crufomate	3.9×10^{3}		HSDB (2015)	Q	99
$C_{12}H_{19}ClNO_3P$					
(ruelene)					
[299-86-5]					
BOFHKBLZOYVHSI-UHFFFAOYSA-N					
phosdiphen	2.6×10^{-2}		MacBean (2012a)	?	
$C_{14}H_{11}O_4Cl_4P$					
[36519-00-3]					
HEMINMLPKZELPP-UHFFFAOYSA-N					
phosphamidon	2.8		Mackay et al. (2006d)	V	
$C_{10}H_{19}ClNO_5P$	2.8		Suntio et al. (1988)	V	12
[13171-21-6]	6.6×10^{6}		HSDB (2015)	Q	99
RGCLLPNLLBQHPF-HJWRWDBZSA-N					
tris(2,3-dibromo-1-propyl) phosphate	3.8×10^{-1}		HSDB (2015)	V	
$C_9H_{15}Br_6O_4P$					
[126-72-7]					
PQYJRMFWJJONBO-UHFFFAOYSA-N					

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
naled $C_4H_7Br_2Cl_2O_4P$ [300-76-5] BUYMVQAILCEWRR-UHFFFAOYSA-N	1.5×10^{-1}		HSDB (2015)	V	
2-bromo-1,1-dimethylethyl 2-bromoethyl 2-chloroethyl phosphate	1.5×10^{3}		Zhang et al. (2010)	Q	287, 288
$C_9H_{18}Br_2ClO_4P$	1.3×10^{-2}		Zhang et al. (2010)	Q	287, 289
[125997-20-8]	4.4×10^{3}		Zhang et al. (2010)	Q	287, 290
GZSKSYDWLZIPOX-UHFFFAOYSA-N	8.2×10^{-1}		Zhang et al. (2010)	Q	287, 291
leptophos	3.7		Mackay and Shiu (1981)	L	
$C_{13}H_{10}O_3BrCl_2P$	3.7		HSDB (2015)	V	
[21609-90-5]	4.0		Mackay et al. (2006d)	V	
CVRALZAYCYJELZ-UHFFFAOYSA-N	4.0		Suntio et al. (1988)	V	12
	2.6×10^{1}		Hilal et al. (2008)	Q	
tributyl phosphorotrithioite	4.3×10^{-1}		HSDB (2015)	Q	99
$C_{12}H_{27}PS_3$	4.3×10^{-1}		Zhang et al. (2010)	Q	287, 288
[150-50-5]	6.0×10^{-4}		Zhang et al. (2010)	Q	287, 289
KLAPGAOQRZTCBI-UHFFFAOYSA-N	1.5×10^{-1}		Zhang et al. (2010)	Q	287, 290
	5.1×10^{-2}		Zhang et al. (2010)	Q	287, 291
bis(2,6,6-trimethylbicyclo[3.1.1]hept-2-enyl) bis(2,6,6-trimethylbicyclo[3.1.1]hept-2-enyl)thiodiphosphonate	8.2×10^{-5}		Zhang et al. (2010)	Q	287, 288
$C_{40}H_{60}P_2S_5$	5.8×10^{4}		Zhang et al. (2010)	Q	287, 289
[68400-79-3]	1.9×10^{5}		Zhang et al. (2010)	Q	287, 290
ZZMOHCWFHCHISQ-UHFFFAOYSA-N	1.6×10^{2}		Zhang et al. (2010)	Q	287, 291
thiometon $C_6H_{15}O_2PS_3$ [640-15-3] OPASCBHCTNRLRM-UHFFFAOYSA-N	3.5×10^{-1}		HSDB (2015)	V	
demeton-S-methyl sulfone $C_6H_{15}O_5PS_2$ [17040-19-6] PZIRJMYRYORVIT-UHFFFAOYSA-N	$<2.3\times10^{10}$		MacBean (2012a)	?	
oxydemeton-methyl $C_6H_{15}O_4PS_2$ [301-12-2] PMCVMORKVPSKHZ-UHFFFAOYSA-N	6.2×10^{7}		HSDB (2015)	Q	99

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
demeton-O-methyl $C_6H_{15}O_3PS_2$ [867-27-6] ZVZQKNVMDKSGGF-UHFFFAOYSA-N	3.2		Ebert et al. (2023)	?	316
demeton-S-methyl $C_6H_{15}O_3PS_2$ [919-86-8] WEBQKRLKWNIYKK-UHFFFAOYSA-N	3.7×10^{2} 3.6×10^{2}		HSDB (2015) Mackay et al. (2006d)	V V	
methacrifos $C_7H_{13}O_5PS$ [62610-77-9] NTAHCMPOMKHKEU-AATRIKPKSA-N	1.0×10^{1}		MacBean (2012a)	?	
phorate $C_7H_{17}O_2PS_3$ [298-02-2] BULVZWIRKLYCBC-UHFFFAOYSA-N	2.1 9.9×10^{-1} 1.5 1.5×10^{-2} 4.5×10^{-2}		HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V V X Q	 12 567 568
salithion $C_8H_9O_3PS$ [3811-49-2] OUNSASXJZHBGAI-UHFFFAOYSA-N	4.7×10^{-1}		MacBean (2012a)	?	
acetoxon $C_8H_{17}O_5PS$ [2425-25-4] ZRCQYAQOWIQUBA-UHFFFAOYSA-N	1.3×10^{4}		HSDB (2015)	Q	99
demeton-O $C_8H_{19}O_3PS_2$ [298-03-3] DGLIBALSRMUQDD-UHFFFAOYSA-N	6.1		MacBean (2012a)	?	12
demeton-S $C_8H_{19}O_3PS_2$ (isosystox) [126-75-0] GRPRVIYRYGLIJU-UHFFFAOYSA-N	2.0×10^{2}		HSDB (2015)	V	
sulfotep $C_8H_{20}O_5P_2S_2$ [3689-24-5] XIUROWKZWPIAIB-UHFFFAOYSA-N	2.2 3.4 9.9×10^{-3} 4.4×10^{-3}		HSDB (2015) Mackay et al. (2006d) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V X Q	 567 568, 571

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tetrakis(hydroxymethyl) phosphonium sulfate $C_8H_{24}O_{12}P_2S$ [55566-30-8] YIEDHPBKGZGLIK-UHFFFAOYSA-L	5.8×10^{17}		HSDB (2015)	Q	99
ethoprophos $C_8H_{19}O_2PS_2$ [13194-48-4] VJYFKVYYMZPMAB-UHFFFAOYSA-N	6.1×10^{1} 6.1×10^{1}		HSDB (2015) Mackay et al. (2006d)	V V	
disulfoton $C_8H_{19}O_2PS_3$ [298-04-4] DOFZAZXDOSGAJZ-UHFFFAOYSA-N	1.1×10^{1} 4.5 4.5 4.5 4.5×10^{-2} 6.4×10^{-1}		Muir et al. (2004) HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Goodarzi et al. (2010)	L V V V X Q	367 12 567 568, 571
endothion $C_9H_{13}O_6PS$ [2778-04-3] YCAGGFXSFQFVQL-UHFFFAOYSA-N	1.5×10^{6}		HSDB (2015)	Q	99
terbufos $C_9H_{21}O_2PS_3$ [13071-79-9] XLNZEKHULJKQBA-UHFFFAOYSA-N	4.1×10^{-1} 4.1×10^{-1} 9.9×10^{-3} 3.0×10^{-1}		HSDB (2015) Mackay et al. (2006d) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V X Q	 567 568
ethion $C_9H_{22}O_4P_2S_4$ [563-12-2] RIZMRRKBZQXFOY-UHFFFAOYSA-N	2.6×10^{1} 3.1×10^{1} 3.1×10^{1} 3.1×10^{-1} 6.8×10^{-1}		HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V V X Q	 12 567 568
fonofos $C_{10}H_{15}OPS_2$ [944-22-9] KVGLBTYUCJYMND-UHFFFAOYSA-N	1.4 1.4 1.4 1.9×10^{5}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Duchowicz et al. (2020)	V V V Q	186
fenthion $C_{10}H_{15}O_3PS_2$ [55-38-9] PNVJTZOFSHSLTO-UHFFFAOYSA-N	6.8 4.5×10^{1} 4.5×10^{1} 4.5×10^{-1} 1.9		HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V V X Q	 12 567 568

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
malathion $C_{10}H_{19}O_6PS_2$ [121-75-5] JXSJBGJIGXNWCI-UHFFFAOYSA-N	2.0×10^{1}	8300	Brockbank (2013)	L	1
	1.5×10^{1}		Chao et al. (2017)	M	
	6.7×10^{2}		Watanabe (1993)	M	
	2.0×10^{3}		Fendinger and Glotfelty (1990)	M	
	4.4×10^{2}		Mackay et al. (2006d)	V	
	2.5×10^{2}		Cotham and Bidleman (1989)	V	
	4.3×10^{2}		Suntio et al. (1988)	V	12
	1.7×10^{2}		Glotfelty et al. (1987)	V	
	7.3×10^{3}		Sanders and Seiber (1983)	V	87
	2.6×10^{1}		Mackay and Shiu (1981)	V	
	4.3		Barcelo and Hennion (1997)	X	567
	1.8		Goodarzi et al. (2010)	Q	568
	1.5×10^{2}		Hilal et al. (2008)	Q	
	2.0×10^{3}		Bartelt-Hunt et al. (2008)	?	21
malaoxon $C_{10}H_{19}O_7PS$ [1634-78-2] WSORODGWGUUOBO-UHFFFAOYSA-N	5.5×10^{6}		HSDB (2015)	Q	99
cadusafos $C_{10}H_{23}O_2PS_2$ [95465-99-9] KXRPCFINVWWFHQ-UHFFFAOYSA-N	7.6		HSDB (2015)	V	
fensulfothion $C_{11}H_{17}O_4PS_2$ [115-90-2] XDNBJTQLKCIJBV-UHFFFAOYSA-N	7.0×10^{4}		HSDB (2015)	Q	99
phenthoate $C_{12}H_{17}O_4PS_2$ [2597-03-7] XAMUDJHXFNRLCY-UHFFFAOYSA-N	1.8×10^{3}		HSDB (2015)	V	
	9.8×10^{1}		Mackay et al. (2006d)	V	
sulprofos $C_{12}H_{19}O_2PS_3$ [35400-43-2] JXHJNEJVUNHLKO-UHFFFAOYSA-N	1.1×10^{1}		HSDB (2015)	V	
	1.1×10^{1}		MacBean (2012a)	?	12
S,S,S-tributyl phosphorotrithioate $C_{12}H_{27}OPS_3$ (DEF) [78-48-8] ZOKXUAHZSKEQSS-UHFFFAOYSA-N	3.4×10^{1}		Fendinger and Glotfelty (1990)	M	
	1.3		Glotfelty et al. (1987)	V	

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
aspon $C_{12}H_{28}O_5P_2S_2$ (tetrapropyl dithiopyrophosphate) [3244-90-4] IIDFEIDMIKSJSV-UHFFFAOYSA-N	6.1		Ebert et al. (2023)	?	318
iprobenphos $C_{13}H_{21}O_3PS$ [26087-47-8] FCOAHACKGGIURQ-UHFFFAOYSA-N	2.6×10^{2}		Watanabe (1993)	M	
propaphos $C_{13}H_{21}O_4PS$ [7292-16-2] PWYIUEFFPNVCMW-UHFFFAOYSA-N	3.4×10^{3} 3.4×10^{3} 3.6×10^{1} 3.4×10^{3}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) MacBean (2012a)	V V Q ?	186
edifenphos $C_{14}H_{15}O_2PS_2$ [17109-49-8] AWZOLILCOUMRDG-UHFFFAOYSA-N	5.0×10^{3} 1.3×10^{4} 1.4×10^{1}		Watanabe (1993) HSDB (2015) Mackay et al. (2006d)	M V V	
systox $C_{16}H_{38}O_6P_2S_4$ [8065-48-3] FAXIJTUDSBIMHY-UHFFFAOYSA-N	5.5×10^{1}		HSDB (2015)	V	
temefos $C_{16}H_{20}O_6P_2S_3$ (temephos) [3383-96-8] WWJZWCUNLNYYAU-UHFFFAOYSA-N	1.7 4.9×10^{3} 4.4		Barcelo and Hennion (1997) HSDB (2015) Goodarzi et al. (2010)	X Q Q	567 99 568
methamidophos $C_2H_8NOPS_2$ [10265-92-6] NNKVPIKMPCQWCG-UHFFFAOYSA-N	1.1×10^{4}		HSDB (2015)	Q	99
acephate $C_4H_{10}NO_3PS$ [30560-19-1] YASYVMFAVPKPKE-UHFFFAOYSA-N	2.0×10^{7} 2.0×10^{7} 1.9×10^{5} 4.4×10^{2}		HSDB (2015) Mackay et al. (2006d) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V X Q	 567 568
dimethoate $C_5H_{12}NO_3PS_2$ [60-51-5] MCWXGJITAZMZEV-UHFFFAOYSA-N	4.1×10^{4} 8.7×10^{3} 9.1×10^{3} 9.0×10^{1} 5.3×10^{2}		HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Barcelo and Hennion (1997) Goodarzi et al. (2010)	V V V X Q	 12 567 568, 569

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
omethoate $C_5H_{12}NO_4PS$ [1113-02-6] PZXOQEXFMJCDPG-UHFFFAOYSA-N	2.1×10^{8}		HSDB (2015)	Q	99
methidathion $C_6H_{11}N_2O_4PS_3$ [950-37-8] MEBQXILRKZHVCX-UHFFFAOYSA-N	1.4×10^{3} 5.8×10^{3} 5.8×10^{3}		HSDB (2015) Glotfelty et al. (1987) Burkhard and Guth (1981)	V V V	
fosthietan $C_6H_{12}NO_3PS_2$ [21548-32-3] RHJOIOVESMTJEK-UHFFFAOYSA-N	2.4×10^{5} 2.4×10^{5}		HSDB (2015) MacBean (2012a)	V ?	
formothion $C_6H_{12}NO_4PS_2$ [2540-82-1] AIKKULXCBHRFOS-UHFFFAOYSA-N	9.0×10^{4}		HSDB (2015)	V	
menazon $C_6H_{12}N_5O_2PS_2$ [78-57-9] SUYHYHLFUHHVJQ-UHFFFAOYSA-N	6.6×10^{3}		HSDB (2015)	V	
ethoate-methyl $C_6H_{14}NO_3PS_2$ [116-01-8] DICRHEJCQXFJBY-UHFFFAOYSA-N	3.5×10^{5}		HSDB (2015)	Q	99
glyphosate-trimesium $C_6H_{16}NO_5PS$ [81591-81-3] RUCAXVJJQQJZGU-UHFFFAOYSA-M	$>2.3\times10^{10}$		MacBean (2012a)	?	
phosfolan $C_7H_{14}NO_3PS_2$ (cyolane) [947-02-4] ILBONRFSLATCRE-UHFFFAOYSA-N	5.1×10^{4}		Ebert et al. (2023)	?	316
methylparathion $C_8H_{10}NO_5PS$ (parathion-methyl) [298-00-0] RLBIQVVOMOPOHC-UHFFFAOYSA-N	5.0×10^{1} 1.7×10^{1} 2.6×10^{2} 1.6×10^{2} 9.9×10^{1} 4.7×10^{1} 9.9×10^{1} 4.7×10^{1} 9.2×10^{1} 2.1×10^{3}		Mackay and Shiu (1981) Chao et al. (2017) Rice et al. (1997b) Fendinger and Glotfelty (1990) Metcalfe et al. (1980) Mackay et al. (2006d) Woodrow et al. (1990) Suntio et al. (1988) Glotfelty et al. (1987) Sanders and Seiber (1983)	L M M M M V V V V V	 12 12 87

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.6×10^{2}		Metcalfe et al. (1980)	V	
	1.3×10^{-1}		Smith and Bomberger (1980)	V	24
	4.7×10^{-1}		Barcelo and Hennion (1997)	X	567
	2.1×10^{1}		Goodarzi et al. (2010)	Q	568
	1.5×10^{1}		Hilal et al. (2008)	Q	
zinophos $C_8H_{13}N_2O_3PS$ (thionazin) [297-97-2] IRVDMKJLOCGUBJ-UHFFFAOYSA-N	1.0×10^{1}		Mackay et al. (2006d)	V	
	1.2×10^{1}		Suntio et al. (1988)	V	12
	1.1×10^{1}		MacBean (2012a)	?	
vamidothion $C_8H_{18}NO_4PS_2$ [2275-23-2] LESVOLZBIFDZGS-UHFFFAOYSA-N	1.1×10^{10}		HSDB (2015)	Q	99
cyanophos $C_9H_{10}NO_3PS$ [2636-26-2] SCKHCCSZFPSHGR-UHFFFAOYSA-N	1.8		HSDB (2015)	V	
fenitrothion $C_9H_{12}NO_5PS$ [122-14-5] ZNOLGFHPUIJIMJ-UHFFFAOYSA-N	8.3×10^{1}		Watanabe (1993)	M	
	1.1×10^{1}		Metcalfe et al. (1980)	M	
	8.3×10^{2}		Mackay et al. (2006d)	V	
	2.8×10^{2}		Suntio et al. (1988)	V	12
	2.7×10^{1}		Mackay and Shiu (1981)	V	
	1.5×10^{1}		Metcalfe et al. (1980)	V	
	2.7		Barcelo and Hennion (1997)	X	567
	4.4×10^{1}		Goodarzi et al. (2010)	Q	568, 569
	5.3		Hilal et al. (2008)	Q	
fosthiazate-1 $C_9H_{18}NO_3PS_2$ [98886-44-3] DUFVKSUJRWYZQP-UHFFFAOYSA-N	7.5×10^{1}		MacBean (2012b)	X	350
	1.0×10^{5}		Keshavarz et al. (2022)	Q	
	5.7×10^{4}		Duchowicz et al. (2020)	Q	
	5.7×10^{4}		Duchowicz et al. (2020)	?	185, 21
	5.7×10^{4}		Maniere et al. (2011)	?	241, 165
prothoate $C_9H_{20}NO_3PS_2$ (trimethoate) [2275-18-5] QTXHFDHVLBDJIO-UHFFFAOYSA-N	1.5×10^{5}		HSDB (2015)	Q	99
amiton $C_{10}H_{24}NO_3PS$ [78-53-5] PJISLFCKHOHLLP-UHFFFAOYSA-N	3.5×10^{4}		Bartelt-Hunt et al. (2008)	?	21

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
azinphos-methyl	3.4×10^{3}		HSDB (2015)	V	
$C_{10}H_{12}N_3O_3PS_2$	3.2×10^{3}		Mackay et al. (2006d)	V	
[86-50-0]	3.1×10^{2}		Suntio et al. (1988)	V	12
CJJOSEISRRTUQB-UHFFFAOYSA-N	3.1		Barcelo and Hennion (1997)	X	567
	4.6×10^{1}		Goodarzi et al. (2010)	Q	568
parathion	1.2×10^{2}		Fendinger and Glotfelty (1990)	M	
$C_{10}H_{14}NO_5PS$	7.1×10^{1}		Mackay et al. (2006d)	V	
(E 605)	5.0×10^{1}		Siebers and Mattusch (1996)	V	12
[56-38-2]	5.0×10^{1}		Siebers et al. (1994)	V	
LCCNCVORNKJIRZ-UHFFFAOYSA-N	8.3×10^{1}		Suntio et al. (1988)	V	12
	4.2×10^{1}		Glotfelty et al. (1987)	V	
	1.6×10^{3}		Sanders and Seiber (1983)	V	87
	8.1		Mackay and Shiu (1981)	V	
	1.3×10^{1}		Burkhard and Guth (1981)	V	
	1.0×10^{1}		Chiou et al. (1980)	V	
	3.3×10^{1}		MacBean (2012b)	X	350
	8.0×10^{-1}		Barcelo and Hennion (1997)	X	567
	3.2×10^{-1}		Goodarzi et al. (2010)	Q	568
	6.5		Hilal et al. (2008)	Q	
	3.4×10^{1}		Bartelt-Hunt et al. (2008)	?	21
isoparathion	6.1×10^{1}		Ebert et al. (2023)	?	318
$C_{10}H_{14}NO_5PS$					
[597-88-6]					
BGWJTLLALYACOG-UHFFFAOYSA-N					
etrimfos	1.6×10^{1}		HSDB (2015)	V	
$C_{10}H_{17}N_2O_4PS$					
[38260-54-7]					
FGIWFCGDPUIBEZ-UHFFFAOYSA-N					
propetamphos	2.1×10^{2}		HSDB (2015)	V	
$C_{10}H_{20}NO_4PS$					
[31218-83-4]					
BZNDWPRGXNILMS-VQHVLOKHSA-N					
mecarbam	1.1×10^{4}		HSDB (2015)	Q	99
$C_{10}H_{20}NO_5PS_2$					
[2595-54-2]					
KLGMSAOQDHLCOS-UHFFFAOYSA-N					
phosmet	1.2×10^{3}		HSDB (2015)	V	
$C_{11}H_{12}NO_4PS_2$	1.3×10^{3}		Mackay et al. (2006d)	V	
[732-11-6]	1.1×10^{3}		Suntio et al. (1988)	V	12
LMNZTLDVJIUSHT-UHFFFAOYSA-N	1.0×10^{1}		Barcelo and Hennion (1997)	X	567
	3.8		Goodarzi et al. (2010)	Q	568
	7.4×10^{2}		Maniere et al. (2011)	?	165

