

Compilation of Henry's law constants (version 5.0.0) 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 46434 values of Henry's law constants for 10173 species, collected from 994 references. It ~~will also be~~ is also 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 a Henry's law constant. In atmospheric chemistry, these constants are needed to describe the ~~distribution-exchange~~ of trace species between the air and liquid cloud droplets ~~or aerosol particles~~, aerosol particles, oceans and other bodies of water. In other areas of environmental research, the constants are needed to calculate the vaporization of contaminants, e.g. 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.

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	$\text{mol m}^{-3} \text{ Pa}^{-1}$	M atm^{-1}	
H_s^{xp}	x/p	Pa^{-1}	atm^{-1}	$H_s^{xp} = H_s^{cp} \times M_{\text{H}_2\text{O}}/\rho_{\text{H}_2\text{O}}$
H_s^{bp}	b/p	$\text{mol kg}^{-1} \text{ Pa}^{-1}$	$\text{mol kg}^{-1} \text{ atm}^{-1}$	$H_s^{bp} = H_s^{cp}/\rho_{\text{H}_2\text{O}}$
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	$\text{Pa m}^3 \text{ mol}^{-1}$	$\text{atm m}^3 \text{ mol}^{-1}$	$H_v^{pc} = 1/H_s^{cp}$
H_v^{px}	p/x	Pa	atm	$H_v^{px} = (\rho_{\text{H}_2\text{O}}/M_{\text{H}_2\text{O}})/H_s^{cp}$
H_v^{pw}	p/w	Pa	atm	$H_v^{pw} = (\rho_{\text{H}_2\text{O}}/M_B)/H_s^{cp}$
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, $\text{M} = \text{mol L}^{-1}$ and $\text{atm} = 101\,325 \text{ Pa}$.

^c Here, $M_{\text{H}_2\text{O}}$ and $\rho_{\text{H}_2\text{O}}$ 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).

This article is a living review describing version 5.0.0¹. Compared to the now obsolete version 4.0 (Sander, 2015), the compilation contains 29084 additional values of Henry’s law constants for 5541 additional species, collected from 305 additional references. In cases where experimental data are available for a large temperature range, the [data-values](#) were refitted to a 3-parameter equation ~~replacing~~ [in addition to](#) 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 the quotient A/G . Here, A and G are quantities describing the equilibrium composition (at infinite dilution) of the aqueous phase and

¹The 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 ACPD.

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 referring to A/G . When referring 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 $T^\ominus = 298.15$ 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:

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

Table 2. Conversion factors between several Henry's law solubility constants H_s (at $T^\ominus = 298.15$ K and $\rho^\ominus = 997$ kg/m³). [For example, the second table entry indicates that \$H_s^{cp} = 1\$ mol m⁻³ Pa⁻¹ \$\Leftrightarrow H_s^{cp} = 101.325\$ M atm⁻¹.](#)

	$H_s^{cp} = \dots \frac{\text{mol}}{\text{m}^3 \text{ Pa}}$	$H_s^{cp} = \dots \frac{\text{M}}{\text{atm}}$	$H_s^{cc} = \dots$	$H_s^{bp} = \dots \frac{\text{mol}}{\text{kg Pa}}$	$H_s^{bp} = \dots \frac{\text{mol}}{\text{kg atm}}$	$H_s^{xp} = \dots \frac{1}{\text{atm}}$	$\alpha = \dots$
$H_s^{cp} = 1 \frac{\text{mol}}{\text{m}^3 \text{ Pa}}$	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
$H_s^{bp} = 1 \frac{\text{mol}}{\text{kg Pa}}$	997.000	1.01021×10^5	2.47152×10^6	1.00000	1.01325×10^5	1825.40	2.26428×10^6
$H_s^{bp} = 1 \frac{\text{mol}}{\text{kg atm}}$	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 $\rho^\ominus = 997$ kg/m³). [For example, the second table entry indicates that \$H_v^{px} = 1\$ atm \$\Leftrightarrow H_v^{pc} = 1.83089\$ m³ Pa mol⁻¹.](#)

	$H_v^{px} = \dots \text{atm}$	$H_v^{pc} = \dots \frac{\text{m}^3 \text{ Pa}}{\text{mol}}$	$H_v^{pc} = \dots \frac{\text{m}^3 \text{ atm}}{\text{mol}}$	$H_v^{cc} = \dots$
$H_v^{px} = 1 \text{ atm}$	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 $\rho^\ominus = 997$ kg/m³). For example, if $H_v^{px} = 5$ atm, then $H_s^{bp} \approx 11$ mol/(kg atm) because $5 \times 11 \approx 55.5084$.

