

Implications of VOC Oxidation in Atmospheric Chemistry: Development of a Comprehensive AI Model for Predicting Reaction Rate Constants

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Figure S1. Learning curve of the Vreact training process

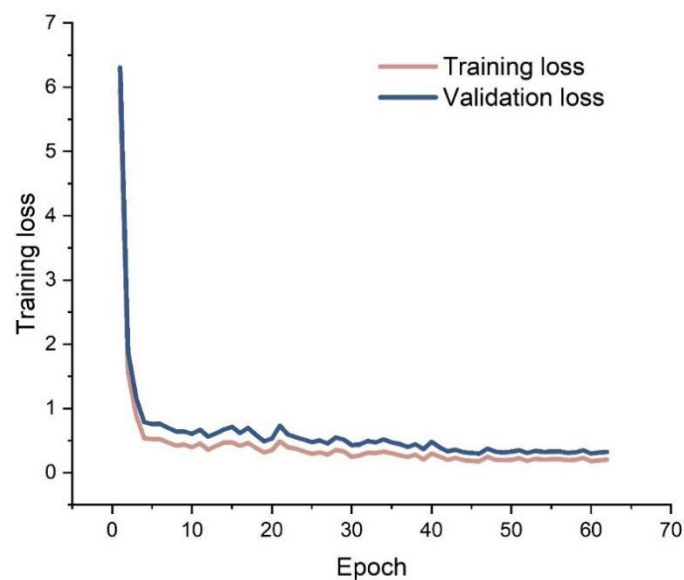


Figure S1 presents the learning curve of the model. The prediction loss on the training set decreases rapidly during the initial phase of training and stabilizes at a very low level. Similarly, the prediction loss on the validation set follows a comparable downward trend and, after a rapid decline, stabilizes at a slightly higher level than that of the training set. The minimal overall difference between the training and validation losses indicates that the model did not experience overfitting and demonstrates strong generalization ability.

Figure S2. User interface of the web platform for predicting VOC reaction rate constants using the Vreact model

The screenshot shows a web browser window with the address bar displaying "vreact.envwind.site:8002". The page is titled "Predicting Rate Constants with the Vreact Model". On the left, there is a navigation sidebar with a "Go to:" section containing radio buttons for "Home" and "Predictor" (which is selected). Below this is a "Contribute" section with a message: "This web platform is free and opensource and you are very welcome to contribute." and a link "Back to Tools". The main content area contains a form with the following elements: a text input field labeled "Type SMILES of VOCs" containing the chemical structure CC(=C)C=C; a "Show" button; a dropdown menu labeled "Choose a radical reaction" with "OH" selected; a section "Return Reaction Rate Constant as" with radio buttons for "ki" (selected) and "lg ki"; a "Predict" button; and a "Show Atom Weights" button.

Navigation:

Go to:

☐ Home

☒ Predictor

Contribute

This web platform is free and opensource and you are very welcome to contribute.

[Back to Tools](#)

Predicting Rate Constants with the Vreact Model

Type SMILES of VOCs

CC(=C)C=C

Show

Choose a radical reaction

OH

Return Reaction Rate Constant as

☒ k_i

☐ $\lg k_i$

Predict

Show Atom Weights

Text S1. Graph representation of molecular structures

The graph $G(V, E)$ comprises a set of vertices (nodes) $i \in V$ and a set of edges $e_{ij} \in E$ that connect vertices i and j . Here, V represents the set of all atoms (nodes) in the molecule, and E represents the set of all chemical bonds (edges) between the atoms. RDKit (version 2023.03.2) is used to calculate atomic and bond features of the molecules. Ten types of atomic information, including element type, chirality, and atomic hybridization type, are calculated for each non-hydrogen atom (Table S2) and converted into a $1 \times l$ feature matrix using one-hot encoding. The feature matrices for all atoms are denoted as X , with dimensions $n \times l$, where n is the number of atoms and l is the feature dimension. Similarly, for each chemical bond represented by edge e_{ij} , four types of bond information, including bond type, conjugation, and whether the bond is in a ring (Table S2), are calculated to generate a $1 \times k$ feature matrix. The feature matrices for all chemical bonds are denoted as Y , with dimensions $2m \times k$, where m is the number of chemical bonds and k is the feature dimension.