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
pirimiphos methyl $C_{11}H_{20}N_3O_3PS$ [29232-93-7] QHOQHJPRIBSPCY-UHFFFAOYSA-N	1.6×10^{1} 1.7×10^{1}		HSDB (2015) Maniere et al. (2011)	V ?	 241, 165
imicyafos $C_{11}H_{21}N_4O_2PS$ [140163-89-9] PPCUNNLZTNMXFO-UHFFFAOYSA-N	1.5×10^{9}		Ebert et al. (2023)	?	318
Agent VX $C_{11}H_{26}NO_2PS$ [50782-69-9] JJIUCEJQJXNMHV-UHFFFAOYSA-N	9.1×10^{2} 2.8×10^{3} 1.2×10^{3}		HSDB (2015) Bartelt-Hunt et al. (2008) Opresko et al. (1998)	V ? ?	 21
ditalimfos $C_{12}H_{14}NO_4PS$ [5131-24-8] MTBZIGHNGSTDJV-UHFFFAOYSA-N	2.3×10^{3}		Ebert et al. (2023)	?	316
quinalphos $C_{12}H_{15}N_2O_3PS$ [13593-03-8] JYQUHIFYBATCCY-UHFFFAOYSA-N	1.1×10^{2}		Ebert et al. (2023)	?	316
phoxim $C_{12}H_{15}N_2O_3PS$ [14816-18-3] ATROHALUCMTWTB-UHFFFAOYSA-N	5.0×10^{1}		Ebert et al. (2023)	?	316
triazophos $C_{12}H_{16}N_3O_3PS$ [24017-47-8] AMFGTOFWMRQMEM-UHFFFAOYSA-N	3.2×10^{2}		HSDB (2015)	V	
azinphos-ethyl $C_{12}H_{16}N_3O_3PS_2$ [2642-71-9] RQVGAIADHNPSME-UHFFFAOYSA-N	1.0×10^{2}		HSDB (2015)	V	
diazinon $C_{12}H_{21}N_2O_3PS$ (dimpylate) [333-41-5] FHIVAFMUCKRCQO-UHFFFAOYSA-N	4.6×10^{1} 9.2×10^{1} 1.5×10^{1} 1.1×10^{1} 8.4×10^{1} 8.8×10^{1} 2.5×10^{1} 1.5×10^{1} 6.7 1.0×10^{2} 1.3×10^{1}	 12000 	Muir et al. (2004) Muir et al. (2004) Feigenbrugel et al. (2004a) Watanabe (1993) Fendinger et al. (1989) Fendinger and Glotfelty (1988) Mackay et al. (2006d) Suntio et al. (1988) Glotfelty et al. (1987) Sanders and Seiber (1983) Burkhard and Guth (1981)	L L M M M M V V V V V	367 366 72 72 12 87

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	1.5×10^{-1}		Barcelo and Hennion (1997)	X	567
	1.7×10^{-1}		Goodarzi et al. (2010)	Q	568
	1.4×10^{2}		Meylan and Howard (1991)	Q	
isoxathion $C_{13}H_{16}NO_4PS$ [18854-01-8] SDMSCIWHRZJSRN-UHFFFAOYSA-N	1.6×10^{2}		HSDB (2015)	Q	99
butamifos $C_{13}H_{21}N_2O_4PS$ [36335-67-8] OEYOMNZEMCPTKN-UHFFFAOYSA-N	3.4×10^{1}		Ebert et al. (2023)	?	316
fenamiphos $C_{13}H_{22}NO_3PS$ [22224-92-6] ZCJPOPBZHLUFHF-UHFFFAOYSA-N	1.1×10^{3}		HSDB (2015)	V	
tebupirimfos $C_{13}H_{23}N_2O_3PS$ [96182-53-5] AWYOMXWDGWUJHS-UHFFFAOYSA-N	3.5		HSDB (2015)	V	
pirimiphos ethyl $C_{13}H_{24}N_3O_3PS$ [23505-41-1] TZBPRYIIJAJUOY-UHFFFAOYSA-N	1.8×10^{-1}		HSDB (2015)	V	
bensulide $C_{14}H_{24}NO_4PS_3$ [741-58-2] RRNIZKPFKNDSRS-UHFFFAOYSA-N	1.1×10^{3}		HSDB (2015)	V	
ethyl *p*-nitrophenyl benzenethiophosphonate $C_{14}H_{14}NO_4PS$ [2104-64-5] AIGRXSNSLVJMEA-UHFFFAOYSA-N	2.2×10^{1}		Duchowicz et al. (2020)	V	186
	2.2×10^{1}		HSDB (2015)	V	
	4.3×10^{7}		Duchowicz et al. (2020)	Q	
pyridaphenthion $C_{14}H_{17}N_2O_4PS$ [119-12-0] CXJSOEPQXUCJSA-UHFFFAOYSA-N	5.1×10^{4}		Ebert et al. (2023)	?	318
piperophos $C_{14}H_{28}NO_3PS_2$ [24151-93-7] UNLYSVIDNRIVFJ-UHFFFAOYSA-N	8.8×10^{2}		Ebert et al. (2023)	?	318

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
isofenphos $C_{15}H_{24}NO_4PS$ [25311-71-1] HOQADATXFBOEGG-UHFFFAOYSA-N	1.2×10^{2} 2.4×10^{2} 1.0×10^{3} 6.9×10^{-1} 2.4×10^{2}		Mackay et al. (2006d) MacBean (2012b) Barcelo and Hennion (1997) Goodarzi et al. (2010) MacBean (2012a)	V X X Q ?	 350 567 568, 569 12
chlormephos $C_5H_{12}ClO_2PS_2$ [24934-91-6] QGTYWWGEWOBMAK-UHFFFAOYSA-N	3.4×10^{-2} 3.4×10^{-2} 3.2×10^{5}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186
chlorethoxyfos $C_6H_{11}Cl_4O_3PS$ [54593-83-8] XFDJMIHUAHSGKG-UHFFFAOYSA-N	2.3		HSDB (2015)	Q	99
ronnel $C_8H_8O_3Cl_3PS$ [299-84-3] JHJOOSLFWRRSGU-UHFFFAOYSA-N	4.8×10^{-1} 1.7×10^{-2} 3.1×10^{-1} 5.7×10^{-2}		Mackay and Shiu (1981) Mackay et al. (2006d) Suntio et al. (1988) Hilal et al. (2008)	L V V Q	 12
tolclofos-methyl $C_9H_{11}Cl_2O_3PS$ [57018-04-9] OBZIQQJJIKNWNO-UHFFFAOYSA-N	1.7×10^{-2} 2.7		Mackay et al. (2006d) Maniere et al. (2011)	V ?	 12, 165
methyl trithion $C_9H_{12}ClO_2PS_3$ [953-17-3] OUCCVXVYGFBXSV-UHFFFAOYSA-N	9.9×10^{1}		HSDB (2015)	Q	99
trichloronate $C_{10}H_{12}Cl_3O_2PS$ [327-98-0] ANIAQSUBRGXWLS-UHFFFAOYSA-N	8.8×10^{-1} 9.0×10^{-1} 2.6×10^{4} 7.5×10^{1}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) MacBean (2012a)	V V Q ?	186
dichlofenthion $C_{10}H_{13}Cl_2O_3PS$ [97-17-6] WGOWCPGHOCIHBW-UHFFFAOYSA-N	1.0×10^{-2} 1.0×10^{-2} 3.2×10^{-5} 3.2×10^{-5} 1.5×10^{1}		Duchowicz et al. (2020) HSDB (2015) Mackay et al. (2006d) Suntio et al. (1988) Duchowicz et al. (2020)	V V V V Q	186 12
prothiofos $C_{11}H_{15}Cl_2O_2PS_2$ [34643-46-4] FITIWKDOCAUBQD-UHFFFAOYSA-N	3.4×10^{-1}		Ebert et al. (2023)	?	318
chlorthiophos $C_{11}H_{15}Cl_2O_3PS_2$ [21923-23-9] JAZJVWLGNLCNDD-UHFFFAOYSA-N	8.2		HSDB (2015)	Q	99

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
carbophenothion	4.9×10^{1}		HSDB (2015)	V	
$C_{11}H_{16}ClO_2PS_3$	2.2×10^{1}		Suntio et al. (1988)	V	12
[786-19-6]					
VEDTXTNSFWUXGQ-UHFFFAOYSA-N					
coumaphos	9.0×10^{1}		HSDB (2015)	V	
$C_{14}H_{16}ClO_5PS$					
[56-72-4]					
BXNANOICGRISHX-UHFFFAOYSA-N					
methylchlorpyrifos	4.1		HSDB (2015)	V	
$C_7H_7NO_3Cl_3PS$	2.5		Mackay et al. (2006d)	V	
[5598-13-0]	2.9		Suntio et al. (1988)	V	12
HRBKVYFZANMGRE-UHFFFAOYSA-N	3.3		Mackay and Shiu (1981)	V	
	6.5×10^{-1}		Hilal et al. (2008)	Q	
	4.3		Maniere et al. (2011)	?	241, 165
dicapthon	1.0×10^{2}		HSDB (2015)	V	
$C_8H_9NO_5ClPS$	4.2×10^{1}		Mackay et al. (2006d)	V	
[2463-84-5]	4.2×10^{1}		Suntio et al. (1988)	V	12
OTKXWJHPGBRXCR-UHFFFAOYSA-N	4.4×10^{1}		Mackay and Shiu (1981)	V	
	6.5		Hilal et al. (2008)	Q	
chlorthion	2.5×10^{2}		HSDB (2015)	V	
$C_8H_9ClNO_5PS$	2.4×10^{2}		MacBean (2012a)	?	
[500-28-7]					
NZNRRXXETLSZRO-UHFFFAOYSA-N					
azamethiphos	3.0×10^{5}		Ebert et al. (2023)	?	318
$C_9H_{10}ClN_2O_5PS$					
[35575-96-3]					
VNKBTWQZTQIWDV-UHFFFAOYSA-N					
isazophos	1.9×10^{1}		HSDB (2015)	V	
$C_9H_{17}ClN_3O_3PS$	1.1×10^{2}		Burkhard and Guth (1981)	V	
[42509-80-8]	7.2×10^{1}		MacBean (2012a)	?	
XRHGWAGWAHHFLF-UHFFFAOYSA-N					
chlorpyrifos	1.8		Muir et al. (2004)	L	367
$C_9H_{11}Cl_3NO_3PS$	2.1		Muir et al. (2004)	L	366
[2921-88-2]	2.2×10^{-1}	7800	Cetin et al. (2006)	M	
SBPBAQFWLVIOKP-UHFFFAOYSA-N	3.1		Rice et al. (1997b)	M	12
	2.4		Fendinger and Glotfelty (1990)	M	
	9.2×10^{-1}		Mackay et al. (2006d)	V	
	1.7		Siebers et al. (1994)	V	
	5.7×10^{-1}		Suntio et al. (1988)	V	12
	8.1×10^{-1}		Glotfelty et al. (1987)	V	
	5.6×10^{-3}		Barcelo and Hennion (1997)	X	567
	3.4		HSDB (2015)	C	
	1.4		Armbrust (2000)	C	
	1.0×10^{-1}		Goodarzi et al. (2010)	Q	568, 569

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Table A10.1: Phosphorus (C, H, O, N, Cl, Br, S, P) (...continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
	2.2×10^{-1}		Hilal et al. (2008)	Q	
	2.5×10^{2}		Meylan and Howard (1991)	Q	
	2.1		Maniere et al. (2011)	?	241, 165
chlorphoxim $C_{12}H_{14}ClN_2O_3PS$ [14816-20-7] GQKRUMZWUHSLJF-NTCAYCPXSA-N	$>2.3\times10^{10}$		MacBean (2012a)	?	
phosazetim $C_{14}H_{11}Cl_2N_2O_4PS$ [4104-14-7] XIBXUAZIZXDFTG-UHFFFAOYSA-N	2.1×10^{3}		HSDB (2015)	Q	99
dialifor $C_{14}H_{17}ClNO_4PS_2$ [10311-84-9] MUMQYXACQUZOFP-UHFFFAOYSA-N	5.5×10^{1}		HSDB (2015)	V	
	7.1		Mackay et al. (2006d)	V	
	7.1		Suntio et al. (1988)	V	12
pyraclofos $C_{14}H_{18}ClN_2O_3PS$ [77458-01-6] QHGVXILFMXYDRS-UHFFFAOYSA-N	2.3×10^{4}		Ebert et al. (2023)	?	318
bromophos $C_8H_8BrCl_2O_3PS$ [2104-96-3] NYQDCVLCJXRDSK-UHFFFAOYSA-N	1.0×10^{-1}		HSDB (2015)	V	
	1.1×10^{-1}		MacBean (2012a)	?	12
bromophos-ethyl $C_{10}H_{12}BrCl_2O_3PS$ [4824-78-6] KWGUFOITWDSNQY-UHFFFAOYSA-N	6.2×10^{-1}		HSDB (2015)	Q	99
profenofos $C_{11}H_{15}BrClO_3PS$ [41198-08-7] QYMMJNLHFKGANY-UHFFFAOYSA-N	4.5×10^{2}		HSDB (2015)	V	
	6.2×10^{2}		Mackay et al. (2006d)	V	
iodofenphos $C_8H_8Cl_2IO_3PS$ [18181-70-9] LFVLUOAHQIVABZ-UHFFFAOYSA-N	2.2		HSDB (2015)	V	
	$>2.3\times10^{10}$		MacBean (2012a)	?	

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A11 Organic species with other elements

A11.1 Sodium (Na)

Table A11.1: Sodium (Na)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
sesone $C_8H_7Cl_2NaO_5S$ (2,4-dichlorophenoxyethyl sulfate) [136-78-7] KISFEBPWFCGRGN-UHFFFAOYSA-M	3.8×10^{5}		HSDB (2015)	Q	99
iodosulfuron-methyl-sodium $C_{14}H_{14}IN_5O_6SNa$ [144550-36-7] JUJFQMPKBJPSFZ-UHFFFAOYSA-M	4.4×10^{10}		Maniere et al. (2011)	?	12, 165
propoxycarbazone-sodium $C_{15}H_{17}N_4O_7NaS$ [181274-15-7] JRQGDDUXDKCWRF-UHFFFAOYSA-M	$>1.0\times10^{10}$		Maniere et al. (2011)	?	12, 165
dioctyl sulfosuccinatesodium salt $C_{20}H_{37}NaO_7S$ (bis(2-ethylhexyl) sodium sulfosuccinate) [577-11-7] APSBXTVYXVQYAB-UHFFFAOYSA-M	2.0×10^{6}		HSDB (2015)	Q	99
dodecylbenzenesulfonic acid sodium salt $C_{18}H_{29}NaO_3S$ (sodium dodecylbenzenesulfonate) [25155-30-0] BWUAQXVVJWAXHR-UHFFFAOYSA-M	1.6×10^{2}		HSDB (2015)	Q	99
D&C yellow 10 $C_{20}H_{17}NO_8Na_2S_2$ [8004-92-0] NYMFWSWVZMTZQO-UHFFFAOYSA-L	3.4×10^{14}		HSDB (2015)	Q	99
D&C yellow 8 $C_{20}H_{10}Na_2O_5$ (fluorescein sodium) [518-47-8] NJDNXYGOVLYJHP-UHFFFAOYSA-L	3.5×10^{10}		HSDB (2015)	Q	447
D&C black 1 $C_{22}H_{14}N_6Na_2O_9S_2$ (amido black 10B) [1064-48-8] HKBVRFLHNUEVRO-DWTBGCDMSA-L	8.2×10^{25}		HSDB (2015)	Q	99

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Table A11.1: Sodium (Na) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
D&C green 5 $C_{28}H_{20}N_2Na_2O_8S_2$ [4403-90-1] FPAYXBWMYIMERV-UHFFFAOYSA-L	3.1×10^{23}		HSDB (2015)	Q	447
FD&C green 2 $C_{37}H_{34}N_2Na_2O_9S3$ [5141-20-8] DGOBMKYRQHEFGQ-UHFFFAOYSA-L	7.0×10^{30}		HSDB (2015)	Q	447

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A11.2 Aluminum (Al)

Table A11.2: Aluminum (Al)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
fosetyl-aluminum $C_6H_{18}AlO_9P_3$ [39148-24-8] ZKZMJOFIHHZSRW-UHFFFAOYSA-K	3.1×10^{9} $>3.1\times10^{9}$		HSDB (2015) Maniere et al. (2011)	V ?	 12, 165

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A11.3 Silicon (Si)

Table A11.3: Silicon (Si)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tetramethylsilane $C_4H_{12}Si$ [75-76-3] CZDYPVPMEAXLPK-UHFFFAOYSA-N	2.3×10^{-6} 2.3×10^{-6} 1.4×10^{-3} 2.4×10^{-6}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Abraham et al. (1990)	V V Q ?	186
tetraethylsilane $C_8H_{20}Si$ [631-36-7] VCZQFJFZMMALHB-UHFFFAOYSA-N	3.8×10^{-6}		Abraham et al. (1990)	?	
trimethylsilanol $(CH_3)_3SiOH$ (TMS) [1066-40-6] AAPLIUHOKVUFCC-UHFFFAOYSA-N	7.0×10^{-2} 2.2×10^{-1}		Xu and Kropscott (2014) Mazzoni et al. (1997)	M V	
silicic acid $Si(OH)_4$ [10193-36-9] RMAQACBXLXPBSY-UHFFFAOYSA-N	2.3×10^{10}	14000	Plyasunov (2012)	M	818
dimethylsilanediol $C_2H_8O_2Si$ [1066-42-8] XCLIHDJZGPCUBT-UHFFFAOYSA-N	2.8×10^{3} 2.9×10^{-1}		Xu and Kropscott (2012) Mazzoni et al. (1997)	M V	12
tetramethyl silicate $C_4H_{12}O_4Si$ [681-84-5] LFQCEHFDDXELDD-UHFFFAOYSA-N	1.5		HSDB (2015)	Q	99
pentamethyldisiloxanol $C_5H_{16}O_2Si_2$ [56428-93-4] FGOLZCPMTWJPOU-UHFFFAOYSA-N	7.3×10^{-4}		Mazzoni et al. (1997)	V	
tetraethyl silicate $C_8H_{20}O_4Si$ [78-10-4] BOTDANWDWHJENH-UHFFFAOYSA-N	4.9×10^{-1}		HSDB (2015)	Q	99
trimethoxysilylpropyl methacrylate $C_{10}H_{20}O_5Si$ [2530-85-0] XDLMVUHYZWKMMD-UHFFFAOYSA-N	3.3×10^{1}		HSDB (2015)	Q	99