	$\frac{H_s^{cp}}{\text{mol}/(\text{m}^3 \text{ Pa})}$	$\frac{H_s^{cp}}{\text{M}/\text{atm}}$	$\frac{H_s^{cc}}{1}$	$\frac{H_s^{bp}}{\text{mol}/(\text{kg Pa})}$	$\frac{H_s^{bp}}{\text{mol}/(\text{kg atm})}$	$\frac{H_s^{xp}}{1/\text{atm}}$	$\frac{\alpha}{1}$
$\frac{H_v^{px}}{\text{atm}}$	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

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

$$\ln H_s = \frac{-\Delta_{\text{sol}}H}{R} \frac{1}{T} + \text{const} \quad (2)$$

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

$$\ln H_s = A + \frac{B}{T} \quad (3)$$

or

$$H_s = \exp(A) \times \exp\left(\frac{B}{T}\right) \quad (4)$$

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:

$$75 \quad H_s = H_s^\ominus \times \exp\left(B \left(\frac{1}{T} - \frac{1}{T^\ominus}\right)\right). \quad (5)$$

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

$$\frac{-\Delta_{\text{sol}}H}{R} = \frac{d \ln H_s}{d(1/T)} = B \quad (6)$$

In this work, the values H_s^\ominus and $d \ln H_s/d(1/T)$ 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 $\Delta_{\text{sol}}H$ can be considered constant. To accommodate a larger temperature range, a third parameter C is often added:

$$\ln H_s = A + \frac{B}{T} + C \times \ln T. \quad (7)$$

Here, the fit parameters A and B are different from those calculated for function (3). The enthalpy of dissolution $\Delta_{\text{sol}}H$ changes linearly with temperature in the 3-parameter fit:

$$85 \quad \frac{-\Delta_{\text{sol}}H}{R} = \frac{d \ln H_s}{d(1/T)} = B - CT \quad (8)$$

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:

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

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:

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

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:

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

100 2.5 Effective Henry's law solubility constants $H_{s,\text{eff}}$

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.

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

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

Once transferred into the aqueous phase, some species are involved in fast equilibria. In these cases, react in the aqueous phase. If these chemical reactions are fast and result in irreversible destruction, Henry's law cannot be applied. If, however, the species enters a fast equilibrium in the aqueous-phase, it is possible to define an "effective" Henry's law constant $H_{s,\text{eff}}$ 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 $H_{s,\text{eff}}$ for aldehydes

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



The total concentration of dissolved methanal is:

$$c_{\text{tot}} = c(\text{HCHO}) + c(\text{H}_2\text{C}(\text{OH})_2) \quad (13)$$

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

$$H_s = \frac{c(\text{HCHO})}{p(\text{HCHO})} \quad (14)$$

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

$$H_{s,\text{eff}} = \frac{c_{\text{tot}}}{p(\text{HCHO})} = \frac{c(\text{HCHO}) + c(\text{H}_2\text{C}(\text{OH})_2)}{p(\text{HCHO})} \quad (15)$$

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

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



Defining the total concentration c_{tot} as

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

the effective Henry's law constant is:

$$H_{s,\text{eff}} = \frac{c_{\text{tot}}}{p(\text{HCl})} = \frac{c(\text{HCl}) + c(\text{Cl}^-)}{p(\text{HCl})} \quad (18)$$

125 Considering the acidity constant

$$K_{\text{a}} = \frac{c(\text{H}^+) c(\text{Cl}^-)}{c(\text{HCl})}, \quad (19)$$

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

$$H_{s,\text{eff}} = H_{\text{s}} \times \left(1 + \frac{K_{\text{a}}}{c(\text{H}^+)} \right) \quad (20)$$

130 Since the factor on the right-hand side contains $c(\text{H}^+)$, the conversion between the intrinsic and the effective Henry's law constant is pH-dependent. Thus, effective Henry's law constants of acids and bases are not material constants but depend on solution pH. Proportionality between $p(\text{HCl})$ and c_{tot} is restricted to conditions under which 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).~~

135 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:

$$H'_{\text{s}} = H_{\text{s}}^{\text{cp}} \times K_{\text{a}} = \frac{c(\text{H}^+) \times c(\text{Cl}^-)}{p(\text{HCl})} \quad (21)$$

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 $H_{s,\text{eff}}$ for halogens

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



The equilibrium constant is:

$$K = \frac{c(\text{HOCl}) c(\text{H}^+) c(\text{Cl}^-)}{c(\text{Cl}_2)} \quad (23)$$

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

$$145 \quad c_{\text{tot}} = c(\text{Cl}_2) + c(\text{HOCl}), \quad (24)$$

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

$$H_{\text{s,eff}} = \frac{c_{\text{tot}}}{p(\text{Cl}_2)} = \frac{c(\text{Cl}_2) + c(\text{HOCl})}{p(\text{Cl}_2)} \quad (25)$$

150 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., $c(\text{HOCl}) \gg c(\text{Cl}_2)$, and the effective Henry’s law solubility constant goes to infinity (see, 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.