Text S2. MPNN message passing and readout phases for molecular graphs

In the molecular graph $G(V, E)$, each node feature is x_i , each edge feature is y_{ij} , and the node state is h_i^t . During the message passing phase of MPNN, the hidden layer node state h_i^t can be updated by the message m_i^{t+1} , with the message function defined as M_t and the vertex update function defined as U_t , where t is the running time step. When $t=0$, $h_i^t=x_i$. The message passing and aggregation from node i and its adjacent nodes and edges obtain the updated state m_i^{t+1} at time $t+1$, as shown in Equation (1). Then, the node embeddings are updated to obtain the hidden state h_i^{t+1} at time $t+1$, as shown in Equation (2). Finally, after T time steps, the readout phase of MPNN is entered, using the readout function R to calculate the feature vector of the entire graph, as shown in Equation (3). M_t , U_t , and R are differentiable functions used for learning. The time step T is a hyperparameter to be determined in subsequent optimization.

$$m_i^{t+1} = \sum_{j \in V} M_t(h_i^t, h_j^t, y_{ij}) \quad (1)$$

$$h_i^{t+1} = U_t(h_i^t, m_i^{t+1}) \quad (2)$$

$$F = R(h_i^T | i \in V) \quad (3)$$

The VOCs molecular feature tensor A' and the oxide molecular feature tensor B' are connected to the original feature tensors A and B , respectively, and the final molecular feature tensors A'' and B'' are obtained through the Set2Set pooling layer. These are then combined and fed into a fully connected layer. The last layer of the fully connected layer is the output layer, which outputs the predicted value of the atmospheric oxidation reaction rate constant $\log_{10}k_i$ for VOCs and oxides. The Smooth L1 Loss function is used to calculate the difference between the model's predicted value and the true value, as shown in Equation (4), where y_i represents the experimental value in the dataset and $\hat{y}_i$ represents the model's predicted value.

$$Loss = \begin{cases} 0.5(y_i - \hat{y}_i)^2, & |y_i - \hat{y}_i| < 1 \\ |y_i - \hat{y}_i| - 0.5, & |y_i - \hat{y}_i| \geq 1 \end{cases} \quad (4)$$

Text S3. Regularization and early stopping techniques in the Vreact model training

The model employs L2 regularization, which adds a penalty term of the sum of the squared weights to the loss function. This restricts the magnitude of the model's parameters to avoid overfitting during training. Early stopping is also used to prevent overfitting. The training stops when the mean squared error on the validation set does not decrease for 15 consecutive training epochs.

Text S4. Model performance evaluation metrics

MSE (Mean Squared Error) is the mean of the squared errors between the predicted data and the original data; the smaller it is, the better the prediction performance. RMSE (Root Mean Squared Error) is the square root of MSE and is also known as the standard error, ensuring consistency in dimensionality. MAE (Mean Absolute Error) is the average of the absolute errors between the predicted data and the original data, used to assess how close the predictions are to the actual values. R^2 (Coefficient of Determination) determines the goodness of fit between the predicted data and the original data, with values ranging from [0,1]; the closer to 1, the better the prediction performance. Moreover, R^2 is not affected by the range of the data itself. The calculation formulas for each evaluation metric are shown in Equations (1) to (4), where m represents the number of samples, y_i represents the experimental values in the dataset, $\hat{y}_i$ represents the model's predicted values, and $\bar{y}$ represents the mean of the experimental values.

$$MSE = \frac{1}{m} \sum_{i=1}^m (y_i - \hat{y}_i)^2 \quad (1)$$

$$RMSE = \sqrt{\frac{1}{m} \sum_{i=1}^m (y_i - \hat{y}_i)^2} \quad (2)$$

$$MAE = \frac{1}{m} \sum_{i=1}^m |y_i - \hat{y}_i| \quad (3)$$

$$R^2 = 1 - \frac{\sum_{i=1}^m (y_i - \hat{y}_i)^2}{\sum_{i=1}^m (y_i - \bar{y})^2} \quad (4)$$

Text S5. Implementation of the Vreact model

The Vreact model was developed using Python (version 3.10.0). Molecular graphs were generated utilizing the open-source deep graph learning framework DGL (version 1.1.0), while RDKit (version 2023.03.2) was employed to compute atomic and chemical bond features, creating the node and edge feature matrices for the molecular graph. The model was constructed using the PyTorch (version 1.21.1) framework and underwent comprehensive training, validation, and evaluation. All aspects of the deep learning model's construction, parameter optimization, training, and analysis were executed on a graphical workstation equipped with an NVIDIA GeForce RTX 3080 GPU.