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Table A11.3: Silicon (Si) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexamethyldisiloxane	1.3×10^{-6}		Xu and Kropscott (2014)	M	
$C_6H_{18}OSi_2$	1.7×10^{-4}		Kochetkov et al. (2001)	M	402, 330
(L2)	3.1×10^{-4}		Kochetkov et al. (2001)	M	402, 331
[107-46-0]	7.7×10^{-7}		David et al. (2000)	M	72
UQEAIHBTYFGYIE-UHFFFAOYSA-N	1.0×10^{-6}		Xu and Kropscott (2014)	V	
	1.0×10^{-6}		Kochetkov et al. (2001)	V	
	4.2×10^{-6}		Mazzoni et al. (1997)	V	
	2.2×10^{-4}		Keshavarz et al. (2022)	Q	
	1.9×10^{-4}		Duchowicz et al. (2020)	Q	
	2.2×10^{-4}		Duchowicz et al. (2020)	?	185, 21
octamethyltrisiloxane	3.4×10^{-7}		Xu and Kropscott (2014)	M	
$C_8H_{24}O_2Si_3$	3.3×10^{-6}		Kochetkov et al. (2001)	M	402, 330
(L3)	2.7×10^{-6}		Kochetkov et al. (2001)	M	402, 331
[107-51-7]	2.8×10^{-7}		Xu and Kropscott (2014)	V	
CXQXSVUQTKDNFP-UHFFFAOYSA-N	2.8×10^{-7}		Kochetkov et al. (2001)	V	
	1.2×10^{-6}		Mazzoni et al. (1997)	V	
	1.3×10^{-5}		Keshavarz et al. (2022)	Q	
	2.5×10^{-5}		Duchowicz et al. (2020)	Q	
	3.0×10^{-6}		Duchowicz et al. (2020)	?	185, 21
decamethyltetrasiloxane	1.4×10^{-7}		Xu and Kropscott (2014)	M	
$C_{10}H_{30}O_3Si_4$	5.8×10^{-7}		Kochetkov et al. (2001)	M	402, 330
(L4)	3.7×10^{-7}		Xu and Kropscott (2014)	V	
[141-62-8]	4.3×10^{-7}		Kochetkov et al. (2001)	V	
YFCGDEUVHLPRCZ-UHFFFAOYSA-N	3.1×10^{-7}		Mazzoni et al. (1997)	V	
	8.1×10^{-7}		Keshavarz et al. (2022)	Q	
	3.3×10^{-6}		Duchowicz et al. (2020)	Q	184
	5.8×10^{-7}		Duchowicz et al. (2020)	?	185, 21
dodecamethylpentasiloxane $C_{12}H_{36}O_4Si_5$ (L5) [141-63-9] FBZANXDWQAVSTQ-UHFFFAOYSA-N	8.7×10^{-8}		Mazzoni et al. (1997)	V	
silthiofam $C_{13}H_{21}NOSSi$ [175217-20-6] MXMXHPPIGKYTAR-UHFFFAOYSA-N	1.9		Maniere et al. (2011)	?	241, 165
tetradecamethylhexasiloxane $C_{14}H_{42}O_5Si_6$ (L6) [107-52-8] ADANNTOYRVPQLJ-UHFFFAOYSA-N	2.7×10^{-8}		Mazzoni et al. (1997)	V	

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Table A11.3: Silicon (Si) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
hexadecamethylheptasiloxane $C_{16}H_{48}O_6Si_7$ (L7) [541-01-5] NFVSFLUJRHRSJG-UHFFFAOYSA-N	7.6×10^{-9}		Mazzoni et al. (1997)	V	
octadecamethyloctasiloxane $C_{18}H_{54}O_7Si_8$ (L8) [556-69-4] VWGDPBQTSZDFMX-UHFFFAOYSA-N	3.3×10^{-9}		Mazzoni et al. (1997)	V	
hexamethylcyclotrisiloxane $C_6H_{18}O_3Si_3$ (D3) [541-05-9] HTDJPCNNEPUOOQ-UHFFFAOYSA-N	5.6×10^{-6}		Mazzoni et al. (1997)	V	
	6.4×10^{-6}		Alton and Browne (2022)	Q	819
	1.6×10^{-5}		Alton and Browne (2022)	Q	820
	2.5×10^{-6}		Alton and Browne (2022)	Q	821
octamethylcyclotetrasiloxane $C_8H_{24}O_4Si_4$ (D4) [556-67-2] HMMGMWAXVFQUOA-UHFFFAOYSA-N	7.3×10^{-7}		Xu and Kropscott (2014)	M	
	8.3×10^{-7}		Xu and Kropscott (2012)	M	87
	1.7×10^{-5}		Kochetkov et al. (2001)	M	297, 330
	1.7×10^{-5}		Kochetkov et al. (2001)	M	297, 331
	1.2×10^{-4}		Hamelink et al. (1996)	M	12
	1.5×10^{-6}		Xu and Kropscott (2014)	V	
	1.6×10^{-6}		Kochetkov et al. (2001)	V	
	8.3×10^{-7}		Mazzoni et al. (1997)	V	
	2.7×10^{-6}		Hamelink et al. (1996)	V	12
	5.4×10^{-7}		Alton and Browne (2022)	Q	819
	1.3×10^{-6}		Alton and Browne (2022)	Q	820
	1.1×10^{-6}		Alton and Browne (2022)	Q	821
	1.3×10^{-5}		Keshavarz et al. (2022)	Q	
	4.2×10^{-5}		Duchowicz et al. (2020)	Q	
	8.4×10^{-5}		Duchowicz et al. (2020)	?	185, 21
decamethylcyclopentasiloxane $C_{10}H_{30}O_5Si_5$ (D5) [541-02-6] XMSXQFUHVRWGNA-UHFFFAOYSA-N	2.8×10^{-7}		Xu and Kropscott (2014)	M	
	3.0×10^{-7}		Xu and Kropscott (2012)	M	
	3.4×10^{-5}		Kochetkov et al. (2001)	M	372, 330
	3.1×10^{-5}		Kochetkov et al. (2001)	M	372, 331
	7.4×10^{-5}		David et al. (2000)	M	72
	2.3×10^{-6}		Xu and Kropscott (2014)	V	
	2.2×10^{-6}		Kochetkov et al. (2001)	V	
	1.5×10^{-6}		Mazzoni et al. (1997)	V	
	2.3×10^{-7}		Alton and Browne (2022)	Q	819
	1.2×10^{-6}		Alton and Browne (2022)	Q	820
	3.1×10^{-6}		Alton and Browne (2022)	Q	821

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Table A11.3: Silicon (Si) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dodecamethylcyclohexasiloxane	4.0×10^{-7}		Xu and Kropscott (2012)	M	79
$C_{12}H_{36}O_6Si_6$	6.8×10^{-5}		Kochetkov et al. (2001)	M	372, 330
(D6)	1.5×10^{-4}		Kochetkov et al. (2001)	M	372, 331
[540-97-6]	3.9×10^{-6}		Kochetkov et al. (2001)	V	
IUMSDRXLFWAGNT-UHFFFAOYSA-N					
tetramethyldisiloxane-1,3-diol	1.8×10^{-1}		Mazzoni et al. (1997)	V	
$C_4H_{14}O_3Si_2$					
[1118-15-6]					
PFEAZKFNWPIFCV-UHFFFAOYSA-N					
hexamethyltrisiloxane-1,5-diol	3.4×10^{-3}		Mazzoni et al. (1997)	V	
$C_6H_{20}O_4Si_3$					
[3663-50-1]					
XYBQTTAROZGWOZ-UHFFFAOYSA-N					
octamethyltetrasiloxane-1,7-diol	2.7×10^{-3}		Mazzoni et al. (1997)	V	
$C_8H_{26}O_5Si_4$					
[3081-07-0]					
VERNMKKMBJGSQB-UHFFFAOYSA-N					
pentamethylcyclotrisiloxanol	1.1×10^{-3}		Mazzoni et al. (1997)	V	
$C_5H_{16}O_4Si_3$	1.2×10^{-1}		Alton and Browne (2022)	Q	819
(D3OH)	2.7×10^{-2}		Alton and Browne (2022)	Q	820
[106916-50-1]	1.5×10^{-3}		Alton and Browne (2022)	Q	821
OGNYSZJXUXVWRE-UHFFFAOYSA-N					
heptamethylcyclotetrasiloxanol	2.3×10^{-4}		Mazzoni et al. (1997)	V	
$C_7H_{22}O_5Si_4$	1.1×10^{-2}		Alton and Browne (2022)	Q	819
(D4OH)	1.1×10^{-2}		Alton and Browne (2022)	Q	820
[5290-02-8]	1.3×10^{-5}		Alton and Browne (2022)	Q	821
MLGUQSFCJNMKPT-UHFFFAOYSA-N					
nonamethylcyclopentasiloxanol	7.0×10^{-5}		Mazzoni et al. (1997)	V	
$C_9H_{28}O_6Si_5$	4.6×10^{-3}		Alton and Browne (2022)	Q	819
(D5OH)	2.0×10^{-2}		Alton and Browne (2022)	Q	820
[5290-04-0]	4.4×10^{-5}		Alton and Browne (2022)	Q	821
DKTKKERLEMHMHS-UHFFFAOYSA-N					
D3FormEst	2.8×10^{-4}		Alton and Browne (2022)	Q	819
$C_6H_{16}O_5Si_3$	3.2×10^{-4}		Alton and Browne (2022)	Q	820
TZIXLALHTGGYNZ-UHFFFAOYSA-N	1.7×10^{-3}		Alton and Browne (2022)	Q	821
D3OHFormEst	5.4		Alton and Browne (2022)	Q	819
$C_5H_{14}O_6Si_3$	9.9		Alton and Browne (2022)	Q	820
RMJPVGNUQFKGPC-UHFFFAOYSA-N	1.2×10^{-2}		Alton and Browne (2022)	Q	821
D3Hydroperoxide	6.9×10^{-2}		Alton and Browne (2022)	Q	819
$C_6H_{18}O_5Si_3$	1.9×10^{-3}		Alton and Browne (2022)	Q	820
JKDUHABXPCJOJB-UHFFFAOYSA-N	8.9×10^{-6}		Alton and Browne (2022)	Q	821

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Table A11.3: Silicon (Si) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
D3EtherHydroperoxide	8.4×10^{-1}		Alton and Browne (2022)	Q	819
$C_6H_{18}O_6Si_3$	1.9×10^{-2}		Alton and Browne (2022)	Q	820
LHGAYMWHCKTFJV-UHFFFAOYSA-N	1.7×10^{-2}		Alton and Browne (2022)	Q	821
D3FormEst2	1.2×10^{-2}		Alton and Browne (2022)	Q	819
$C_6H_{14}O_7Si_3$	9.2×10^{-3}		Alton and Browne (2022)	Q	820
WKTLUKWDJJZJCN-UHFFFAOYSA-N	2.0×10^{-2}		Alton and Browne (2022)	Q	821
D3OH2O1	2.4×10^{3}		Alton and Browne (2022)	Q	819
$C_4H_{14}O_5Si_3$	2.9		Alton and Browne (2022)	Q	820
UGEQNRIYBONGCP-UHFFFAOYSA-N	1.8×10^{-1}		Alton and Browne (2022)	Q	821
D4FormEst	2.4×10^{-5}		Alton and Browne (2022)	Q	819
$C_8H_{22}O_6Si_4$	8.5×10^{-5}		Alton and Browne (2022)	Q	820
PWVQOGDRWKITJQ-UHFFFAOYSA-N	8.8×10^{-5}		Alton and Browne (2022)	Q	821
D4OHFormEst	4.6×10^{-1}		Alton and Browne (2022)	Q	819
$C_7H_{20}O_7Si_4$	3.1		Alton and Browne (2022)	Q	820
AXBVNNKTZSENOJ-UHFFFAOYSA-N	1.2×10^{-4}		Alton and Browne (2022)	Q	821
1,1,1,3,5,5,5- heptamethyltrisiloxane $C_7H_{22}O_2Si_3$ [1873-88-7] QNWOFLWXQGHSRH-UHFFFAOYSA-N	1.1×10^{-7}		Ebert et al. (2023)	?	318
D4Hydroperoxide	5.8×10^{-3}		Alton and Browne (2022)	Q	819
$C_8H_{24}O_6Si_4$	4.4×10^{-4}		Alton and Browne (2022)	Q	820
IEOAKTNTPADFJB-UHFFFAOYSA-N	1.8×10^{-6}		Alton and Browne (2022)	Q	821
D4EtherHydroperoxide	7.1×10^{-2}		Alton and Browne (2022)	Q	819
$C_8H_{24}O_7Si_4$	4.5×10^{-3}		Alton and Browne (2022)	Q	820
BKBHFCQPJIYNBR-UHFFFAOYSA-N	1.5×10^{-5}		Alton and Browne (2022)	Q	821
D4FormEst2	1.0×10^{-3}		Alton and Browne (2022)	Q	819
$C_8H_{20}O_8Si_4$	1.8×10^{-3}		Alton and Browne (2022)	Q	820
WJOJQLFAIHHNFX-UHFFFAOYSA-N	2.9×10^{-4}		Alton and Browne (2022)	Q	821
D4OH2	2.1×10^{2}		Alton and Browne (2022)	Q	819
$C_6H_{20}O_6Si_4$	1.0		Alton and Browne (2022)	Q	820
ONAQLRRZBYFKLA-UHFFFAOYSA-N	8.3×10^{-5}		Alton and Browne (2022)	Q	821
D5FormEst	1.0×10^{-5}		Alton and Browne (2022)	Q	819
$C_{10}H_{28}O_7Si_5$	1.2×10^{-4}		Alton and Browne (2022)	Q	820
IGERVNZEGVJPED-UHFFFAOYSA-N	6.4×10^{-5}		Alton and Browne (2022)	Q	821
glycidoxypropyltrimethoxysilane $C_9H_{20}O_5Si$ [2530-83-8] BPSIOYPQMFLKFR-UHFFFAOYSA-N	1.4×10^{2}		Ebert et al. (2023)	?	318

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Table A11.3: Silicon (Si) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
D5OHFormEst	2.0×10^{-1}		Alton and Browne (2022)	Q	819
$C_9H_{26}O_8Si_5$	5.6		Alton and Browne (2022)	Q	820
KNIXZSAQQHGMJX-UHFFFAOYSA-N	4.7×10^{-5}		Alton and Browne (2022)	Q	821
D5Hydroperoxide	2.5×10^{-3}		Alton and Browne (2022)	Q	819
$C_{10}H_{30}O_7Si_5$	6.3×10^{-4}		Alton and Browne (2022)	Q	820
VGMLSGIAATVHBV-UHFFFAOYSA-N	1.1×10^{-6}		Alton and Browne (2022)	Q	821
D5EtherHydroperoxide	3.1×10^{-2}		Alton and Browne (2022)	Q	819
$C_{10}H_{30}O_8Si_5$	6.8×10^{-3}		Alton and Browne (2022)	Q	820
GSAPDUDDTPAQSH-UHFFFAOYSA-N	1.1×10^{-5}		Alton and Browne (2022)	Q	821
D5FormEst2	4.5×10^{-4}		Alton and Browne (2022)	Q	819
$C_{10}H_{26}O_9Si_5$	2.5×10^{-3}		Alton and Browne (2022)	Q	820
QFORSIVEJZTNKQ-UHFFFAOYSA-N	2.0×10^{-4}		Alton and Browne (2022)	Q	821
isobutyltriethoxysilane $C_{10}H_{24}O_3Si$ [17980-47-1] ALVYUZIFSCKIFP-UHFFFAOYSA-N	5.5×10^{-3}		Ebert et al. (2023)	?	316
methyltris(trimethylsiloxy)silane $C_{10}H_{30}O_3Si_4$ [17928-28-8] RGMZNZABJYWAEC-UHFFFAOYSA-N	2.9×10^{-8}		Ebert et al. (2023)	?	316
vinyltris(2-methoxyethoxy)silane $C_{11}H_{24}O_6Si$ [1067-53-4] WOXXJEVNDJOOLV-UHFFFAOYSA-N	5.9×10^{2}		Ebert et al. (2023)	?	318
tetrakis(trimethylsiloxy)silane $C_{12}H_{36}O_4Si_5$ [3555-47-3] VNRWTCZXQWOWIG-UHFFFAOYSA-N	2.6×10^{-8}		Ebert et al. (2023)	?	318
2-(3,4-epoxycyclohexyl) ethyltriethoxysilane $C_{14}H_{28}O_4Si$ [10217-34-2] UDUKMRHNZZLJRB-UHFFFAOYSA-N	9.9		Ebert et al. (2023)	?	318
D5OH2	8.9×10^{1}		Alton and Browne (2022)	Q	819
$C_8H_{26}O_7Si_5$	2.5		Alton and Browne (2022)	Q	820
AGIASGIZCMBNMT-UHFFFAOYSA-N	1.3×10^{-4}		Alton and Browne (2022)	Q	821
hexamethyldisilazane $C_6H_{19}NSi_2$ [999-97-3] FFUAGWLWBBFQJT-UHFFFAOYSA-N	1.1×10^{-1}		HSDB (2015)	Q	99

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Table A11.3: Silicon (Si) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
D3Organonitrate $C_6H_{17}NO_6Si_3$ WGZJMUDCTAXYSF-UHFFFAOYSA-N	2.4×10^{-3} 1.6×10^{-4} 1.0×10^{-4}		Alton and Browne (2022) Alton and Browne (2022) Alton and Browne (2022)	Q Q Q	819 820 821
D3EtherOrganonitrate $C_6H_{17}NO_7Si_3$ CJWFNCZCCFYEKP-UHFFFAOYSA-N	2.9×10^{-2} 1.7×10^{-3} 1.4×10^{-3}		Alton and Browne (2022) Alton and Browne (2022) Alton and Browne (2022)	Q Q Q	819 820 821
D4Organonitrate $C_8H_{23}NO_7Si_4$ CYMCLGYPZZKOOI-UHFFFAOYSA-N	2.0×10^{-4} 4.1×10^{-5} 7.5×10^{-6}		Alton and Browne (2022) Alton and Browne (2022) Alton and Browne (2022)	Q Q Q	819 820 821
D4EtherOrganonitrate $C_8H_{23}NO_8Si_4$ XHFUWVKWVPBCDO-UHFFFAOYSA-N	2.4×10^{-3} 3.8×10^{-4} 1.6×10^{-5}		Alton and Browne (2022) Alton and Browne (2022) Alton and Browne (2022)	Q Q Q	819 820 821
(3-aminopropyl)triethoxysilane $C_9H_{23}NO_3Si$ [919-30-2] WYTZZXDRDKSJID-UHFFFAOYSA-N	1.2×10^{2}		Ebert et al. (2023)	?	318
D5Organonitrate $C_{10}H_{29}NO_8Si_5$ KWHVDACCYNMOAR-UHFFFAOYSA-N	8.7×10^{-5} 4.9×10^{-5} 1.2×10^{-5}		Alton and Browne (2022) Alton and Browne (2022) Alton and Browne (2022)	Q Q Q	819 820 821
D5EtherOrganonitrate $C_{10}H_{29}NO_9Si_5$ BQINUVFPZWRRBW-UHFFFAOYSA-N	1.1×10^{-3} 5.7×10^{-4} 2.9×10^{-5}		Alton and Browne (2022) Alton and Browne (2022) Alton and Browne (2022)	Q Q Q	819 820 821
silafluofen $C_{25}H_{29}FO_2Si$ [105024-66-6] HPYNBECUCCGGPA-UHFFFAOYSA-N	4.0×10^{-1}		Ebert et al. (2023)	?	318
flusilazole $C_{16}H_{15}F_2N_3Si$ [85509-19-9] FQKUGOMFVDPBIZ-UHFFFAOYSA-N	2.7×10^{1} 4.4×10^{2}		Barcelo and Hennion (1997) Goodarzi et al. (2010)	X Q	567 568, 571
simeconazole $C_{14}H_{20}FN_3OSi$ [149508-90-7] YABFPHSQTSFWQB-UHFFFAOYSA-N	4.0×10^{3}		Ebert et al. (2023)	?	318
dichloromethylsilane CH_4Cl_2Si (methyldichlorosilane) [75-54-7] NWKBSEBOBPHMKL-UHFFFAOYSA-N	7.6×10^{-4}		HSDB (2015)	Q	99

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Table A11.3: Silicon (Si) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
etacelasil $C_{11}H_{25}O_6ClSi$ [37894-46-5] SLZWEMYSYKOWCG-UHFFFAOYSA-N	2.9×10^3		MacBean (2012a)	?	