155 Instead of extrapolating to infinite dilution, the total chlorine solubility is sometimes reported at the fixed partial pressure of $p(\text{Cl}_2) = 101325 \text{ Pa}$. However, even in the vicinity of 101325 Pa , the total chlorine concentration c_{tot} is not proportional to $p(\text{Cl}_2)$.

In order to convert experimentally determined chlorine solubilities to the intrinsic constant $H_{\text{s}}(\text{Cl}_2)$, 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

160 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 amount 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:

$$\log_{10} \left(\frac{H_{\text{s}0}^{bp}}{H_{\text{s}}^{bp}} \right) = K_{\text{s}} \times b(\text{salt}) \quad (26)$$

170 where $H_{\text{s}0}^{bp}$ = Henry’s law constant in pure water, H_{s}^{bp} = Henry’s law constant in the salt solution, K_{s} = molality-based Sechenov [constant parameter for a given salt](#), and $b(\text{salt})$ = molality of the salt. [For mixed electrolyte solutions with more than one salt, an extension of the Sechenov equation developed by Schumpe \(1993\) and Weisenberger and Schumpe \(1996\) can be used. Sechenov parameters are not suitable for systems in which a species reacts irreversibly with the salt \(e.g., \$\text{N}_2\text{O}_5 + \text{Cl}^-\$ \).](#)

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~~ is also 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~~ considered. 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 $\text{mol}/(\text{m}^3 \text{Pa})$. In cases where the conversion involves the temperature-dependent density of water, the parameterization by Bettin and Spieweck (1990) was used to calculate $\rho_{\text{H}_2\text{O}}$ at the temperature T . The temperature-dependent vapor pressure of water p_{sat} was calculated using the parameterization by Buck (1981).

Inorganic substances are sorted according to the elements they contain. The order chosen is: O, H, N, F, Cl, Br, I, S, rare gases, others. Compounds with several of these elements are put into the last of the applicable sections. For example, nitril chloride which contains O, N and Cl, is listed in the Cl section. Carbon-containing compounds (including CO and CO₂) 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 $T^\ominus = 298.15$ K. Values are rounded to two significant digits and given in the unit $\text{mol}/(\text{m}^3 \text{Pa})$.

The column labeled " $d \ln H_s / d(1/T)$ " 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 $\Delta_{\text{sol}}H$ is temperature-dependent, the value of $d \ln H_s / d(1/T)$ is calculated at $T^\ominus = 298.15$ K. If a 3-parameter fit according to Eq. (7) allows the parameterization over a larger temperature range, it is presented in the notes.

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 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. Note, however, that recent measurements which are newer than the latest review article should always be considered.

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

- 205 “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 ($\Delta_{\text{sol}}G = -RT \ln H$, see Sander (1999) for details).
- 210 “X” The original paper was not available for this study. The data listed here ~~was~~were 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~~using 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.
- 215 “?” The cited paper doesn’t clearly state how the value was obtained.
- “W” The value is probably ~~wrong, as explained in the note~~wrong. It is not listed in the table, in order to avoid spreading of erroneous data. More information can be found in the notes.

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.

220

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.

225 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).

230

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
- 235 – 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)
- 240 – Brennan et al. (1998): Comparison of predictive methods
- Sander (1999): QPPR, QSPR, thermodynamic calculations
- Fogg and Sangster (2003): Miscellaneous methods
- 245 – 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>
- 250 – 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:
- 255 http://geckoa.lisa.u-pec.fr/generateur_form.php
- The Pesticide Properties Database (PPD):
<https://www.ars.usda.gov/Services/docs.htm?docid=14199>
- HENRYWIN, a program to calculate Henry's law constants:
- 260 <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>

265 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_{tot} 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:

$$\begin{aligned}
 270 \quad P_{\text{tot}} &= p_{\text{solute}} + p_{\text{water}} \\
 &= xH_{\text{v}}^{p_x} + (1-x)p_{\text{sat}} \\
 &= x(H_{\text{v}}^{p_x} - p_{\text{sat}}) + p_{\text{sat}}
 \end{aligned} \tag{27}$$

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 $\frac{dP}{dx} = \frac{dp_{\text{tot}}}{dx}$ (i.e., the slope of a plot P_{tot} vs x) can be used to obtain the Henry’s law constant:

$$275 \quad \frac{dP}{dx} = \frac{dp_{\text{tot}}}{dx} = H_{\text{v}}^{p_x} - p_{\text{sat}} \Rightarrow H_{\text{v}}^{p_x} = \frac{dP}{dx} + p_{\text{sat}} \tag{28}$$

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: the uniform format H_s^{cp} with the unit mol/(m³ 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.

290 – 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 is also~~ available at <https://www.henrys-law.org>, will be continuously 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 [isoprene](#), HCl, Br₂, ~~and or~~ BrCl, there is a large uncertainty in the value of the Henry's law constants. I always welcome ~~information emails informing me~~ 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/jn-0-1-2023-supplement>.

300 *Competing interests.* The author declares no competing interests.

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Appendix A: Appendix with data tables

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