Table S1. Distribution of VOCs reactions with atmospheric oxidants across datasets

Dataset	Total	•OH	O ₃	•Cl	NO ₃
Training set	2240	1090	257	583	310
Validation set	281	140	28	72	41
Internal test set	281	133	26	80	42

Table S2. Atomic features and bond features used in molecular graph representation

	Atom features	Description	Length
Atom	Atom type	[C, N, O, S, F, P, Cl, Br, I, Si]	10
	Implicit valence	[0,1]	2
	Radical electrons	[0,1]	2
	Degree	[0,1,2,3,4,5,6]	7
	Formal charge	[-1,0,1]	3
	Hybridization	[sp, sp ² , sp ³ , sp ³ d]	4
	FCFP	Molecular fingerprint	6
	Number of hydrogens	[0,1,2,3,4]	5
	Chirality	[R, S]	2
	Possibility of chirality	Possibility of atomic chirality	1
Bond	Bond type	[single, double, triple, aromatic]	4
	Bond is in conjugation	Part of conjugation	1
	Bond is in ring	Part of ring	1
	Bond stereochemistry	[stereonone, stereoany, stereoz, stereo]	4

Table S3. Hyperparameter search space and optimal settings for the Vreact model

Hyperparameter	Search range	Optimal settings
lr	0.005~0.005	0.00454
$batchsize$	8~256	115
$weight\ decay$	0~0.01	0.00231
p	0~0.5	0.0107
T	4~10	6

Table S4. Experimental and predicted $\log_{10}k_i$ values for VOCs on the internal test dataset

Oxidants	VOCs chemical name	Experimental $\log_{10}k_i$	Prediction $\log_{10}k_i$
•OH	chloro(difluoro)methane	-14.328	-14.251
•OH	1,2-bis(difluoromethoxy)-1,1,2,2-tetrafluoroethane	-14.328	-15.158
•OH	acetyl fluoride	-14.131	-13.580
•OH	1,1,1,2,3,3-hexafluoro-3-(2,2,2-trifluoroethoxy)propane	-14.061	-13.729
•OH	1,1,2,2,2-pentafluoroethyl formate	-13.921	-14.021
•OH	1-bromo-2-chloro-1,1,2-trifluoroethane	-13.854	-13.772
•OH	(E)-1,2,3,3,4,4,5,5-octafluorocyclopentane	-13.845	-13.933
•OH	1,1,2,3,3-pentafluoropropane	-13.745	-14.068
•OH	(E)-1,1,2,2-tetrafluoro-3,4-dichlorocyclobutane	-13.487	-13.575
•OH	1-chloro-2,2,3,3-tetrafluorocyclobutane	-13.344	-13.535
•OH	methylphosphonic dichloride	-13.194	-13.659
•OH	perfluorocyclopentene	-13.139	-12.814
•OH	methyl chlorodifluoroacetate	-13.006	-13.338
•OH	methyl 2,2-difluoroacetate	-12.876	-13.116
•OH	1-ethoxy-1,1,2,3,3,3-hexafluoropropane	-12.854	-12.674
•OH	trifluoromethoxyethane	-12.824	-12.863
•OH	1,1,1,2-tetrafluoro-2-methoxyethane	-12.796	-12.840
•OH	acetone	-12.729	-11.997
•OH	1,1,2-trichloroethane	-12.721	-12.799
•OH	2,2-difluoroethanol	-12.569	-12.324
•OH	tribromomethane	-12.569	-12.713
•OH	1,2-dibromo-3-chloropropane	-12.393	-12.314
•OH	1,2-dichloropropane	-12.337	-12.126
•OH	2-formyloxyethyl formate	-12.315	-11.829
•OH	3,3,3-trifluoro-2-(trifluoromethyl)propene	-12.125	-11.820
•OH	2-bromopropane	-12.120	-11.717
•OH	tetramethylsilane	-11.966	-11.549
•OH	3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluoro-1-decene	-11.893	-11.600
•OH	(Z)-1,3,3,3-tetrafluoropropene	-11.889	-11.787
•OH	(Z)-1,2,3,3,3-pentafluoroprop-1-ene	-11.886	-11.809
•OH	3,3,4,4,4-pentafluoro-1-butene	-11.854	-11.374
•OH	pentanenitrile	-11.830	-11.572
•OH	butanoic acid	-11.745	-11.603
•OH	perfluoro-1-butene	-11.712	-12.124