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A11.4 Calcium (Ca)

Table A11.4: Calcium (Ca)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
prohexadione-calcium $C_{20}H_{22}O_{10}Ca$ [127277-53-6] VQIYODJWCVPJRC-UHFFFAOYSA-N	5.2×10^4		Maniere et al. (2011)	?	241, 165

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A11.5 Zinc (Zn)

Table A11.5: Zinc (Zn)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
zineb $C_4H_6N_2S_4Zn$ [12122-67-7] AMHNZOICSMBGDH-UHFFFAOYSA-L	2.7×10^3 $>3.7\times10^3$ $>1.9\times10^2$		Mackay et al. (2006d) MacBean (2012b) Maniere et al. (2011)	V X ?	 350 12, 165
ziram $C_6H_{12}N_2S_4Zn$ [137-30-4] DUBNHZYBDBBJHD-UHFFFAOYSA-L	1.6×10^4 2.1×10^5 1.8×10^2		HSDB (2015) Mackay et al. (2006d) Maniere et al. (2011)	V V ?	 165
mancozeb $C_8H_{12}MnN_4S_8Zn$ [8018-01-7] CHNQZRKUZPNOOH-UHFFFAOYSA-J	1.6×10^1		Maniere et al. (2011)	?	12, 165

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A11.6 Arsenic (Sn)

Table A11.6: Arsenic (Sn)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
methylarsine CH_5As [593-52-2] IDDBICIFODFKQO-UHFFFAOYSA-N	9.0×10^{-6}		Ebert et al. (2023)	?	318
ethylarsine C_2H_7As [593-59-9] OSAGMAAQMRQLLW-UHFFFAOYSA-N	1.5×10^{-5}		Ebert et al. (2023)	?	316
diethyl arsine $C_4H_{11}As$ [692-42-2] JZCIYTSNUPIOMK-UHFFFAOYSA-N	2.2×10^{-5}		HSDB (2015)	Q	99
phenylarsine oxide C_6H_5AsO [637-03-6] BQVCCPGCDUSGOE-UHFFFAOYSA-N	9.0×10^{-1}		Bartelt-Hunt et al. (2008)	?	21
diphenylarsanylformonitrile $C_{13}H_{10}AsN$ [23525-22-6] BDHNJKLLVSRGDK-UHFFFAOYSA-N	1.1×10^{3}		Ebert et al. (2023)	?	318
dichloro(methyl)arsane CH_3AsCl_2 [593-89-5] VXRMBBLRHSRVDK-UHFFFAOYSA-N	5.1×10^{-3}		Ebert et al. (2023)	?	318
lewisite $C_2H_2AsCl_3$ [541-25-3] GIKLTQKNOXNBNY-OWOJBTEDSA-N	4.5×10^{-2} 3.1×10^{-2} 5.2×10^{-3} 3.7×10^{-2}		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020) Bartelt-Hunt et al. (2008)	V V Q ?	186 21
diphenylchloroarsine $C_{12}H_{10}AsCl$ [712-48-1] YHHKGKCOLGRKKB-UHFFFAOYSA-N	6.1×10^{1}		Ebert et al. (2023)	?	318
lewisite oxide C_2H_2AsClO [3088-37-7] MVCVAGFCWDFQQX-OWOJBTEDSA-N	5.2×10^{-3}		Bartelt-Hunt et al. (2008)	?	21

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Table A11.6: Arsenic (Sn) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\mathrm{mol}}{\mathrm{m^3\,Pa}}\right]$	$\frac{\mathrm{d}\ln H_s^{cp}}{\mathrm{d}(1/T)}$ [K]	Reference	Type	Note
phenyldichloroarsine $C_6H_5AsCl_2$ [696-28-6] UDHDFEGCOJAVRE-UHFFFAOYSA-N	3.3×10^{-1}		HSDB (2015)	Q	99
adamsite $C_{12}H_9AsClN$ [578-94-9] PBNSPNYJYOYWTA-UHFFFAOYSA-N	3.0×10^{2}		HSDB (2015)	Q	99

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A11.7 Selenium (Se)

Table A11.7: Selenium (Se)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dimethyl selenide C_2H_6Se [593-79-3] RVIXKDRPFPUUOO-UHFFFAOYSA-N	1.2×10^{-2} 4.3×10^{-3} 5.7×10^{-3}		Keshavarz et al. (2022) Duchowicz et al. (2020) Duchowicz et al. (2020)	Q Q ?	 185, 21
dimethyl diselenide $C_2H_6Se_2$ [7101-31-7] VLXBWPOEOIIREY-UHFFFAOYSA-N	1.4×10^{-3}		Ebert et al. (2023)	?	318
2-amino-4-(methylselenyl)butyric acid $C_5H_{11}NO_2Se$ (selenium methionine) [1464-42-2] RJFAYQIBOAGBLC-UHFFFAOYSA-N	2.9×10^{5}		HSDB (2015)	Q	99

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A11.8 Tin (Sn)

Table A11.8: Tin (Sn)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tetramethylstannane $C_4H_{12}Sn$ (tetramethyltin) [594-27-4] VXKWYPOMXBVZSJ-UHFFFAOYSA-N	9.4×10^{-6} 9.7×10^{-6} 1.2×10^{-5}	3800	Abraham and Nasehzadeh (1981) Abraham et al. (1990) Abraham (1979)	M ? ?	
tetraethylstannane $C_8H_{20}Sn$ (tetraethyltin) [597-64-8] RWWNQEOPUOCKGR-UHFFFAOYSA-N	1.6×10^{-5} 6.1×10^{-6} 5.7×10^{-6} 1.1×10^{-5}	 6100 	HSDB (2015) Abraham et al. (1990) Abraham and Nasehzadeh (1981) Abraham (1979)	Q ? ? ?	99 822
tetrabutylstannane $C_{16}H_{36}Sn$ (tetra-butyl tin) [1461-25-2] AFCAKJKUYFLYFK-UHFFFAOYSA-N	1.6×10^{-6}		HSDB (2015)	Q	99
triphenyltin hydroxide $C_{18}H_{16}OSn$ [76-87-9] BFWMWWXRWVJXSE-UHFFFAOYSA-M	2.3×10^{1} 3.8×10^{-1}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186
hexabutyldistannoxane $C_{24}H_{54}OSn_2$ (bis(tributyltin)oxide) [56-35-9] APQHKWPGGHMYKJ-UHFFFAOYSA-N	7.6×10^{1}		HSDB (2015)	V	
hexakis(2-methyl-2-phenylpropyl)distannoxane $C_{60}H_{78}OSn_2$ (fenbutatin oxide) [13356-08-6] HOXINJBQVZWYGZ-UHFFFAOYSA-N	4.9×10^{3}		HSDB (2015)	V	
fentin acetate $C_{20}H_{18}O_2Sn$ [900-95-8] WDQNIWFZKXZFAY-UHFFFAOYSA-M	2.0×10^{3}		Ebert et al. (2023)	?	365
1-(tricyclohexylstannyl)1H-1,2,4-triazole $C_{20}H_{35}N_3Sn$ (azocyclotin) [41083-11-8] ONHBDDJJTDTLIR-UHFFFAOYSA-N	4.6×10^{6} 4.6×10^{6} 1.2		Duchowicz et al. (2020) HSDB (2015) Duchowicz et al. (2020)	V V Q	186

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A11.9 Mercury (Hg)

Table A11.9: Mercury (Hg)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
dimethylmercury	1.3×10^{-3}	2700	Talmi and Mesmer (1975)	M	
C_2H_6Hg	2.1×10^{-3}		Abraham et al. (2008)	C	
[593-74-8]	1.3×10^{-3}	2700	WHO (1990)	C	
ATZBPOVXVPIOMR-UHFFFAOYSA-N	1.0×10^{-3}	3000	Abraham et al. (2008)	Q	218
	1.5×10^{-3}		Schroeder and Munthe (1998)	?	21
	1.3×10^{-3}	2700	Schroeder and Munthe (1998)	?	21
	3.1×10^{-3}		Iverfeldt and Persson (1985)	?	219
diethylmercury	1.0×10^{-3}	3800	Abraham et al. (2008)	Q	218
$C_4H_{10}Hg$					
[627-44-1]					
SPIUPAOJDZNUJH-UHFFFAOYSA-N					
dipropylmercury	5.6×10^{-4}	4600	Abraham et al. (2008)	Q	218
$C_6H_{14}Hg$					
[628-85-3]					
UZTYYBPPVOXULF-UHFFFAOYSA-N					
diisopropylmercury	3.9×10^{-4}	4600	Abraham et al. (2008)	Q	218
$C_6H_{14}Hg$					
[1071-39-2]					
UVUGOJQWNVFTRT-UHFFFAOYSA-N					
dibutylmercury	2.9×10^{-4}	5400	Abraham et al. (2008)	Q	218
$C_8H_{18}Hg$					
[629-35-6]					
CCYKQVBIPYDCKS-UHFFFAOYSA-N					
diphenylmercury	2.8×10^{2}	8800	Abraham et al. (2008)	Q	218
$C_{12}H_{10}Hg$					
[587-85-9]					
HWMTUNCVVYPZHZ-UHFFFAOYSA-N					
hydroxymethylmercury	9.8×10^{2}	7700	Iverfeldt and Persson (1985)	M	
CH_3HgOH	1.5×10^{3}		Shon et al. (2005)	?	823
[1184-57-2]					
KRZWEBVPFGCYMY-UHFFFAOYSA-M					
phenyl mercuric ethanoate	1.5×10^{4}		Suntio et al. (1988)	V	12
$C_8H_8HgO_2$					
[62-38-4]					
XEBWQGVWTUSTLN-UHFFFAOYSA-M					
(3-cyanoguanidino)methylmercury	7.0×10^{4}		HSDB (2015)	Q	99
$C_3H_6N_4Hg$					
(methylmercuric dicyanamide)					
[502-39-6]					
JVJUWCMBRUMDDQ-UHFFFAOYSA-N					

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Table A11.9: Mercury (Hg) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
chloromethylmercury CH_3HgCl [115-09-3] BABMCXWQNSQAOC-UHFFFAOYSA-M	2.2×10^{1} 1.5×10^{1} 2.0×10^{1} 2.6×10^{1} 1.5×10^{1}	1800 4100 5300	Iverfeldt and Lindqvist (1982) Talmi and Mesmer (1975) WHO (1990) Abraham et al. (2008) Schroeder and Munthe (1998) Iverfeldt and Persson (1985)	M M C Q ? ?	33, 824 87 33 214 80, 21 219
chloroethylmercury C_2H_5HgCl [107-27-7] QWUGXIXRFGEYBD-UHFFFAOYSA-M	1.5×10^{1}	5600	Abraham et al. (2008)	Q	218
chloropropylmercury C_3H_7HgCl [2440-40-6] ZLAYJSKLDWSALK-UHFFFAOYSA-M	1.2×10^{1}	5900	Abraham et al. (2008)	Q	218
chloroisopropylmercury C_3H_7HgCl [30615-19-1] YOKZNQICWABELX-UHFFFAOYSA-M	9.9	6000	Abraham et al. (2008)	Q	218
chlorobutylmercury C_4H_9HgCl [543-63-5] OKPMTXZRMGMMOO-UHFFFAOYSA-M	8.8	6300	Abraham et al. (2008)	Q	218
chloropentylmercury $C_5H_{11}HgCl$ [544-15-0] UHFZINPMKCNPQL-UHFFFAOYSA-M	7.0	6700	Abraham et al. (2008)	Q	218
chlorophenylmercury C_6H_5HgCl [100-56-1] AWGTVRDHKJQFAX-UHFFFAOYSA-M	3.8×10^{2} 9.2×10^{2}	 7400	Abraham et al. (2008) Abraham et al. (2008)	V Q	 218
2-methoxyethylmercury chloride $CH_3OC_2H_4HgCl$ (aretan) [123-88-6] VJTAZCKMHINUKO-UHFFFAOYSA-M	3.9×10^{3}	8600	Abraham et al. (2008)	Q	218
bromomethylmercury CH_3HgBr [506-83-2] ZDHHIJSLJCLMPX-UHFFFAOYSA-M	 3.7	4800	Abraham et al. (2008) Iverfeldt and Persson (1985)	Q ?	214 219

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Table A11.9: Mercury (Hg) (. . . continued)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
bromoethylmercury C_2H_5HgBr [107-26-6] UREACWLAXSOUKG-UHFFFAOYSA-M	3.0	5200	Abraham et al. (2008)	Q	218
bromophenylmercury C_6H_5HgBr [1192-89-8] PUPHNPSAIJQNEE-UHFFFAOYSA-M	1.8×10^{2}	6900	Abraham et al. (2008)	Q	218
iodomethylmercury CH_3HgI [143-36-2] JVDIOYBHEYUIBM-UHFFFAOYSA-M	2.0 5.8×10^{-1}	4800	Abraham et al. (2008) Iverfeldt and Persson (1985)	Q ?	218 219
iodoethylmercury C_2H_5HgI [2440-42-8] BYIGJUQTUPMNMF-UHFFFAOYSA-M	2.5	5200	Abraham et al. (2008)	Q	218
iodophenylmercury C_6H_5HgI [823-04-1] BISBXZWWFIOZSX-UHFFFAOYSA-M	9.0×10^{1}	6700	Abraham et al. (2008)	Q	218

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A11.10 Lead (Pb)

Table A11.10: Lead (Pb)

Substance Formula (Trivial Name) [CAS Registry Number] InChIKey	H_s^{cp} (at $T^{\ominus}$) $\left[\frac{\text{mol}}{\text{m}^3\,\text{Pa}}\right]$	$\frac{\text{d}\ln H_s^{cp}}{\text{d}(1/T)}$ [K]	Reference	Type	Note
tetramethyl lead $C_4H_{12}Pb$ [75-74-1] XOOGZRUBTYCLHG-UHFFFAOYSA-N	1.6×10^{-5}		HSDB (2015)	V	
ethyltrimethylplumbane $C_5H_{14}Pb$ [1762-26-1] KHQJREYATBQBHY-UHFFFAOYSA-N	2.8×10^{-5}		HSDB (2015)	Q	99
diethyldimethylplumbane $C_6H_{16}Pb$ (diethyldimethyl lead) [1762-27-2] OLOAJSHVLXNSQV-UHFFFAOYSA-N	2.1×10^{-5}		HSDB (2015)	Q	99
triethylmethylplumbane $C_7H_{18}Pb$ (methyltriethyl lead) [1762-28-3] KGFRUGHBHNUHOS-UHFFFAOYSA-N	1.6×10^{-5}		HSDB (2015)	Q	99
tetraethyl lead $C_8H_{20}Pb$ [78-00-2] MRMOZBOQVYRSEM-UHFFFAOYSA-N	1.3×10^{-5} 1.3×10^{-5}	6400	Feldhake and Stevens (1963) Abraham (1979)	M ?	
trimethyl lead chloride C_3H_9ClPb [1520-78-1] HPQRSQFZILKRDH-UHFFFAOYSA-M	2.5		Ebert et al. (2023)	?	316
triethyl lead chloride $C_6H_{15}ClPb$ [1067-14-7] UQWYUMLFPUILRT-UHFFFAOYSA-M	2.1×10^{5} 1.1×10^{-3}		Duchowicz et al. (2020) Duchowicz et al. (2020)	V Q	186

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Appendix: Notes

1) A detailed temperature dependence with more than one parameter is available in the original publication. Here, only the temperature dependence at 298.15 K according to the van 't Hoff equation is presented.

2) Clever et al. (2014) recommend the data from Rettich et al. (2000).

3) Vapor pressure data for water from Wagner and Pruss (1993) was needed to calculate H_s.

4) The data from Millero et al. (2002a) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-130.91491 + 6700.12242/T + 17.04684 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

5) Almost the same data were also published in Millero et al. (2002b).

6) The data from Millero et al. (2002b) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-118.73105 + 6163.97787/T + 15.22401 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

7) Almost the same data were also published in Millero et al. (2002a).

8) The data from Rettich et al. (2000) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-179.13831 + 8707.17767/T + 24.33473 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

9) The data from Sherwood et al. (1991) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-197.67462 + 9515.09306/T + 27.11204 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

10) The data from Rettich et al. (1981) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-178.21340 + 8672.23354/T + 24.19307 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

11) Measured at high temperature and extrapolated to $T^{\ominus}$ = 298.15 K.

12) Value at T = 293 K.

13) Value at T = 273 K.

14) Value at T = 310 K.

15) The data from Murray and Riley (1969) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-180.22078 + 8760.50130/T + 24.49289 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

16) The data from Shoor et al. (1969) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-91.44799 + 4548.67245/T + 11.38821 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

17) The data from Carpenter (1966) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-130.04464 + 6687.45227/T + 16.90114 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

18) The data from Morrison and Billett (1952) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-167.89288 + 8254.02144/T + 22.62741 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

19) The data from Winkler (1891b) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-155.30315 + 7638.78869/T + 20.77945 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

20) Calculated using machine learning matrix completion methods (MCMs).

21) Several references are given in the list of Henry's law constants but not assigned to specific species.

22) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-161.84252 + 7966.66767/T + 21.73409 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

23) The partial pressure of water vapor (needed to convert some Henry's law constants) was calculated using the formula given by Buck (1981). The quantities A and α from Dean and Lange (1999) were assumed to be identical.

24) Value at "room temperature".

25) Clever et al. (2014) recommend the data from Battino (1981).

26) Battino (1981) concludes that ozone aqueous chemistry needs further clarification. Data from Roth and Sullivan (1981) are recommended, in spite of limitations and assumptions of the data.

27) Roth and Sullivan (1981) found that H_s depends on the concentration of OH^-.

28) Value at T = 291 K.

29) Value given here as quoted by Durham et al. (1981).

30) Lide and Frederikse (1995) present an unusually low value for the Henry solubility of ozone. They refer to Battino (1981) as the source but the quoted value cannot be found there.

31) Parker (1992) assume that the free energy of solvation of atomic hydrogen is equal to that of He because of a similar van der Waals radius.

32) Roduner and Bartels (1992) say that the free energy of solvation $\Delta G^{\mathrm{H}}_{\mathrm{solv}}$ (and therefore Henry's law constant) of atomic hydrogen is approximated well by that of molecular hydrogen. However, they apparently do not give a value for $\Delta G^{\mathrm{H}}_{\mathrm{solv}}$.

33) Fitting the temperature dependence $\mathrm{d}\ln H/\mathrm{d}(1/T)$ produced a low correlation coefficient ($r^2 < 0.9$). The data should be treated with caution.

34) Data digitized from Figs. 2 and 3. in Schmidt (1979).

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35) The data from Gordon et al. (1977) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-158.95051 + 6959.76267/T + 21.73478\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

36) The data from Crozier and Yamamoto (1974) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-129.44163 + 5676.58091/T + 17.31002\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

37) The data presented for hydrogen in Tab. II of Shoor et al. (1969) appear to be incorrect and are not reproduced here.

38) Value at T = 303 K.

39) The data from Morrison and Billett (1952) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-94.36490 + 4110.23880/T + 12.07743\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

40) The data from Braun (1900) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(171.59451 - 6856.02728/T - 28.14739\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

41) The data from Winkler (1891a) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-103.47250 + 4506.63123/T + 13.44160\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

42) Fitting the temperature dependence $\mathrm{d}\ln H/\mathrm{d}(1/T)$ produced a very low correlation coefficient ($r^2 < 0.5$). The data should be treated with caution.

43) The paper by Bunsen (1855a) was written in German. English versions with the same data were published by Bunsen (1855b) and Bunsen (1855c).

44) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-98.78036 + 4298.15060/T + 12.74131\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

45) Young (1981a) recommend the data from Muccitelli and Wen (1978).

46) The data from Muccitelli and Wen (1978) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-103.11330 + 4676.56978/T + 13.28348\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

47) Calculated from correlation between the polarizabilities and solubilities of stable gases. The temperature dependence is an estimate of the upper limit.

48) Jacob (1986) assumed the temperature dependence to be the same as for water.

49) In the abstract, Schwartz (1984) gives a range of 9.9 $\mathrm{mol/(m^3\,Pa)} < H_s^{cp} < 3.0\times10^1$ $\mathrm{mol/(m^3\,Pa)}$. The mean value of this range (2.0×10^1 $\mathrm{mol/(m^3\,Pa)}$) has been used by Lelieveld and Crutzen (1991), Pandis and Seinfeld (1989), and Jacob (1986).

50) The value of $H_s^{\ominus}$ was taken from Schwartz (1984).

51) Erratum for page 264 of Fogg and Sangster (2003): The second value from their Ref. [10] refers to 291.15 K, not 281.15 K.

52) This value is a correction of the solubility published by Lind and Kok (1986).

53) This value was measured at low pH. It is superseded by a later publication of the same group (Lind and Kok, 1994).

54) Pandis and Seinfeld (1989) cite an incorrect value from Lind and Kok (1986), see erratum by Lind and Kok (1994).

55) The data from Rettich et al. (1984) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-187.67954 + 8903.42524/T + 25.60079\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

56) The data from Murray et al. (1969) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-174.95275 + 8370.22025/T + 23.67878\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

57) The data from Morrison and Billett (1952) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-193.68175 + 9249.63150/T + 26.45117\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

58) Value at T = 311 K.

59) The data from Braun (1900) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(291.66324 - 11637.66767/T - 46.44134\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

60) The data from Winkler (1891b) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-164.15156 + 7906.86704/T + 22.05399\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

61) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-163.64571 + 7887.30480/T + 21.97696\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

62) Tsuji et al. (1990) provide effective Henry's law constants at several pH values. Here, only the value at pH 5.8 is shown for the (acidic) S-compounds, and the value at pH 8.6 for the alkaline N-compounds.

63) Value given here as quoted by Betterton (1992).

64) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(206.08500 - 7165.18642/T - 32.18383\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

65) Bone et al. (1983) gives Carter et al. (1968) as the source. However, no data were found in that reference.

66) There is a typo in Sander et al. (2011): The value for A should be -10.19, not 10.19.

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67) Modarresi et al. (2007) use different descriptors for their calculations. They conclude that GA/RBFN is the best QSPR model. Only these results are shown here.

68) Incorrect data are given by Burkholder et al. (2019) for HN_3. The correct parameter for the temperature dependence is: A = -10.19 (R. E. Huie, pers. comm. 2021).

69) Incorrect data are given by Burkholder et al. (2015) for HN_3. The correct parameter for the temperature dependence is: A = -10.19 (R. E. Huie, pers. comm. 2021).

70) Solubility in sea water.

71) The data from Weiss and Price (1980) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-180.63611 + 9824.20147/T + 24.46112\ln(T))\ \mathrm{mol/(m^3\,Pa)}$ with T in K.

72) Value at T = 296 K.

73) The data from Roth (1897) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-125.17909 + 7706.80638/T + 15.96486\ln(T))\ \mathrm{mol/(m^3\,Pa)}$ with T in K.

74) Value given here as quoted by Gabel and Schultz (1973).

75) Value given here as quoted by Sy and Hasbrouck (1964).

76) The H298 and A,B,C data listed in Table 5.4 of Sander et al. (2011) are inconsistent, with 94 % difference.

77) The H298 and A,B,C data listed in Table 5.4 of Sander et al. (2006) are inconsistent, with 94 % difference.

78) A minus sign is missing in the fitting parameter presented by Young (1981b). It should be -62.8086, not 62.8086.

79) Value at T = 297 K.

80) Value at T = 288 K.

81) The data from Winkler (1901) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-184.00012 + 8924.34832/T + 25.13228\ln(T))\ \mathrm{mol/(m^3\,Pa)}$ with T in K.

82) The data from Loomis (1928) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-223.88313 + 10620.37030/T + 31.13453\ln(T))\ \mathrm{mol/(m^3\,Pa)}$ with T in K.

83) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-160.19223 + 7888.02642/T + 21.56401\ln(T))\ \mathrm{mol/(m^3\,Pa)}$ with T in K.

84) Incorrect data are given by Burkholder et al. (2019) for NO. The correct parameters for the temperature dependence are: A = -163.86, B = 8234, C = 22.816 (R. E. Huie, pers. comm. 2021).

85) Incorrect data are given by Burkholder et al. (2015) for NO. The correct parameters for the temperature dependence are: A = -163.86, B = 8234, C = 22.816 (R. E. Huie, pers. comm. 2021).

86) The fitting parameters A, B, C, and D in Table I of Wilhelm et al. (1977) do not reproduce the data in their Table III.

87) Value at T = 295 K.

88) Pandis and Seinfeld (1989) refer to Schwartz (1984) as the source but the quoted value cannot be found there.

89) Value obtained by estimating the diffusion coefficient for NO_3 to be $D = 1.0\times10^{-5}\ \mathrm{cm^2/s}$.

90) Jacob (1986) assume that NO_3 has the same Henry's law constant as HNO_3.

91) Seinfeld and Pandis (1998) probably refer to the incorrect value given by Pandis and Seinfeld (1989).

92) Calculated from the solvation free energy.

93) Calculated from the solvation free energy.

94) Calculated from the solvation free energy.

95) This value was extrapolated from data at T = 230 K and T = 273 K.

96) Robinson et al. (1997) applied an empirical correlation between Henry's law solubilities and boiling points from Schwartz and White (1981).

97) Estimate based on the relation between boiling points and Henry's law constants for other nitrogen oxides from Schwartz and White (1981).

98) Fast, irreversible hydrolysis is assumed, which is equivalent to an infinite effective Henry's law constant.

99) Calculated based on the method by Meylan and Howard (1991).

100) Lelieveld and Crutzen (1991) assume the temperature dependence to be the same as for $a(H^+)a(NO_3^-)/p(HNO_3)$ in Schwartz and White (1981).

101) $H_s' = 2.6\times10^7\times\exp\left(8700\ \mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

102) $H_s' = 2.4\times10^7\times\exp\left(8700\ \mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

103) Pandis and Seinfeld (1989) refer to Schwartz (1984) as the source but it is probably from Schwartz and White (1981).

104) The value is incorrect. See erratum by Brimblecombe and Clegg (1989).

105) Möller and Mauersberger (1992) assumed the solubility of HNO_4 to be comparable to that of HNO_3.

106) $H_s' = 9.4\times10^1\times\exp\left(7400\ \mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

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107) The data from Dean et al. (1973) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-164.52717 + 8214.77776/T + 21.97482 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

108) The data from Ashton et al. (1968) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-279.21972 + 13536.60588/T + 38.97386 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

109) The data from Dean et al. (1973) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-318.29953 + 15733.17858/T + 44.55320 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

110) The value presented here appears to be the total solubility of chlorine (i.e., the sum of Cl_2 and HOCl) at a partial pressure of $p(Cl_2) = 101325$ Pa. This is different from Henry's law constant, which is defined at extrapolation to infinite dilution.

111) Young (1983) recommends values calculated from Table 1 of Adams and Edmonds (1937). Thus, the data refer to effective values that take into account the hydrolysis in the aqueous-phase:

$$H_{s,\mathrm{eff}} = ([Cl_2] + [HOCl])/p(Cl_2)$$

In addition, the values apply to a partial pressure of $p(Cl_2) = 101325$ Pa, and not to infinite dilution.

112) The same experimental data were also published by Whitney and Vivian (1941b).

113) The data from Yakovkin (1900) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-122.31264 + 7690.40834/T + 15.63947 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

114) Leaist (1986) converted the total solubility of chlorine in pure water from Adams and Edmonds (1937) to an intrinsic Henry's law constant.

115) Adams and Edmonds (1937) re-analyzed the data from Yakovkin (1900) and Arkadiev (1918), considering deviations from the perfect gas law. They calculated the total solubility of chlorine (i.e., the sum of Cl_2 and HOCl) at several partial pressures of Cl_2. This is different from Henry's law constant, which is defined at extrapolation to infinite dilution.

116) Arkadiev (1918) re-analyzed the measurements of Yakovkin (1900). In addition to the data between 15 °C and 83.4 °C, he also analyzed the experimental results at 0 °C and obtained a dimensionless Henry solubility of $H_s^{cc} = 4.115$ at that temperature.

117) The value of ΔH° listed in Table 2 of Bartlett and Margerum (1999) is incorrect. The correct value can be found in the text on page 3411.

118) Wilhelm et al. (1977) present a fitting function for Cl_2 based on four papers which are cited in the footnotes of Table I. However, Bunsen (1855b) and Bunsen (1855c) don't contain any data for Cl_2, and the data from Whitney and Vivian (1941a) and Whitney and Vivian (1941b) are inconsistent with the fitting function.

119) Calculated from the free energy of solution by Schwarz and Dodson (1984).

120) $H_s' = 2.0 \times 10^7 \ \frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

121) $H_s' = 2.0 \times 10^7 \times \exp\left(9000\ \mathrm{K}\left(\frac{1}{T} - \frac{1}{T^\ominus}\right)\right) \frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

122) $H_s' = 2.0 \times 10^7 \times \exp\left(9000\ \mathrm{K}\left(\frac{1}{T} - \frac{1}{T^\ominus}\right)\right) \frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

123) $H_s' = 2.0 \times 10^7 \times \exp\left(9000\ \mathrm{K}\left(\frac{1}{T} - \frac{1}{T^\ominus}\right)\right) \frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

124) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(9.16427 + 45.13997/T - 1.92853 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

125) Pandis and Seinfeld (1989) refer to Marsh and McElroy (1985) as the source but the quoted value cannot be found there.

126) This value was extrapolated from data at T = 215 K and T = 263 K.

127) Value at pH = 6.5.

128) Value at T = 200 K.

129) Secoy and Cady (1941) measured the gas/aqueous equilibrium constant $p(Cl_2O)/c(HOCl)^2$ but not the intrinsic Henry's law constant of Cl_2O.

130) Ourisson and Kastner (1939) measured the gas/aqueous equilibrium constant $p(Cl_2O)/c(HOCl)^2$ but not the intrinsic Henry's law constant of Cl_2O.

131) The data from this work were fitted to the 3-parameter equation: $H_s^{cp} = \exp(1680.49677 - 69933.08019/T - 254.37188 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

132) The gas/aqueous equilibrium constant $p(Cl_2O)/c(HOCl)^2$ was combined with the temperature-dependent aqueous-phase hydration constant $c(HOCl)^2/c(Cl_2O)$ from Roth (1929) in order to calculate the intrinsic Henry's law constant of Cl_2O.

133) Data for the equilibrium between gaseous Cl_2O and aqueous HOCl were taken from Secoy and Cady (1941).

134) Data for the equilibrium between gaseous Cl_2O and aqueous HOCl were taken from Ourisson and Kastner (1939).

135) Value at T = 277 K.

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136) The recommended value from Wilhelm et al. (1977) appears to be dubious as it refers to Secoy and Cady (1941) who do not provide a value for the intrinsic Henry's law constant of Cl_2O.

137) Young (1983) cites data from Secoy and Cady (1941). However, that paper only describes the equilibrium between gas-phase Cl_2O and aqueous-phase HOCl. A Henry's law constant of Cl_2O is not provided. In addition, the values given by Young (1983) are not extrapolated to infinite dilution but to 1 atm partial pressure of Cl_2O. It is not explained how the nonlinear pressure dependence was extrapolated to 1 atm.

138) Wilhelm et al. (1977) cite Secoy and Cady (1941) as the source for their value. However, that paper only describes the equilibrium between gas-phase Cl_2O and aqueous-phase HOCl. A Henry's law constant of Cl_2O is not provided.

139) Even though Haller and Northgraves (1955) have been cited several times as the source of the ClO_2 solubility data, they did not perform any measurements. They took the data from the 1952 edition of the Kirk-Othmer Encyclopedia of Chemical Technology which apparently reproduced data from Holst (1944).

140) Derived as a fitting parameter used in numerical modeling.

141) Robinson et al. (1997) assumed that the entropy of vaporization is the same for HOCl and $ClNO_3$ according to Trouton's rule. On their page 3592, they mention a value of 7 M/atm at 250 K. However, checking their Fig. 9 and applying the temperature-dependence equation from their Tab. 3, it seems that the value of 7 M/atm refers to 298 K, not 250 K.

142) Dubik et al. (1987) measured the solubility in concentrated salt solutions (natural brines).

143) Value given here as quoted by McCoy et al. (1990).

144) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-148.75612 + 9709.79389/T + 19.53402\ln(T))\ \mathrm{mol/(m^3\,Pa)}$ with T in K.

145) $H_s' = 8.2\times10^9 \times \exp\left(10000\ \mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

146) $H_s' = 1.3\times10^{10} \times \exp\left(10000\ \mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

147) $H_s' = 7.0\times10^9 \times \exp\left(10000\ \mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

148) Chameides and Stelson (1992) give a value of $H_s' = 7.1\times10^9 \times \exp\left(6100\ \mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$. They refer to Jacob (1986) and Chameides (1984) as the source but this value cannot be found there.

149) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-60.28318 + 2830.41867/T + 8.66642\ln(T))\ \mathrm{mol/(m^3\,Pa)}$ with T in K.

150) The value is from Table 1 of the paper. However, *J. Geophys. Res.* forgot to print the tables and I received them directly from the author.

151) The value presented for HOBr is incorrect. A corrected version was later published by Burkholder et al. (2019).

152) Fickert (1998) extracted a value from wetted-wall flow tube experiments. However, it was later discovered that under the experimental conditions no evaluation of H_s is possible (J. Crowley, pers. comm., 1999).

153) Value at T = 275 K.

154) Value at T = 290 K.

155) Calculated using data from Wagman et al. (1982) and the aqueous-phase equilibrium $Cl_2 + Br_2 \rightleftharpoons 2\ BrCl$ from Wang et al. (1994).

156) Thompson and Zafiriou (1983) quote a paper as the source that gives only the solubility but not the Henry's law constant.

157) Calculated from the free energy of solution by Schwarz and Bielski (1986).

158) $H_s' = 2.5\times10^{10} \times \exp\left(9800\ \mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

159) $H_s' = 2.1\times10^{10} \times \exp\left(9800\ \mathrm{K}\left(\frac{1}{T}-\frac{1}{T^\ominus}\right)\right)\frac{\mathrm{mol^2}}{\mathrm{m^6\,Pa}}$

160) Saiz-Lopez et al. (2014) refer to Saiz-Lopez et al. (2008) as the source but the quoted value cannot be found there.

161) It is unclear to which isomer the value of the Henry's law constant refers to.

162) Assumed to be infinity by analogy with INO_3.

163) Thompson and Zafiriou (1983) assume that $H_s^{cp}(\mathrm{HOI})$ is between 4.4×10^{-1} mol/(m^3 Pa) and 4.4×10^{2} mol/(m^3 Pa).

164) Badia et al. (2019) assume that INO_2 has the same Henry's law constant as $BrNO_2$.

165) Data taken from the AGRITOX database file agritox-20210608.zip.

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166) Fogg and Young (1988) provide two different fitting functions: One for $T < 283.2$ K and one for $T > 283.2$ K. At $T = 283.2$ K, the functions have different values and different slopes. Here, only the function that is valid at $T^{\ominus}$ is used.

167) The data from Clarke and Glew (1971) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-133.37135 + 7422.07576/T + 17.82903 \ln(T))$ mol/(m^3 Pa) with T in K.

168) The data from Schoenfeld (1855) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(98.96644 - 3021.28876/T - 16.78233 \ln(T))$ mol/(m^3 Pa) with T in K.

169) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-122.57010 + 6962.28299/T + 16.20245 \ln(T))$ mol/(m^3 Pa) with T in K.

170) The parameter fit for the temperature dependence is incorrect. A corrected version was later presented by Iliuta and Larachi (2007).

171) The data from Clarke and Glew (1971) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-152.96053 + 8324.82999/T + 20.73129 \ln(T))$ mol/(m^3 Pa) with T in K.

172) Obtained with D_2O as solvent.

173) Value at T = 353 K.

174) The data from Schoenfeld (1855) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(265.79241 - 9131.99684/T - 42.01987 \ln(T))$ mol/(m^3 Pa) with T in K.

175) Value given here as quoted by Rodríguez-Sevilla et al. (2002).

176) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(153.05871 - 4328.05304/T - 25.05397 \ln(T))$ mol/(m^3 Pa) with T in K.

177) Marti et al. (1997) give partial pressures of H_2SO_4 over a concentrated solution (e.g., 2.6×10^{-9} Pa for 54.1 weight-percent at 298 K). Extrapolating this to dilute solutions can only be considered an order-of-magnitude approximation for H_s.

178) Ayers et al. (1980) give partial pressures of H_2SO_4 over concentrated solutions at high temperatures. Extrapolating this to dilute solutions can only be considered an order-of-magnitude approximation for H_s.

179) Gmitro and Vermeulen (1964) give partial pressures of H_2SO_4 over a concentrated solution (e.g., 10^{-7} mmHg for 70 weight-percent at 298 K). Extrapolating this to dilute solutions can only be considered an order-of-magnitude approximation for H_s.

180) Clegg et al. (1998) estimate a Henry's law constant of 5×10^{11} atm^{-1} at 303.15 K for the reaction $H_2SO_4(g) \rightleftharpoons 2\ H^+(aq) + SO_4^{2-}(aq)$ but don't give a definition for it. Probably it is defined as $x^2(H^+) \times x(SO_4^{2-})/p(H_2SO_4)$, where x is the aqueous-phase mixing ratio.

181) The data from Bullister et al. (2002) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-281.50843 + 14256.43847/T + 38.73689 \ln(T))$ mol/(m^3 Pa) with T in K.

182) The data presented for SF6 in Tab. II of Shoor et al. (1969) appear to be incorrect and are not reproduced here.

183) The data from Ashton et al. (1968) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-431.90650 + 20715.81650/T + 61.33841 \ln(T))$ mol/(m^3 Pa) with T in K.

184) Value from the validation set for checking whether the model is satisfactory for compounds that are absent from the training set.

185) Experimental value, extracted from HENRYWIN.

186) Estimation based on the quotient between vapor pressure and water solubility, extracted from HENRYWIN.

187) The data presented for helium in Tab. II of Shoor et al. (1969) appear to be incorrect and are not reproduced here.

188) The data from Morrison and Johnstone (1954) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-267.15298 + 11440.04263/T + 37.95994 \ln(T))$ mol/(m^3 Pa) with T in K.

189) The data from Lannung (1930) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(84.35043 - 4135.59197/T - 14.55881 \ln(T))$ mol/(m^3 Pa) with T in K.

190) Calculated employing molecular force field models for the solutes from Warr et al. (2015).

191) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-153.15219 + 6434.36008/T + 20.89911 \ln(T))$ mol/(m^3 Pa) with T in K.

192) The data from Morrison and Johnstone (1954) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-171.84866 + 7492.61303/T + 23.58966 \ln(T))$ mol/(m^3 Pa) with T in K.

193) The data from Lannung (1930) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-40.04033 + 1266.80589/T + 4.12574 \ln(T))$ mol/(m^3 Pa) with T in K.

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194) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-150.94728 + 6639.96438/T + 20.42365\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

195) The data from Rettich et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-178.55165 + 8674.63293/T + 24.26764\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

196) The data from Murray and Riley (1970) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-151.84230 + 7548.13106/T + 20.24085\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

197) The data from Shoor et al. (1969) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-177.19900 + 8740.49327/T + 23.99118\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

198) The data from Ashton et al. (1968) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-160.52023 + 7898.05096/T + 21.56102\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

199) The data from Morrison and Johnstone (1954) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-159.49603 + 7859.86242/T + 21.39868\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

200) The data from Lannung (1930) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-183.19260 + 8856.79081/T + 24.97248\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

201) Calculated employing molecular force field models for the solutes from Vrabec et al. (2001).

202) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-143.77232 + 7158.59719/T + 19.05403\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

203) The data from Morrison and Johnstone (1954) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-153.87925 + 7855.39037/T + 20.51280\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

204) Two series of measurements with considerably different results are presented by von Antropoff (1910) for krypton.

205) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-220.92114 + 10903.79433/T + 30.49407\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

206) The value b for Xe given by Himmelblau (1960) in their Table III is incorrect. Most likely, only a minus sign is missing.

207) The data from Morrison and Johnstone (1954) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-165.83721 + 8808.62019/T + 22.15186\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

208) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-199.40126 + 10306.10786/T + 27.18844\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

209) The data from Lewis et al. (1987) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(5.03587 + 1555.37916/T - 3.42648\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

210) Calculated employing molecular force field models for the solutes from Mick et al. (2016).

211) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-240.66156 + 12686.97685/T + 33.12171\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

212) The data from Sisi et al. (1971) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-81.82525 + 4954.57763/T + 10.19950\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

213) Solubility in natural sea water. Measurements at different salinities were also performed, but only at a fixed temperature of 296.15 K.

214) Temperature dependence calculated using linear free energy relationships (LFER).

215) Petersen et al. (1998) give the invalid unit "$\mathrm{mol\,L^{-1}\,ppm^{-1}}$". Here, it is assumed that "ppm" is used as a synonym for "10^{-6} atm".

216) Shon et al. (2005) refer to Petersen et al. (1998) as the source but a different value is listed there.

217) Value at T = 333 K.

218) Calculated using linear free energy relationships (LFER).

219) More than one reference is given as the source of this value.

220) Hedgecock et al. (2005) refer to Hedgecock and Pirrone (2004) as the source but this value cannot be found there.

221) Clever and Young (1987) recommend the data from Rettich et al. (1981).

222) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-133.87728 + 6629.97157/T + 17.62624\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

223) The data from Scharlin and Battino (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-206.41168 + 10058.77208/T + 28.34417\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

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224) The data from Shoor et al. (1969) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-201.05778 + 9920.37989/T + 27.48020 \ln(T))$ mol/(m^3 Pa) with T in K.

225) The same value was also published in McAuliffe (1963).

226) The same value was also published in McAuliffe (1966).

227) The data from Morrison and Billett (1952) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-195.92072 + 9624.37184/T + 26.74976 \ln(T))$ mol/(m^3 Pa) with T in K.

228) The data from Winkler (1901) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-203.15902 + 9951.75251/T + 27.82679 \ln(T))$ mol/(m^3 Pa) with T in K.

229) Yao et al. (2002) compared two QSPR methods and found that radial basis function networks (RBFNs) are better than multiple linear regression. In their paper, they provide neither a definition nor the unit of their Henry's law constants. Comparing the values with those that they cite from Yaws (1999), it is assumed that they use the variant H_v^{px} and the unit atm.