•OH	2-chloro-2-fluoroacetaldehyde	-11.678	-11.544
•OH	3-picoline	-11.638	-11.651
•OH	isopropylcyclopropane	-11.583	-11.029
•OH	3,3,3-trifluoropropanal	-11.569	-11.773
•OH	3-methyl-2-pentyl nitrate	-11.553	-11.249
•OH	1,4-naphthoquinone	-11.538	-10.512
•OH	3-methyl-2-butanone	-11.523	-11.342
•OH	4-chlorobiphenyl	-11.471	-11.192
•OH	ethyl levulinate	-11.465	-11.042
•OH	dodecamethyltetrasiloxane	-11.458	-10.970
•OH	di-tert-butyl ether	-11.432	-11.286
•OH	dimethoxypropane	-11.387	-10.907
•OH	acrylonitrile	-11.385	-10.822
•OH	1,3,5-trioxane	-11.268	-11.112
•OH	3-methylhexane	-11.201	-10.930
•OH	3,4-diethylhexane	-11.160	-10.761
•OH	2-methyl-2-pentanol	-11.149	-10.990
•OH	1-butyne	-11.125	-11.271
•OH	methylcyclopentane	-11.121	-10.977
•OH	bis(2-chloroethyl) ether	-11.119	-11.154
•OH	2-ethoxy-2-methylpropane	-11.061	-10.997
•OH	1-pentyne	-11.017	-11.111
•OH	diacetylene	-11.000	-11.126
•OH	oxetane	-10.987	-11.026
•OH	2-pentanol	-10.959	-10.664
•OH	4-methyl-1,3-dioxane	-10.947	-10.817
•OH	2-nonanone	-10.914	-10.748
•OH	4-methyl-2H-furan-5-one	-10.900	-10.429
•OH	4-methyl-2-pentanone	-10.871	-11.122
•OH	cyclooctane	-10.858	-10.721
•OH	1,3-dioxepane	-10.854	-10.727
•OH	menthol	-10.830	-10.568
•OH	ethyl acrylate	-10.799	-10.659
•OH	3-fluoropropene	-10.796	-10.577
•OH	1,1,3-trimethoxypropane	-10.777	-10.425
•OH	2-acetylbenzaldehyde	-10.770	-10.554
•OH	5-hydroxy-2-heptanone	-10.721	-10.501
•OH	(E)-decalin	-10.721	-10.719
•OH	3-hydroxypropanal	-10.701	-10.523
•OH	m-ethyltoluene	-10.691	-10.785

•OH	1,2-propanediol	-10.678	-10.738
•OH	9,10-dihydroanthracene	-10.674	-10.438
•OH	3,3-dimethylbutanal	-10.670	-10.647
•OH	3-hydroxy-2-hexanone	-10.658	-10.718
•OH	5-hydroxy-2-octanone	-10.638	-10.403
•OH	methyl-1,4-benzoquinone	-10.638	-10.492
•OH	fenchol	-10.604	-10.756
•OH	phenylmethanol	-10.569	-11.053
•OH	t-butylsulfide	-10.538	-11.245
•OH	2-butoxyethanol	-10.523	-10.557
•OH	3-methyl-2-cyclohexen-1-one	-10.509	-10.176
•OH	methylsilane	-10.482	-11.498
•OH	(E)-2-butenedial	-10.462	-10.579
•OH	1,2-pentadiene	-10.444	-10.271
•OH	isochroman	-10.432	-10.645
•OH	furan	-10.416	-10.396
•OH	2-chloroethyl vinyl ether	-10.381	-10.090
•OH	N,N-diisopropylaniline	-10.357	-10.305
•OH	triethyl phosphate	-10.330	-10.553
•OH	3-methyl-3-buten-2-one	-10.301	-10.439
•OH	1-dodecene	-10.298	-10.235
•OH	(E)-4-hydroperoxy-2-hexenal	-10.292	-10.427
•OH	5-hexen-3-one	-10.286	-10.235
•OH	5-hexen-2-one	-10.284	-10.243
•OH	(Z)-2-butenedial	-10.237	-10.612
•OH	dimethyl sulfoxide	-10.229	-10.642
•OH	4-hexen-2-one	-10.222	-10.031
•OH	2-methyl-1-butene	-10.215	-10.170
•OH	4-hydroxy-3-methyl-3-penten-2-one	-10.215	-10.102
•OH	3-methyl-1-penten-3-ol	-10.208	-10.339
•OH	2-methyl-3-buten-2-ol	-10.201	-10.450
•OH	1-penten-3-ol	-10.199	-10.243
•OH	n-butyl methacrylate	-10.182	-10.330
•OH	isopropenyl acetate	-10.173	-10.378
•OH	(E)-2-penten-1-ol	-10.170	-10.082
•OH	(Z/E)-2-heptene	-10.168	-10.061
•OH	dimethylamine	-10.166	-10.191
•OH	(E)-2-hexenyl acetate	-10.162	-10.149
•OH	2-methyl-1-octene	-10.154	-10.099
•OH	methyl ketene	-10.143	-10.177