230) English and Carroll (2001) provide several calculations. Here, the preferred value with explicit inclusion of hydrogen bonding parameters from a neural network is shown.

231) Value from the training dataset.

232) Calculated with a principal component analysis (PCA), see Suzuki et al. (1992) for details.

233) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-185.72813 + 9197.97387/T + 25.21142 \ln(T))$ mol/(m^3 Pa) with T in K.

234) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-109.51433 + 6313.03876/T + 13.60483 \ln(T))$ mol/(m^3 Pa) with T in K.

235) The data from Morrison and Billett (1952) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-215.51394 + 10861.98666/T + 29.50128 \ln(T))$ mol/(m^3 Pa) with T in K.

236) The data from Winkler (1901) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-277.60377 + 13887.90452/T + 38.63046 \ln(T))$ mol/(m^3 Pa) with T in K.

237) Value given here as quoted by Gharagheizi et al. (2010).

238) Calculated using linear free energy relationships (LFER).

239) Calculated using SPARC Performs Automated Reasoning in Chemistry (SPARC).

240) Calculated using COSMOtherm.

241) Temperature is not specified.

242) Value from the training dataset.

243) Calculated using the GROMHE model.

244) Calculated using the SPARC approach.

245) Calculated using the HENRYWIN method.

246) Calculated using a combination of a group contribution method and neural networks.

247) Modarresi et al. (2005) use different descriptors for their calculations. They conclude that COSA and ANN are the best QSPR models, but COSA is not ideal for hydrocarbons with low solubility. Only results obtained with ANN are shown here.

248) Yaffe et al. (2003) present QSPR results calculated with the fuzzy ARTMAP (FAM) and with the back-propagation (BK-Pr) method. They conclude that FAM is better. Only the FAM results are shown here.

249) Value from the training set.

250) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-249.13770 + 12672.58357/T + 34.34947 \ln(T))$ mol/(m^3 Pa) with T in K.

251) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-275.67877 + 14048.75446/T + 38.16041 \ln(T))$ mol/(m^3 Pa) with T in K.

252) The data from Morrison and Billett (1952) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-257.69118 + 13189.22089/T + 35.51019 \ln(T))$ mol/(m^3 Pa) with T in K.

253) The H298 and A,B,C data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 14 % difference.

254) The H298 and A,B,C data listed in Table 5-4 of Burkholder et al. (2015) are inconsistent, with 14 % difference.

255) The H298 and A,B,C data listed in Table 5.4 of Sander et al. (2011) are inconsistent, with 14 % difference.

256) The H298 and A,B,C data listed in Table 5.4 of Sander et al. (2006) are inconsistent, with 14 % difference.

257) The data from Morrison and Billett (1952) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-257.40529 + 13425.82235/T + 35.27658 \ln(T))$ mol/(m^3 Pa) with T in K.

258) Value given here as quoted by Dupeux et al. (2022).

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259) Calculated using the COSMO-RS method.

260) Value from the validation dataset.

261) The H298 and A,B,C data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 6 % difference.

262) The H298 and A,B,C data listed in Table 5-4 of Burkholder et al. (2015) are inconsistent, with 6 % difference.

263) The H298 and A,B,C data listed in Table 5.4 of Sander et al. (2011) are inconsistent, with 6 % difference.

264) The H298 and A,B,C data listed in Table 5.4 of Sander et al. (2006) are inconsistent, with 6 % difference.

265) Fogg and Sangster (2003) cite an incorrect fitting function from Hayduk (1986).

266) The fitting function and the data in the table on page 34 of Hayduk (1986) are inconsistent by a factor of about three. A comparison with the original measurements by Wetlaufer et al. (1964) shows that the data in the table are correct. Refitting the data suggests that the third fitting parameter should be 52.4651, not 53.4651.

267) Value from the test set.

268) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 15 % difference.

269) The data from Jou and Mather (2000) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-400.38105 + 20169.61328/T + 56.35286 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

270) Jou and Mather (2000) also contains high-temperature data. However, only data up to 373.2 K were used here to calculate the temperature dependence.

271) Value from the validation dataset.

272) Value from the test set.

273) The data from Shoor et al. (1969) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-311.59148 + 15699.27148/T + 43.32183 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

274) Value from the test dataset.

275) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

276) Apparently, the values in Table 2 of Park et al. (1997) show $\log_{10}(K_{\mathrm{aw}})$ and not K_{aw} as their figure caption states.

277) Extrapolated from data measured between 40 °C and 80 °C.

278) Data are taken from the report by Howe et al. (1987).

279) Value from the training set.

280) In their Table 8, Staudinger and Roberts (1996) incorrectly cite a value given by Ashworth et al. (1988).

281) The same data were also published in Hansen et al. (1995).

282) Hansen et al. (1993) found that the solubility of 2-methylhexane increases with temperature.

283) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 5 % difference.

284) The data from Dohányosová et al. (2004) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-670.94997 + 33188.34075/T + 95.95541 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

285) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 21 % difference.

286) The data from Dohányosová et al. (2004) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-792.29258 + 38089.35992/T + 114.36667 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

287) Data taken from the supplement.

288) Calculated using the EPI Suite (v4.0) method.

289) Calculated using the SPARC (v4.2) method.

290) Calculated using the COSMOtherm (v2.1) method.

291) Calculated using the ABSOLV (ADMEBoxes v4.1) method.

292) Mackay et al. (2006a) list a vapor pressure p, a solubility c, and a Henry's law constant calculated as p/c. However, the data are internally inconsistent and deviate by more than 10 %.

293) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 23 % difference.

294) Value at T = 294 K.

295) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 13 % difference.

296) The data listed in Tabs. 2 and 3 of Dewulf et al. (1999) are inconsistent, with 5 % difference.

297) Value at T = 301 K.

298) Value given here as quoted by Staudinger and Roberts (1996).

299) Value from the test set for true external validation.

300) The data from Dohányosová et al. (2004) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-365.40645 + 19821.40051/T + 50.78223 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

301) The data from Dohányosová et al. (2004) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-383.72514 + 20514.87228/T + 53.42859 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

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302) The data from Dohányosová et al. (2004) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-369.42853 + 19642.40603/T + 51.34116 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

303) Haynes (2014) refer to Mackay and Shiu (1981) but that article lists this value for 1,4-dimethylcyclohexane, not for 1,2-dimethylcyclohexane.

304) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

305) The data from Dohányosová et al. (2004) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-346.32561 + 18710.63122/T + 47.87398 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

306) The data from Maaßen (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-187.57836 + 9639.75245/T + 25.50544 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

307) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-166.44394 + 8613.39266/T + 22.39721 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

308) The data from Morrison and Billett (1952) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-175.14997 + 9028.26949/T + 23.67675 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

309) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-221.00286 + 11107.47493/T + 30.50401 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

310) The data from Maaßen (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-168.51157 + 9378.22622/T + 22.33127 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

311) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-241.54655 + 12718.75981/T + 33.18333 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

312) The data from Serra and Palavra (2003) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-261.78355 + 13728.91505/T + 36.10688 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

313) According to Donahue and Prinn (1993), the value is incorrect.

314) Wang et al. (2017) provide separate data for *cis* and *trans*. However, since both isomers are identified by the same SMILES string in their study, it is unclear how the stereochemistry has been taken into account.

315) Values for the Henry's law constants shown in Fig. 3 of Martins et al. (2017) were obtained from S. Pinho (pers. comm., 2022).

316) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from multiple sources and obtained from experimental vapor pressure and water solubility.

317) The data from Dohányosová et al. (2004) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-169.70973 + 10843.51763/T + 21.91320 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

318) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from a single database or data collection and obtained from experimental vapor pressure and water solubility.

319) Approximate value extracted from Fig. 1 of Maillard and Rosenthal (1952).

320) The same article was also published in Monatshefte für Chemie 23, 489–501 (1902).

321) Value given here as quoted by Fogg et al. (2001).

322) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-143.25283 + 7542.89338/T + 19.33269 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

323) Regression and individual data points of Simpson and Lovell (1962) are inconsistent, with 5 % difference.

324) Using the theoretical initial concentration (H0), see Zhang et al. (2013) for details.

325) Average of all duplicates (H1), see Zhang et al. (2013) for details.

326) Sieg et al. (2009) also provide data for supercooled water. Here, only data above 0 °C were used to calculate the temperature dependence.

327) Extrapolated from data above 298 K.

328) It was found that H_s changes with the concentration of the solution.

329) The data from Görgényi et al. (2002) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-346.88030 + 18421.52810/T + 48.91393 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

330) Value obtained by applying a modified batch air-stripping method, otherwise called the vapor entry loop (VEL) method, see Kochetkov et al. (2001) for details.

331) Value obtained by applying the static head space (HS) method, see Kochetkov et al. (2001) for details.

332) The data from Khalfaoui and Newsham (1994b) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-129.36095 + 8999.48627/T + 16.29087 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

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333) The data from Robbins et al. (1993) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(189.41389 - 5855.10843/T - 30.90289\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

334) Value at T = 302 K.

335) The data from Cooling et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-231.38331 + 13640.47358/T + 31.46504\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

336) Calculated using G_h and H_h from Table 2 in Andon et al. (1954). Note that the thermodynamic functions in that table are not based on their α in Table 1. Instead, the expression $\exp(-G_h/(RT))$ yields the Henry's law constant H_s^{xp} in the unit $1/\mathrm{atm}$.

337) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 11 % difference.

338) Values for salt solutions are also available from this reference.

339) The data from Görgényi et al. (2002) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-468.28203 + 24099.39947/T + 66.85565\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

340) Value obtained by applying the EPICS method, see Ayuttaya et al. (2001) for details.

341) Value obtained by applying the static cell (linear form) method, see Ayuttaya et al. (2001) for details.

342) Value obtained by applying the direct phase concentration ratio method, see Ayuttaya et al. (2001) for details.

343) Value obtained by applying the static cell (nonlinear form) method, see Ayuttaya et al. (2001) for details.

344) The data from Robbins et al. (1993) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-573.76928 + 28956.65188/T + 82.51911\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

345) The temperature dependence is recalculated using the data in Table 4 of Lamarche and Droste (1989) and not taken from their Table 5.

346) Apparently, the vapor pressure of toluene was used to calculate its Henry's law constant. However, no source is provided.

347) Value given here as quoted by Dewulf et al. (1995).

348) The data from Robbins et al. (1993) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-1350.74178 + 64760.28328/T + 197.85937\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

349) The data from Schwardt et al. (2021) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(100.47045 - 2603.76722/T - 17.31043\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

350) Value given here as quoted by HSDB (2015).

351) The regression parameters for ethylbenzene in Tab. 1 of Schwardt et al. (2021) are wrong. Corrected values from Schwardt et al. (2022) are used here.

352) The data from Schwardt et al. (2021) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-176.88587 + 11290.74921/T + 23.22869\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

353) Different types of Henry's law constants of Ryu and Park (1999) are inconsistent, with 14 % difference.

354) The data from Robbins et al. (1993) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-371.46947 + 20514.07888/T + 51.95086\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

355) The value listed as A for diethylbenzene is probably not A but the Henry's law volatility constant H_v^{px} at 298 K.

356) Yaffe et al. (2003) list this species twice in their table, with different values. As it is unclear which is correct, the data are not reproduced here.

357) Erratum for page 365 of Fogg and Sangster (2003): Data from Kondoh and Nakajima (1997) are cited incorrectly, giving the same values at 308.2 K and 318.2 K, respectively.

358) Value from the external prediction set.

359) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 8 % difference.

360) Because of discrepancies between the values shown in Tables 4 and 5 of Shiu and Ma (2000), the data are not used here.

361) Effective Henry's law constants at several pH values are provided by van Ruth and Villeneuve (2002). Here, only the value at pH 3 is shown.

362) The values of Dewulf et al. (1999) are not used here because, according to them, the calculated regression does not match the theoretical expectation for this species.

363) Calculated using the COSMO-RS method.

364) Value given here as quoted by Haynes (2014).

365) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from a single database or data collection and measured directly.

366) Literature-derived value.

367) Final adjusted value.

368) Value given here as quoted by Petrasek et al. (1983).

369) Calculated using COSMOtherm.

370) Calculated using the COSMO-RS method.

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371) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from a single original paper and obtained from experimental vapor pressure and water solubility.

372) Value at T = 299 K.

373) Value at T = 283 K.

374) Cargill (1990) recommends the data from Rettich et al. (1982).

375) The data from Rettich et al. (1982) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-188.21737 + 8974.05844/T + 25.72558 \ln(T))$ mol/(m^3 Pa) with T in K.

376) The data from Douglas (1967) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-180.92848 + 8514.05914/T + 24.68060 \ln(T))$ mol/(m^3 Pa) with T in K.

377) Solubility in sea water at 20.99 % chlorinity.

378) The data from Winkler (1901) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-163.07031 + 7890.85881/T + 21.94517 \ln(T))$ mol/(m^3 Pa) with T in K.

379) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-161.93492 + 7852.78262/T + 21.76812 \ln(T))$ mol/(m^3 Pa) with T in K.

380) The data from Zheng et al. (1997) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-144.44443 + 8071.06186/T + 19.20040 \ln(T))$ mol/(m^3 Pa) with T in K.

381) The data from Murray and Riley (1971) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-167.86941 + 9146.24434/T + 22.67331 \ln(T))$ mol/(m^3 Pa) with T in K.

382) The data from Morrison and Billett (1952) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-126.83009 + 7302.88179/T + 16.55553 \ln(T))$ mol/(m^3 Pa) with T in K.

383) The data from Bohr (1899) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-140.70007 + 7951.73013/T + 18.60961 \ln(T))$ mol/(m^3 Pa) with T in K.

384) As mentioned by Fogg and Sangster (2003), the fitting equation by Scharlin (1996) is erroneous. It appears that a correction factor of about 10^6 is necessary for consistency with their own data in Tab. 1.

385) The data from Dean and Lange (1999) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-138.54120 + 7859.16351/T + 18.28486 \ln(T))$ mol/(m^3 Pa) with T in K.

386) Keßel et al. (2017) provide data at several pH values. Here, only the value at pH 2 is shown because hydrolyses occurs in more alkaline solutions.

387) The H298 and A,B,C data listed in Table 5.4 of Sander et al. (2011) are inconsistent, with 92 % difference.

388) This paper supersedes earlier work with more concentrated solutions (Butler et al., 1933).

389) Value given here as quoted by Gaffney et al. (1987).

390) Value given here as quoted by Hine and Weimar (1965).

391) The H298 and A,B,C data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 10 % difference.

392) The H298 and A,B,C data listed in Table 5-4 of Burkholder et al. (2015) are inconsistent, with 10 % difference.

393) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 8 % difference.

394) The H298 and A,B,C data listed in Table 5.4 of Sander et al. (2011) are inconsistent, with 10 % difference.

395) Extrapolated from data above 298 K.

396) Koga (1995) found that *tert*-butanol does not obey Henry's law at $c > 3.8$ mM.

397) Incorrect data are given by Burkholder et al. (2019) for 2-methyl-2-propanol. The correct parameter for the temperature dependence is: C = 37.98 (R. E. Huie, pers. comm. 2021).

398) Incorrect data are given by Burkholder et al. (2015) for 2-methyl-2-propanol. The correct parameter for the temperature dependence is: C = 37.98 (R. E. Huie, pers. comm. 2021).

399) Calculated for an aqueous solution containing 60 % ethanol by volume as the solvent.

400) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

401) Value obtained by Saxena and Hildemann (1996) using the group contribution method.

402) Value at T = 300 K.

403) The error given by Suzuki et al. (1992) is not the difference between the observed and the calculated value, as it should be. It is unclear which of the numbers is wrong.

404) The species is probably 2,3-dimethyl-2-butanol and not 2,3-dimethylbutanol as listed in Hine and Mookerjee (1975).

405) Rumble (2021) refers to Moore et al. (1995) as the source but this value cannot be found there.

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406) It is assumed here that entry number 72 in Table 1 of Yaws et al. (1997) refers to 2-methyl-1-heptanol, not 2-methyl-2-heptanol.

407) KWAC and KAWp from Table 2 of Lei et al. (2007) are inconsistent, with 10 % difference.

408) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 8 % difference.

409) Different types of Henry's law constants of Yaws and Yang (1992) are inconsistent, with 16 % difference.

410) Different types of Henry's law constants of Yaws and Yang (1992) are inconsistent, with 10 % difference.

411) Value at T = 307 K.

412) Value given here as quoted by Mackay et al. (1995).

413) Calculated using SPARC Performs Automated Reasoning in Chemistry (SPARC). It is assumed here that the value refers to T = 298.15 K.

414) Value given here as quoted by Hine and Mookerjee (1975).

415) Value at T = 373 K.

416) Value at T = 281 K.

417) It is assumed here that the thermodynamic data refers to the units $[\mathrm{mol\,dm^{-3}}]$ and $[\mathrm{atm}]$ as standard states.

418) Value given here as quoted by Shiu et al. (1994).

419) HSDB (2015) refer to Abraham et al. (1994b) as the source but this value cannot be found there. Maybe the value is taken from Abraham et al. (1990).

420) Mackay et al. (2006c) list a vapor pressure p, a solubility c, and a Henry's law constant calculated as p/c. However, the data are internally inconsistent and deviate by more than 10 %.

421) Betterton (1992) gives Buttery et al. (1969) as the source. However, no data were found in that reference.

422) Intermediate of estimates employing the bond method from the EPI HENRYWIN software.

423) Although Mansfield (2020) writes that his "Table 6 summarizes numerical calculations for formaldehyde and acetaldehyde assuming the values given in Tables 4 and 5", different values for the Henry's law constants are shown in these tables.

424) Saxena and Hildemann (1996) say that this value is unreliable.

425) Calculated using the free energy perturbation (FEP) method.

426) Calculated using the thermodynamic integration (TI) method.

427) Calculated using the Bennett acceptance ratio (BAR) method.

428) Saxena and Hildemann (1996) give a range of $9.9\times10^2\ \mathrm{mol/(m^3\,Pa)} < H_\mathrm{s}^{cp} < 5.9\times10^4\ \mathrm{mol/(m^3\,Pa)}$.

429) Saxena and Hildemann (1996) give a range of $5.9\times10^6\ \mathrm{mol/(m^3\,Pa)} < H_\mathrm{s}^{cp} < 3.9\times10^9\ \mathrm{mol/(m^3\,Pa)}$.

430) The formula of 1,2-butanediol is incorrectly given as "$\mathrm{HOCH(OH)C_2H_5}$" by Burkholder et al. (2019).

431) The formula of 1,2-butanediol is incorrectly given as "$\mathrm{HOCH(OH)C_2H_5}$" by Burkholder et al. (2015).

432) Saxena and Hildemann (1996) give a range of $9.9\times10^2\ \mathrm{mol/(m^3\,Pa)} < H_\mathrm{s}^{cp} < 4.9\times10^4\ \mathrm{mol/(m^3\,Pa)}$.

433) Saxena and Hildemann (1996) give a range of $3.9\times10^2\ \mathrm{mol/(m^3\,Pa)} < H_\mathrm{s}^{cp} < 3.9\times10^4\ \mathrm{mol/(m^3\,Pa)}$.

434) Calculated based on atmospheric measurements.

435) Calculated using EPI.

436) Calculated using SPARC.

437) Henry's law constants calculated using the GROMHE model. Temperature-dependences calculated with the method of Kühne et al. (2005).

438) Isaacman-VanWertz et al. (2016) refer to Raventos-Duran et al. (2010) as the source but the quoted value cannot be found there.

439) Calculated using GROMHE.

440) Isaacman-VanWertz et al. (2016) refer to a paper by Hilal et al. as the source but the quoted value cannot be found there.

441) Calculated using SPARC.

442) Calculated using the bond contribution of HENRYWIN.

443) Compernolle and Müller (2014b) recommend H_s^{cp} for 1,7-heptanediol in the range of $4.5\times10^4\ \mathrm{mol/(m^3\,Pa)} < H_\mathrm{s}^{cp} < 8.3\times10^4\ \mathrm{mol/(m^3\,Pa)}$.

444) Compernolle and Müller (2014b) recommend H_s^{cp} for 1,9-nonanediol in the range of $2.4\times10^4\ \mathrm{mol/(m^3\,Pa)} < H_\mathrm{s}^{cp} < 3.9\times10^4\ \mathrm{mol/(m^3\,Pa)}$.

445) Compernolle and Müller (2014b) recommend H_s^{cp} for 1,10-decanediol in the range of $2.5\times10^4\ \mathrm{mol/(m^3\,Pa)} < H_\mathrm{s}^{cp} < 3.0\times10^4\ \mathrm{mol/(m^3\,Pa)}$.

446) Value given here as quoted by Hilal et al. (2008).

447) Calculated using the EPI Suite method (https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface).

448) Value for the temperature range from 261 K to 281 K.

449) Value at T = 278 K.

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450) Leriche et al. (2000) assume $H_s(\mathrm{ROO}) = H_s(\mathrm{ROOH}) \times H_s(\mathrm{HO_2})/H_s(\mathrm{H_2O_2})$.

451) Lelieveld and Crutzen (1991) assume $H_s(\mathrm{CH_3OO}) = H_s(\mathrm{HO_2})$.

452) Jacob (1986) assumes $H_s(\mathrm{CH_3OO}) = H_s(\mathrm{CH_3OOH}) \times H_s(\mathrm{HO_2})/H_s(\mathrm{H_2O_2})$.

453) Calculated using EVAPORATION and AIOMFAC.

454) Calculated using the GROMHE model.

455) Effective value that takes into account the hydration of HCHO:

$$H_s = ([\mathrm{HCHO}] + [\mathrm{CH_2(OH)_2}])/p(\mathrm{HCHO})$$

456) Data from Table 1 by Zhou and Mopper (1990) were used to redo the regression analysis. The data for acetone in their Table 2 are incorrect.

457) Dong and Dasgupta (1986) found that the Henry's law constant for HCHO is not a true constant but increases with increasing concentration. Note that their expression does not converge asymptotically to a constant value at infinite dilution.

458) Ledbury and Blair (1925) (and also Blair and Ledbury (1925)) measured the solubility of HCHO at very high concentrations around 5 to 15 M. Their value of H_s increases with HCHO concentration. Lelieveld and Crutzen (1991), Hough (1991), and Pandis and Seinfeld (1989) all use these solubility data but do not specify how they extrapolated to lower concentrations. Since the concentration range is far from typical values in atmospheric chemistry, the value is not reproduced here.

459) Value given here as quoted by Möller and Mauersberger (1992).

460) Effective value that takes into account the hydration of the aldehyde:

$$H_s = ([\mathrm{RCHO}] + [\mathrm{RCH(OH)_2}])/p(\mathrm{RCHO})$$

461) The data from Wieland et al. (2015) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(25.01220 + 3596.11696/T - 6.81730\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

462) Value given here as quoted by Bone et al. (1983).

463) Value suitable for the conditions of a case study in Mexico City.

464) Volkamer et al. (2009) found average effective Henry's law constants for CHOCHO in the range $1.6{\times}10^6$ $\mathrm{mol/(m^3\,Pa)} < H_s^{cp} < 5.9{\times}10^6$ $\mathrm{mol/(m^3\,Pa)}$ for solutions containing ammonium sulfate and/or fulvic acid. A salting-in effect by fulvic acid was observed even in the absence of sulfate.

465) Solubility in sulfate aerosol.

466) Woo and McNeill (2015) say that the Henry's law constant was updated based on advances in the literature since McNeill et al. (2012) but do not provide further details.

467) Value at T = 372 K.

468) The data from Wieland et al. (2015) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-176.35942 + 12895.73116/T + 22.70566\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

469) The formula of propenal is incorrectly given as "$\mathrm{CH_2CHO}$" by Burkholder et al. (2019).

470) The temperature dependence parameter C for 2-butenal is missing in Burkholder et al. (2019). The correct value is: C = 24.42 (R. E. Huie, pers. comm. 2021).

471) The data from Buttery et al. (1971) for trans-2-octenal are incorrectly cited by Betterton (1992).

472) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

473) Calculated under the assumption that ΔG and ΔH are based on $[\mathrm{mol/l}]$ and $[\mathrm{atm}]$ as the standard states.

474) Calculated using the experimental value adjusted (EVA) method, see McFall et al. (2020) for details.

475) Value at T = 359 K.

476) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 5 % difference.

477) Calculated from the slope of $y_{\mathrm{ac}}P$ vs x_{ac}, using data from Tab. VIII in Lichtenbelt and Schram (1985).

478) Value at T = 313 K.

479) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

480) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 7 % difference.

481) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

482) Table S2 in the supplement of Wu et al. (2022a) contains incorrect data for 3-octanone. Here, the corrected data (S. Wu, pers. comm. 2022) were used: 2.88E-2 and 1.52E-2 at 25 °C and 35 °C, respectively.

483) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 7 % difference.

484) The value listed as A for 2,6,8-trimethyl-4-nonanone is probably not A but the Henry's law volatility constant H_v^{px} at 298 K.

485) The data from Wieland et al. (2015) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(116.85779 - 1341.05519/T - 19.91967\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

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486) The data from Wieland et al. (2015) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-74.84087 + 9452.88617/T + 7.41865 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

487) The value given here was measured at a liquid phase mixing ratio of 1 µmol/mol. Servant et al. (1991) found that the Henry's law constant changes at higher concentrations.

488) Abraham (1984) smoothed the values from a plot of enthalpy against carbon number.

489) The value of $H_s^{\ominus}$ was taken from Keene and Galloway (1986).

490) Calculated using thermodynamic data from Latimer (1952).

491) Value at pH = 4.

492) Calculated using HENRYWIN 3.2 (bond contribution method).

493) At pH 7.

494) At pH 10.8.

495) Value at T = 289 K.

496) Value at T = 338 K.

497) Pecsar and Martin (1966) is quoted as the source. However, only activity coefficients and no vapor pressures are listed there.

498) The H298 and A,B,C data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 6 % difference.

499) The formula of methyl ethanoate is incorrectly given as "$CH_3C(O)CH_3$" by Burkholder et al. (2015).

500) The H298 and A,B data listed in Table 5-4 of Burkholder et al. (2015) are inconsistent, with 74 % difference.

501) The same data were also published in Kieckbusch and King (1979a).

502) The H298 and A,B,C data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 7 % difference.

503) The formula of propyl ethanoate is incorrectly given as "$CH_3C(O)C_3H_8$" by Burkholder et al. (2019).

504) Katritzky et al. (1998) list this species twice in their table, with different values. As it is unclear which of them is correct, the data are not reproduced here.

505) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 5 % difference.

506) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

507) The value listed as A for n-heptyl acetate is probably not A but the Henry's law volatility constant H_v^{px} at 298 K.

508) The value listed as A for n-octyl acetate is probably not A but the Henry's law volatility constant H_v^{px} at 298 K.

509) Betterton (1992) gives Kieckbusch and King (1979b) as the source. However, no data were found in that reference.

510) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

511) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 5 % difference.

512) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

513) The data from Wieland et al. (2015) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(34.46832 + 3269.29552/T - 8.76905 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

514) Burkholder et al. (2019) refer to Dohnal et al. (2010) but the quoted value cannot be found there.

515) Burkholder et al. (2015) refer to Dohnal et al. (2010) but the quoted value cannot be found there.

516) Dipropyl phthalate is listed twice with different values.

517) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 9 % difference.

518) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 17 % difference.

519) Hwang et al. (2010) present regression parameters in their Tab. 6 and values extrapolated to 298.15 K in their Tab. 5. However, I was not able to reproduce their calculation. The data shown here are from my own regression of the measured data between 318.15 K and 333.15 K.

520) The data from Haimi et al. (2006) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(752.39274 - 29351.83448/T - 115.55407 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

521) Different types of Henry's law constants of Arp and Schmidt (2004) are inconsistent, with 5 % difference.

522) The data from Robbins et al. (1993) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-4264.16032 + 202439.46180/T + 628.54371 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

523) The data from Haimi et al. (2006) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(224.10069 - 4205.03828/T - 37.65761 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

524) The data from Haimi et al. (2006) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-780.30940 + 40758.59752/T + 112.07468 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

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525) The data from Haimi et al. (2006) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-565.00561 + 31411.46240/T + 79.73748\ln(T))$ mol/(m^3 Pa) with T in K.

526) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from a single original paper and obtained from experimental vapor pressure and the infinite-dilution activity coefficient.

527) The data from Haimi et al. (2006) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-1125.52184 + 56732.54277/T + 163.04749\ln(T))$ mol/(m^3 Pa) with T in K.

528) The data from Haimi et al. (2006) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-1315.53726 + 64110.36765/T + 191.89554\ln(T))$ mol/(m^3 Pa) with T in K.

529) The value listed as A for di-n-pentyl ether is probably not A but the Henry's law volatility constant H_v^{px} at 298 K.

530) The value listed as A for di-n-hexyl ether is probably not A but the Henry's law volatility constant H_v^{px} at 298 K.

531) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 5 % difference.

532) The data from Wieland et al. (2015) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-157.10556 + 10203.60762/T + 20.42555\ln(T))$ mol/(m^3 Pa) with T in K.

533) Betterton (1992) gives Hine and Weimar (1965) as the source. However, no data were found in that reference.

534) Betterton (1992) gives Vitenberg et al. (1975) as the source. However, no data were found in that reference.

535) Based on gas chromatograph retention indices (GC-RIs).

536) Warneck (2005) refers to Saxena and Hildemann (1996) as the source but the quoted value cannot be found there.

537) The formula of hydroxyethanoic acid is incorrectly given as "HC(OH)C(O)OH" by Burkholder et al. (2019).

538) The formula of hydroxyethanoic acid is incorrectly given as "HC(OH)C(O)OH" by Burkholder et al. (2015).

539) Temperature dependencies in Tabs. 1 and 2 of Ashworth et al. (1988) are inconsistent, with 31 % difference.

540) Compernolle and Müller (2014a) recommend H_s^{cp} for tartaric acid in the range of 6.9×10^{14} mol/(m^3 Pa) $< H_s^{cp} < 9.2\times10^{15}$ mol/(m^3 Pa).

541) Chan et al. (2010) give a range of 1.9×10^5 mol/(m^3 Pa) $< H_s^{cp} < 9.5\times10^6$ mol/(m^3 Pa).

542) Calculated using the HENRYWIN program and calibration to 1,3-propanediol.

543) The value was chosen for a model study because it gave the best agreement with measurements.

544) Center of the range (2.3...4.0) mol/(m^3 Pa).

545) Calculated based on the method by Hine and Mookerjee (1975).

546) Compernolle and Müller (2014a) recommend H_s^{cp} for citric acid in the range of 2.0×10^{14} mol/(m^3 Pa) $< H_s^{cp} < 5.9\times10^{15}$ mol/(m^3 Pa).

547) The data from Wieland et al. (2015) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-96.39127 + 11107.87195/T + 10.76466\ln(T))$ mol/(m^3 Pa) with T in K.

548) In their Fig. 5b, Kish et al. (2013) apply an unspecified factor to the Henry's law constant, and it is not clear if the temperature dependence shown there is correct (Y. Liu, pers. comm. 2014).

549) Calculated using the method from Nguyen (2013).

550) Calculated from the slope of y_1P vs x_1, using the tabulated VLE data from Kim et al. (2008) between 40 °C and 100 °C. Only dilute solutions with $x_1 \le 0.1$ were considered.

551) Value at T = 309 K.

552) The data from Christie and Crisp (1967) for dipropylamine are incorrectly cited by Betterton (1992).

553) Value at T = 323 K.

554) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

555) Value at T = 308 K.

556) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 5 % difference.

557) Value at T = 285 K.

558) Mackay et al. (2006d) list a vapor pressure p, a solubility c, and a Henry's law constant calculated as p/c. However, the data are internally inconsistent and deviate by more than 10 %.

559) Calculated using $\Delta G_s^{g\to H_2O}$ and $\Delta H_s^{g\to H_2O}$ from Table IV of Arnett and Chawla (1979). Since some of the values in this table are taken directly from Andon et al. (1954), it is assumed that the thermodynamic properties are defined in the same way. Since $\Delta H_s^{g\to H_2O}$ is defined relative to pyridine, a value of -11.93 kcal/mol from Arnett et al. (1977) was added.

560) Due to an apparently incorrect definition of the Henry's law constant by Andon et al. (1954),

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Staudinger and Roberts (2001) quote incorrect values from that paper.

561) The data from Wieland et al. (2015) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-12.48322 + 7833.96799/T - 2.23379\ln(T))\ \mathrm{mol/(m^3\ Pa)}$ with T in K.

562) Value given here as quoted by Feigenbrugel and Le Calvé (2021).

563) Value calculated from the solubility of 9.4×10^{-3} mol/L and the vapor pressure of 0.255 mmHg, as shown on pages 7142-7143 of Arnett and Chawla (1979). It is inconsistent with the entry in Table IV of that paper.

564) Value given here as quoted by Ma et al. (2010a).

565) Nguyen (2013) refer to Kim et al. (2008) as the source but this value cannot be found there.

566) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 7 % difference.

567) Value given here as quoted by Goodarzi et al. (2010).

568) Goodarzi et al. (2010) compared several QSPR methods and found that the Levenberg-Marquardt algorithm with Bayesian regularization produces the best results. Values obtained with other methods can be found in their supplement.

569) Value from the validation set.

570) At pH 5.

571) Value from the test set.

572) At pH 10.

573) At pH 9.

574) At pH 5.2.

575) At pH 7.4.

576) At pH 9.3.

577) At pH 4.

578) Kames and Schurath (1992) were unable to assign the values to the isomers.

579) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from a single original paper and measured directly.

580) The same data were also published in Fischer and Ballschmiter (1998a).

581) The formula of 1,3-propanediol dinitrate is incorrectly given as "$O_2NO_2CH_2CH_2CH_2ONO_2$" by Burkholder et al. (2019).

582) The formula of 1,3-propanediol dinitrate is incorrectly given as "$O_2NO_2CH_2CH_2CH_2ONO_2$" by Burkholder et al. (2015).

583) Comparing the value with that from the cited publication (Kames and Schurath, 1995), it can be seen that the unit and the temperature listed in Table 3 of Warneck et al. (1996) are incorrect.

584) The data from Kames and Schurath (1995) for peroxyacetyl nitrate are incorrectly cited by Schurath et al. (1996).

585) The data from Kames and Schurath (1995) for peroxypropionyl nitrate are incorrectly cited by Schurath et al. (1996).

586) The data from Kames and Schurath (1995) for peroxy-n-butyl nitrate are incorrectly cited by Schurath et al. (1996).

587) The data from Kames and Schurath (1995) for peroxymethacryloyl nitrate are incorrectly cited by Schurath et al. (1996).

588) The data from Kames and Schurath (1995) for peroxy-i-butyl nitrate are incorrectly cited by Schurath et al. (1996).

589) Estimate based on Raventos-Duran et al. (2010).

590) Effective value at pH 3.

591) The value at $T^{\ominus}$ is the intrinsic Henry's law constant but the temperature dependence refers to the effective Henry's law constant at pH 3.08.

592) Burkholder et al. (2019) refer to Borduas et al. (2016) but the quoted value cannot be found there.

593) The values for nitroethane in Tabs. VI and VIII of Friant and Suffet (1979) differ by a factor of 10. Apparently, the value in Tab. VIII is wrong.

594) The data listed in Tabs. 2 and 3 of Dewulf et al. (1999) are inconsistent, with 27 % difference.

595) Mackay et al. (2006d) list two values for dinoseb which differ by a factor of 1000. It is unclear which number is correct (if any) and the data are not reproduced here.

596) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

597) The data from Glew and Moelwyn-Hughes (1953) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-135.82151 + 7593.40134/T + 18.05983\ln(T))\ \mathrm{mol/(m^3\ Pa)}$ with T in K.

598) The data from Maaßen (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-163.70243 + 8973.31702/T + 22.17142\ln(T))\ \mathrm{mol/(m^3\ Pa)}$ with T in K.

599) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-142.70480 + 8025.53525/T + 19.04459\ln(T))\ \mathrm{mol/(m^3\ Pa)}$ with T in K.

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600) The data from Zheng et al. (1997) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-190.61883 + 10088.26604/T + 25.94088\ln(T))$ mol/(m^3 Pa) with T in K.

601) The data from Maaßen (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-177.44258 + 9554.69077/T + 23.94054\ln(T))$ mol/(m^3 Pa) with T in K.

602) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-350.64777 + 16708.21486/T + 49.40261\ln(T))$ mol/(m^3 Pa) with T in K.

603) The data from Scharlin and Battino (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-552.21779 + 25529.81258/T + 79.59510\ln(T))$ mol/(m^3 Pa) with T in K.

604) The data from Scharlin and Battino (1994) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-552.21779 + 25529.81258/T + 79.59510\ln(T))$ mol/(m^3 Pa) with T in K.

605) The data from Wen and Muccitelli (1979) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-356.93310 + 16943.80173/T + 50.37092\ln(T))$ mol/(m^3 Pa) with T in K.

606) The data from Ashton et al. (1968) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-320.94892 + 15261.58540/T + 45.04995\ln(T))$ mol/(m^3 Pa) with T in K.

607) The data from Morrison and Johnstone (1954) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-174.44927 + 8434.85415/T + 23.34667\ln(T))$ mol/(m^3 Pa) with T in K.

608) The H298 and A,B data listed in Table 5-7 of Burkholder et al. (2019) are inconsistent, with 8 % difference.

609) The H298 and A,B data listed in Table 5-7 of Burkholder et al. (2015) are inconsistent, with 8 % difference.

610) The data from Zheng et al. (1997) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-203.78636 + 11097.46295/T + 27.89781\ln(T))$ mol/(m^3 Pa) with T in K.

611) The data from Maaßen (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-184.82864 + 10260.68840/T + 25.06659\ln(T))$ mol/(m^3 Pa) with T in K.

612) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-175.64793 + 9805.36391/T + 23.71997\ln(T))$ mol/(m^3 Pa) with T in K.

613) The data from Zheng et al. (1997) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-244.13803 + 12963.44791/T + 33.68869\ln(T))$ mol/(m^3 Pa) with T in K.

614) The data from Maaßen (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-225.56576 + 12186.49271/T + 30.88527\ln(T))$ mol/(m^3 Pa) with T in K.

615) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-208.89051 + 11387.65726/T + 28.42219\ln(T))$ mol/(m^3 Pa) with T in K.

616) The data from Chang and Criddle (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-1003.84803 + 45506.40253/T + 147.89569\ln(T))$ mol/(m^3 Pa) with T in K.

617) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-164.25882 + 9381.26592/T + 21.50848\ln(T))$ mol/(m^3 Pa) with T in K.

618) The data from Wen and Muccitelli (1979) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-499.57565 + 23563.38593/T + 71.28478\ln(T))$ mol/(m^3 Pa) with T in K.

619) Value at T = 287 K.

620) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-78.74672 + 5836.90728/T + 8.41930\ln(T))$ mol/(m^3 Pa) with T in K.

621) The data from Clever et al. (2005) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-588.11467 + 28143.61522/T + 84.26598\ln(T))$ mol/(m^3 Pa) with T in K.

622) In their Table 13, Clever et al. (2005) list Ostwald coefficients that are probably incorrect by a factor of 100. Therefore, these values are not used. Instead, H_s is calculated using the mol fraction x_1 from the same table.

623) The data from Scharlin and Battino (1994) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-630.69809 + 30309.09484/T + 90.46889\ln(T))$ mol/(m^3 Pa) with T in K.

624) The data from Wen and Muccitelli (1979) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-673.45393 + 31915.35190/T + 97.01332\ln(T))$ mol/(m^3 Pa) with T in K.

625) The data from Maaßen (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-197.14327 + 10473.25304/T + 26.34780\ln(T))$ mol/(m^3 Pa) with T in K.

626) Calculated using the COSMO-RS method.

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627) Value given here as quoted by Kanakidou et al. (1995).

628) Comparing with Abraham et al. (1994a), it seems that the compound called "trifluoroethanol" by Goss (2005) refers to 2,2,2-trifluoroethanol.

629) Comparing with Abraham et al. (1994a), it seems that the compound called "hexafluoropropanol" by Goss (2005) refers to 1,1,1,3,3,3-hexafluoro-2-propanol.

630) Value at T = 284 K.

631) Measured in aqueous hydrochloric acid and extrapolated to pure water as the solvent at 25 °C. Measurements were also made at other temperatures, however, those were not extrapolated to pure water as the solvent.

632) Calculated using the EPI Suite Bond estimation method.

633) Calculated using the new SPARC method, see Arp et al. (2006) for details.

634) Calculated using the COSMOtherm method, see Arp et al. (2006) for details.

635) A refit yields: A = -18.99, B = 5493, and H(298 K) = 0.57 M/atm (R. E. Huie, pers. comm. 2021).

636) A refit yields: A = -18.99, B = 5493, and H(298 K) = 0.57 M/atm (R. E. Huie, pers. comm. 2021).