•OH	(E)-2-octene	-10.141	-10.069
•OH	indene	-10.108	-10.070
•OH	(E)-2-decene	-10.108	-10.057
•OH	2-methyl-1-tridecene	-10.077	-10.067
•OH	2-vinylfuran	-10.056	-9.911
•OH	2-methyl-2-pentene	-10.051	-9.861
•OH	alpha-copaene	-10.046	-9.969
•OH	catechol	-10.000	-9.999
•OH	benzene oxide	-10.000	-9.999
•OH	morpholine	-9.959	-10.383
•OH	2,3,5-trimethylphenol	-9.865	-9.827
•OH	N,N-dimethylaniline	-9.830	-10.367
•OH	3-methyl-2-buten-1-ol	-9.796	-9.882
•OH	limonene	-9.783	-9.663
•OH	gamma-terpinene	-9.770	-9.709
•OH	citronellol	-9.770	-9.715
•OH	beta-caryophyllene	-9.699	-9.578
•OH	O,O-diethyl methylphosphonothioate	-9.690	-10.482
•OH	3,4-dihydroxy-3-hexene-2,5-dione	-9.569	-10.605
•Cl	1,1,2-trifluoro-2-(trifluoromethoxy)ethane	-14.886	-14.717
•Cl	2-chloro-1,1,1-trifluoroethane	-14.187	-13.916
•Cl	3,3,4,4,5-pentafluoro-2,5-bis(1,1,1,2,3,3,3-heptafluoropropan-2-yl)oxolan-2-yl formate	-13.873	-13.563
•Cl	perfluoro-n-heptyl formate	-13.854	-13.424
•Cl	perfluoroisopropyl formyl ether	-13.833	-13.748
•Cl	3,3-dichloro-1,1,1-trifluoro-2-propanone	-13.638	-13.605
•Cl	3-chloro-1,1,1-trifluoro-2-propanone	-13.250	-13.264
•Cl	formyl acetate	-13.000	-12.629
•Cl	chloro(fluoro)methane	-12.959	-12.829
•Cl	1,1,1,2,2,3,3-heptafluoro-3-methoxypropane	-12.933	-13.402
•Cl	methyl nitrate	-12.620	-12.833
•Cl	chloromethane	-12.310	-11.995
•Cl	1,1,1,2,2,3,3,4,4-nonafluoro-6-iodohexane	-11.903	-11.769
•Cl	acetone	-11.678	-11.055
•Cl	2,2,3,3,3-pentafluoropropanal	-11.678	-11.015
•Cl	isopropyl nitrate	-11.420	-11.356
•Cl	1,1,1-trifluoro-2-propanol	-11.347	-11.202
•Cl	methyl isocyanate	-11.213	-12.813
•Cl	2,2,2-trichloroacetaldehyde	-11.194	-11.222
•Cl	ethyl 2-chloropropanoate	-11.129	-10.434