637) A refit yields: A = -21.67, B = 5776, and H(298 K) = 0.10 M/atm (R. E. Huie, pers. comm. 2021).

638) The H298 and A,B data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 29 % difference.

639) A refit yields: A = -21.67, B = 5776, and H(298 K) = 0.10 M/atm (R. E. Huie, pers. comm. 2021).

640) The H298 and A,B data listed in Table 5-4 of Burkholder et al. (2015) are inconsistent, with 29 % difference.

641) The H298 and A,B data listed in Table 5.4 of Sander et al. (2011) are inconsistent, with 29 % difference.

642) The data from Clever et al. (2005) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(289.52696 - 11352.27202/T - 46.16631\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

643) The Ostwald coefficient given by Clever et al. (2005) at 313.2 K is probably incorrect. Therefore, the Ostwald coefficients are not used. Instead, H_s is calculated using the mol fraction x_1 from the same table.

644) Extrapolated based on number of carbons.

645) Measured with the wetted-wall column at room temperature.

646) The H298 and A,B data listed in Table 5.4 of Sander et al. (2011) are inconsistent, with 9 % difference.

647) The H298 and A,B data listed in Table 5.4 of Sander et al. (2006) are inconsistent, with 9 % difference.

648) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-251.05500 + 13259.10200/T + 35.01685\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

649) The same data were also published in McConnell et al. (1975).

650) The data from Glew and Moelwyn-Hughes (1953) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-171.13914 + 9743.00524/T + 23.09616\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

651) Values at different temperatures are from different sources. Thus a temperature dependence was not calculated.

652) Chiang et al. (1998) show vinyl chloride in their Table 2 but most probably they meant to refer to dichloromethane instead.

653) The data from Wright et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-444.17924 + 22456.73010/T + 63.76504\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

654) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 7 % difference.

655) The data from Görgényi et al. (2002) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-378.59438 + 20174.67146/T + 53.50889\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

656) The data from Moore et al. (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(32.52949 + 1878.33965/T - 7.88669\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

657) The data from Wright et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-109.09283 + 8000.75665/T + 13.39152\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

658) Probably an interpolation of the data from Balls (1980).

659) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 5 % difference.

660) The data from Bullister and Wisegarver (1998) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-704.15798 + 34144.64622/T + 102.06046\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

661) The data from Wright et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-426.63883 + 22457.44484/T + 60.22986\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

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662) The data from Maaßen (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-221.58683 + 12291.19608/T + 30.42274 \ln(T))$ mol/(m^3 Pa) with T in K.

663) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-233.85465 + 12927.81251/T + 32.20905 \ln(T))$ mol/(m^3 Pa) with T in K.

664) The data from Görgényi et al. (2002) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-372.18420 + 19566.35271/T + 52.67600 \ln(T))$ mol/(m^3 Pa) with T in K.

665) The data from Wright et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-1295.59488 + 61538.96732/T + 190.02999 \ln(T))$ mol/(m^3 Pa) with T in K.

666) The data from Wright et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-309.75754 + 17275.24359/T + 43.35857 \ln(T))$ mol/(m^3 Pa) with T in K.

667) The data from Robbins et al. (1993) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(313.50875 - 12121.71831/T - 49.20602 \ln(T))$ mol/(m^3 Pa) with T in K.

668) The data from Wright et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(255.46482 - 8896.18926/T - 40.90189 \ln(T))$ mol/(m^3 Pa) with T in K.

669) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 5 % difference.

670) The data from Schwardt et al. (2021) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(200.57633 - 7128.32092/T - 31.87111 \ln(T))$ mol/(m^3 Pa) with T in K.

671) The data from Wright et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-304.31063 + 17046.46392/T + 42.59182 \ln(T))$ mol/(m^3 Pa) with T in K.

672) The data from Schwardt et al. (2021) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-1784.40256 + 88283.19114/T + 260.26556 \ln(T))$ mol/(m^3 Pa) with T in K.

673) The data from Wright et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(608.52671 - 23622.70039/T - 93.86675 \ln(T))$ mol/(m^3 Pa) with T in K.

674) The value for A in the table of Kondoh and Nakajima (1997) is incorrect. Recalculating the regression, it can be seen that it should be 13.95 and not 1.395.

675) The data from Wright et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(2638.58362 - 114985.14319/T - 396.08684 \ln(T))$ mol/(m^3 Pa) with T in K.

676) The H298 and A,B data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 9 % difference.

677) The data from Wright et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-573.71583 + 28877.33987/T + 82.70652 \ln(T))$ mol/(m^3 Pa) with T in K.

678) The data from Sarraute et al. (2006) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-503.53929 + 28223.72051/T + 70.89539 \ln(T))$ mol/(m^3 Pa) with T in K.

679) As explained by Miller and Stuart (2003), the measurements were performed at 296 K.

680) Value for T = 295...298 K.

681) Value for T = 293...298 K.

682) The data from Schwardt et al. (2021) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-20.66741 + 2604.13624/T + 0.71646 \ln(T))$ mol/(m^3 Pa) with T in K.

683) Mackay et al. (2006b) list a vapor pressure p, a solubility c, and a Henry's law constant calculated as p/c. However, the data are internally inconsistent and deviate by more than 10 %.

684) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

685) The data from Schwardt et al. (2021) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-214.72727 + 12076.60512/T + 29.20360 \ln(T))$ mol/(m^3 Pa) with T in K.

686) A typo in Ashworth et al. (1988) has been corrected, the correct value was presented by Howe et al. (1987).

687) The data from Wright et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-332.68901 + 17925.88529/T + 46.77838 \ln(T))$ mol/(m^3 Pa) with T in K.

688) The data from Schwardt et al. (2021) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-6.68864 + 2211.35284/T - 1.35565 \ln(T))$ mol/(m^3 Pa) with T in K.

689) The data from Khalfaoui and Newsham (1994b) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-593.56757 + 30300.79738/T + 85.11672 \ln(T))$ mol/(m^3 Pa) with T in K.

690) The data from Wright et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-294.54970 + 16409.35487/T + 40.82700 \ln(T))$ mol/(m^3 Pa) with T in K.

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691) The data from Cooling et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-511.78322 + 26710.11950/T + 72.88403 \ln(T))$ mol/(m^3 Pa) with T in K.

692) The data from Schwardt et al. (2021) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-265.05147 + 15058.79780/T + 36.44507 \ln(T))$ mol/(m^3 Pa) with T in K.

693) The data from Görgényi et al. (2002) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-480.92432 + 24776.46284/T + 68.60174 \ln(T))$ mol/(m^3 Pa) with T in K.

694) The data from Knauss et al. (2000) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-389.28726 + 21123.08804/T + 54.69871 \ln(T))$ mol/(m^3 Pa) with T in K.

695) The data from Khalfaoui and Newsham (1994b) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-511.93773 + 26713.30359/T + 72.90551 \ln(T))$ mol/(m^3 Pa) with T in K.

696) The data from Robbins et al. (1993) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(176.56015 - 5511.47473/T - 28.96682 \ln(T))$ mol/(m^3 Pa) with T in K.

697) The data from Wright et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(681.41357 - 27448.54898/T - 104.63745 \ln(T))$ mol/(m^3 Pa) with T in K.

698) The data from Cooling et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-574.03630 + 29404.80442/T + 82.22224 \ln(T))$ mol/(m^3 Pa) with T in K.

699) The data from Schwardt et al. (2021) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-330.94781 + 18207.73829/T + 46.05991 \ln(T))$ mol/(m^3 Pa) with T in K.

700) The data from Knauss et al. (2000) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-281.09217 + 15955.08953/T + 38.60107 \ln(T))$ mol/(m^3 Pa) with T in K.

701) The data from Robbins et al. (1993) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-1145.60543 + 55089.35358/T + 167.32916 \ln(T))$ mol/(m^3 Pa) with T in K.

702) The data from Wright et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-224.85290 + 13463.70772/T + 30.65123 \ln(T))$ mol/(m^3 Pa) with T in K.

703) Henry's law constants were evaluated using data from Florida sandy field soil.

704) According to Thomas et al. (2006), theoretical Henry's law constants were calculated using the "normal boiling point, the critical temperature, and the enthalpy of volatilization at the normal boiling point".

705) Haynes (2014) refer to Mackay and Shiu (1981) but that article lists this value for 1-chloro-2-methylpropane (the saturated compound), not for 1-chloro-2-methylpropene.

706) The regression parameters for chlorobenzene in Tab. 1 of Schwardt et al. (2021) are wrong. Corrected values from Schwardt et al. (2022) are used here.

707) The data from Schwardt et al. (2021) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-266.69788 + 14811.78372/T + 37.00246 \ln(T))$ mol/(m^3 Pa) with T in K.

708) The data from Khalfaoui and Newsham (1994b) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-757.46460 + 35956.18738/T + 110.75693 \ln(T))$ mol/(m^3 Pa) with T in K.

709) The data from Cooling et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-820.00716 + 38880.20610/T + 120.01460 \ln(T))$ mol/(m^3 Pa) with T in K.

710) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 8 % difference.

711) Erratum for page 344 of Fogg and Sangster (2003): Their reference [89] does not contain 1,2-dichlorobenzene.

712) The data listed in Tabs. 2 and 3 of Dewulf et al. (1999) are inconsistent, with 7 % difference.

713) The data listed in Tabs. 2 and 3 of Dewulf et al. (1999) are inconsistent, with 7 % difference.

714) Rumble (2021) refers to Oliver (1985) as the source but this value cannot be found there.

715) Value for T = 298...303 K.

716) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from multiple sources and obtained from the experimental octanol/water partition coefficient and the octanol/air partition coefficient.

717) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from a single database or data collection and obtained from the experimental octanol/water partition coefficient and the octanol/air partition coefficient.

718) Odabasi and Adali (2016) provide the parameters A and B for an equation to calculate temperature-dependent Henry's law constants. Values

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calculated with this equation at 298 K are slightly different than those measured at 298 K and given as H in their table 1. Here, the values H and B are used.

719) Modified gas-stripping method (MGSM), see Lau et al. (2006) for details.

720) Integrated gas-stripping method (IGSM), see Lau et al. (2006) for details.

721) Calculated with the principal component regression (PCR) method, see Fang Lee (2007) for details.

722) Calculated with the partial least-square regression (PLSR) method, see Fang Lee (2007) for details.

723) The same data were also published in Dunnivant et al. (1988).

724) Value given here as quoted by Dunnivant et al. (1988).

725) Calculated using the EPICS method.

726) Calculated using the "Direct" method.

727) Westcott et al. (1981) give a range of 1.9×10^{-2} $\mathrm{mol/(m^3\,Pa)} < H_s^{cp} < 3.2\times10^{-2}$ $\mathrm{mol/(m^3\,Pa)}$.

728) Westcott et al. (1981) give a range of 2.8×10^{-2} $\mathrm{mol/(m^3\,Pa)} < H_s^{cp} < 9.0\times10^{-2}$ $\mathrm{mol/(m^3\,Pa)}$.

729) Erratum for page 350 of Fogg and Sangster (2003): The equation describing the recommended temperature-dependent data appears to be incorrect and is not used here.

730) Value at pH = 4.

731) When comparing H in Table 4 with K_{gw} in Table 5 of Pfeifer et al. (2001), it can be seen that the values refer to $K_{gw} \times 100$ and not $K_{gw}/100$.

732) Measured at pH 1.

733) The same data were also published in Brandsch et al. (1993).

734) Erratum for page 376 of Fogg and Sangster (2003): Data from Santl et al. (1994) are cited incorrectly, it should be 3.64, not 3.84.

735) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 8 % difference.

736) Although pronamide and propyzamide are the same species, Mackay et al. (2006d) list two different values for them. It is unclear which number is correct (if any) and the data are not reproduced here.

737) The value at 20 °C was calculated from published values of vapor pressure and water solubility. Data between 25 °C and 40 °C were calculated from the measured evaporation rate.

738) At pH 5.4.

739) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from multiple sources and measured directly.

740) The data from Zheng et al. (1997) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-206.94328 + 11372.60160/T + 28.22232\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

741) The data from Maaßen (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-200.57402 + 11192.93914/T + 27.21798\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

742) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-208.06388 + 11491.48483/T + 28.35421\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

743) The data from Chang and Criddle (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-1756.79407 + 80807.02552/T + 259.24906\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

744) The data from McLinden (1989) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-387.81156 + 19950.78638/T + 54.91348\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

745) The temperature dependence was recalculated from the data on p. 20 of McLinden (1989).

746) The data from McLinden (1989) for HCFC-22 are incorrectly cited by Kanakidou et al. (1995).

747) The H298 and A,B data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 5 % difference.

748) The H298 and A,B data listed in Table 5-4 of Burkholder et al. (2015) are inconsistent, with 5 % difference.

749) The H298 and A,B data listed in Table 5.4 of Sander et al. (2011) are inconsistent, with 5 % difference.

750) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(100.23590 - 3339.68982/T - 17.66849\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

751) The data from Scharlin and Battino (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-291.40685 + 14224.53456/T + 40.73325\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

752) The data from Scharlin and Battino (1994) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-291.40685 + 14224.53456/T + 40.73325\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

753) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-147.53824 + 8643.05363/T + 18.97752\ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

754) The data from Scharlin and Battino (1995) were fitted to the 3-parameter equation: $H_s^{cp} =$

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$\exp(-211.99699+11400.41036/T+28.66283\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

755) The data from Scharlin and Battino (1994) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-211.99699+11400.41036/T+28.66283\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

756) The data from Maaßen (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-278.68448+15169.41095/T+38.36974\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

757) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-129.78084+8533.77911/T+16.20428\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

758) The data from Bu and Warner (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-415.59157+21411.24346/T+58.50528\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

759) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(0.13353+5070.08549/T-4.84639\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

760) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-113.07654+6884.36758/T+13.75470\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

761) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-149.62353+7869.46528/T+19.40044\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

762) The data from Chang and Criddle (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-402.28495+20229.16189/T+57.28419\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

763) The data from Maaßen (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-277.88370+14905.51805/T+38.38688\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

764) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-195.56650+11207.08869/T+26.12575\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

765) The data from Maaßen (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-249.15404+13774.89590/T+34.23234\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

766) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-210.55601+11968.42846/T+28.54087\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

767) The data from Maaßen (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-155.04312+9704.04801/T+20.06575\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

768) The data from Maaßen (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-270.78344+14413.03953/T+37.48366\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

769) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-184.96240+10541.13831/T+24.70437\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

770) The data from Chang and Criddle (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-190.58060+10602.65774/T+25.66197\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

771) The data from Maaßen (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-237.50724+13032.41274/T+32.48569\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

772) The data from Reichl (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-200.95912+11406.81841/T+27.03092\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

773) The data from Smith et al. (1981b) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(678.00770-27346.39638/T-103.92351\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

774) Kanakidou et al. (1995) assume $H_s(\mathrm{CClF_2OONO_2})$ = $H_s(\mathrm{PAN})$.

775) The H298 and A,B data listed in Table 5-4 of Burkholder et al. (2019) are inconsistent, with 11 % difference.

776) The data from De Bruyn and Saltzman (1997) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-521.17646+25057.64644/T+75.60914\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

777) The data from Glew and Moelwyn-Hughes (1953) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-184.73597+10636.09284/T+25.03175\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

778) Values at 298 K in Table C2 and C5 of Brockbank (2013) are inconsistent, with 6 % difference.

779) The data from Moore et al. (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-395.20167+20638.03484/T+56.40082\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

780) The data from Wright et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-82.06673+6867.92071/T+9.56720\ln(T))$ $\mathrm{mol}/(\mathrm{m}^3\,\mathrm{Pa})$ with T in K.

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781) The data from Moore et al. (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-408.59491 + 21699.59623/T + 58.19801 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

782) The data from Wright et al. (1992) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(1124.79951 - 46767.40872/T - 170.54217 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

783) Erratum for page 274 of Fogg and Sangster (2003): The value in the table is k_H, not $\ln k_H$.

784) Value at T = 50 K.

785) Rumble (2021) refers to Hiatt (2013) as the source but this value cannot be found there.

786) Haynes (2014) refer to Mackay et al. (1993) as the source but this value cannot be found there.

787) The data from Sarraute et al. (2006) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-370.06283 + 22192.71634/T + 51.12683 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

788) Erratum for page 321 of Fogg and Sangster (2003): Data from Yates and Gan (1998) are cited with a typo. The value at 313.2 K should probably be 4.78×10^{-6}, not 4.78×10^{-2}.

789) Ebert et al. (2023) present "curated experimental" Henry's law constants from the literature but do not provide any references. It is only mentioned that the value is from a single original paper and obtained from the experimental octanol/water partition coefficient and the octanol/air partition coefficient.

790) Diaz et al. (2005) also cite a Henry's law constant from Pfeifer et al. (2001) even though this species is not mentioned there. There might be a mix up of the different haloanisoles.

791) Erratum for page 285 of Fogg and Sangster (2003): The data in their table look strange (9.70R) and are not used here.

792) The data from Moore et al. (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-76.31131 + 7250.73360/T + 8.15388 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

793) The data from Moore et al. (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-265.18008 + 15516.80509/T + 36.54803 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

794) The data from Moore et al. (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-229.06923 + 13418.39257/T + 31.15669 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

795) The data from Glew and Moelwyn-Hughes (1953) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-384.31677 + 19391.25580/T + 54.93602 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

796) The data from Moore et al. (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-247.93525 + 14910.30572/T + 34.08071 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

797) The regression given by Fogg and Sangster (2003) does not produce the data in their table. Thus the regression was recalculated.

798) The value listed as A for iodobenzene is probably not A but the Henry's law volatility constant H_v^{px} at 298 K. For the value of B, a minus sign is probably missing.

799) The data from Moore et al. (1995) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-242.58767 + 14043.89458/T + 33.48497 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

800) Karagodin-Doyennel et al. (2021) probably assume that CH_2BrI has the same Henry's law constant as CH_2ClI.

801) The data from Haimi et al. (2006) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-266.45850 + 15036.99733/T + 36.80758 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

802) Yaws et al. (2003) present Henry's law constants based on water solubility and vapor pressure. The water solubility is calculated using a correlation to the boiling point. For the vapor pressures, no references are provided.

803) The data from Zin et al. (2016) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-419.66332 + 22034.35758/T + 59.55571 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

804) The data from Haimi et al. (2006) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-166.97891 + 10357.07398/T + 22.04420 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

805) The data from Haimi et al. (2006) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-406.56800 + 21428.82541/T + 57.60207 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

806) The data from Zin et al. (2016) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(10.26074 + 2303.75755/T - 4.36399 \ln(T))$ $\mathrm{mol/(m^3\,Pa)}$ with T in K.

807) Presumably, the species called "42-methyl-2-butanethiol" in Table 1 of Yao et al. (2002) should be 2-methyl-2-butanethiol.

808) Schäfer and Lax (1962) present data based on Booth and Jolley (1943). However, these data appear to be incorrect.

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809) Booth and Jolley (1943) converted data from Rex (1906) to another unit. However, this was apparently not done correctly.

810) Booth and Jolley (1943) present data from Chancel and Parmentier (1885). However, in that paper only the solubility at an unknown partial pressure of CS_2 was measured.

811) Value extracted from their Figure 46.

812) The data from Haimi et al. (2006) were fitted to the 3-parameter equation: $H_s^{cp} = \exp(-233.39763 + 13839.16150/T + 31.85189 \ln(T))\ \mathrm{mol/(m^3\ Pa)}$ with T in K.

813) $H'_s = 6.4 \times 10^{14}\ \frac{\mathrm{mol^2}}{\mathrm{m^6\ Pa}}$

814) It is unclear how Fogg and Sangster (2003) obtained the data. Apparently, limiting activity coefficients γ^∞ were taken from Trampe and Eckert (1993) but a source for vapor pressure data is not mentioned. Also, the γ^∞ values listed in the table are different from those found in the original paper.

815) At pH 3.9.

816) At pH 4.8.

817) Mackay et al. (2006d) list two values for thiobencarb which differ by a large factor. It is unclear which number is correct (if any) and the data are not reproduced here.

818) Extrapolated from data at elevated temperatures.

819) Calculated using HENRYWIN 3.21.

820) Calculated using vapor pressures and water solubilities from HENRYWIN 3.21.

821) Calculated using vapor pressures and water solubilities from the EPA Toxicity Estimation Software Tool (TEST).

822) Wilhelm et al. (1977) and Abraham (1979) are quoted as the source. However, the data cannot be found there.

823) Shon et al. (2005) refer to Petersen et al. (1998) as the source but this value cannot be found there.

824) The value from their experiment 7 at 10 °C is not used in the determination of the temperature dependence because of very different ionic strengths and concentrations for that experiment.

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