•Cl	2-methylpropionyl chloride	-11.107	-11.112
•Cl	1-nitrooxy-2-butanol	-11.061	-10.297
•Cl	1-nitropropane	-11.004	-11.179
•Cl	ethyl formate	-10.992	-10.789
•Cl	isopropyl formate	-10.801	-10.699
•Cl	5-nitrooxy-2-pentanol	-10.688	-10.097
•Cl	furfural	-10.456	-9.927
•Cl	1,1,1,2,2-pentafluoro-3-methoxypropane	-10.377	-11.188
•Cl	2,2,2-trifluoroethyl butanoate	-10.299	-10.522
•Cl	(E)-1-chloro-3,3,3-trifluoroprop-1-ene	-10.282	-10.518
•Cl	hexamethylcyclotrisiloxane	-10.252	-10.403
•Cl	methyl thiolformate	-10.244	-9.712
•Cl	chloro(iodo)methane	-10.236	-11.52
•Cl	dichlorosilane	-10.154	-11.555
•Cl	pentanenitrile	-10.151	-10.185
•Cl	formaldehyde	-10.143	-10.541
•Cl	3-pentanone	-10.097	-9.996
•Cl	N-methylformamide	-10.066	-9.887
•Cl	2,4-dimethylbenzaldehyde	-10.061	-9.705
•Cl	N-methylacetamide	-10.046	-10.001
•Cl	(Z)-1,2-dichloroethene	-10.041	-10.253
•Cl	bis(2-chloroethyl) ether	-10.000	-9.716
•Cl	acrylonitrile	-9.987	-9.813
•Cl	cyclopentanone	-9.959	-10.313
•Cl	2,2-dimethylpropane	-9.959	-10.081
•Cl	n-propyl isobutyrate	-9.951	-9.790
•Cl	3-methyl-2-butanol	-9.921	-9.612
•Cl	ethyl 3-methylbutanoate	-9.903	-9.935
•Cl	1-bromobutane	-9.854	-9.973
•Cl	methyl t-butyl ether	-9.824	-9.863
•Cl	2-methylpropanal	-9.807	-9.704
•Cl	n-butyl n-butanoate	-9.770	-9.820
•Cl	alpha-methylstyrene	-9.733	-9.501
•Cl	2-ethoxyethanol	-9.711	-9.481
•Cl	1,4-benzoquinone	-9.710	-9.716
•Cl	n-pentanethiol	-9.706	-9.444
•Cl	3-pentanol	-9.699	-9.620
•Cl	2-methylbutane	-9.678	-9.834
•Cl	allyl cyanide	-9.661	-9.636
•Cl	2,4,4-trimethyl-1-pentanol	-9.628	-9.552

•Cl	3-methyl-2-butenal	-9.611	-9.331
•Cl	5-methyl-2-hexanol	-9.605	-9.503
•Cl	4-pentenenitrile	-9.576	-9.539
•Cl	propene	-9.569	-9.451
•Cl	methylamine	-9.538	-10.137
•Cl	trimethylsilylmethanol	-9.530	-9.438
•Cl	3-buten-2-ol	-9.523	-9.408
•Cl	menthol	-9.469	-9.575
•Cl	2-methyl-3-butyn-2-ol	-9.456	-9.927
•Cl	(E)-2-hexen-1-ol	-9.454	-9.143
•Cl	1,2-dimethylnaphthalene	-9.443	-9.641
•Cl	2-methyl-2-butene	-9.420	-9.013
•Cl	n-heptane	-9.420	-9.588
•Cl	ethylcyclohexane	-9.411	-9.473
•Cl	3-octen-1-ol	-9.384	-9.040
•Cl	1-ethenoxypropane	-9.374	-9.066
•Cl	n-octane	-9.357	-9.522
•Cl	3-methyl-2-buten-1-ol	-9.348	-9.031
•Cl	1-octene	-9.260	-9.231
•Cl	2-methoxy-1-propene	-9.153	-9.028
O ₃	dichlorvos	-18.770	-17.001
O ₃	o-cresol	-18.585	-16.888
O ₃	E 1,3-dichloropropene	-18.174	-18.557
O ₃	(Z)-3-hexene-2,5-dione	-17.745	-17.182
O ₃	(E)-2-formylcinnamaldehyde	-17.745	-17.738
O ₃	(E)-2-nonenal	-17.688	-17.007
O ₃	3-methyl-1-penten-3-ol	-17.284	-16.730
O ₃	3-buten-1-ol	-17.256	-16.842
O ₃	(E)-3-hexene-2,5-dione	-17.081	-17.735
O ₃	2-methyl-1-octene	-16.860	-16.574
O ₃	1-nonen-3-ol	-16.724	-16.767
O ₃	2-methyl-1,5-hexadiene	-16.684	-16.417
O ₃	alpha-cedrene	-16.553	-15.729
O ₃	3-octen-2-one	-16.458	-16.773
O ₃	1-hydroxy-2-methylbut-3-en-2-yl nitrate	-16.276	-17.121
O	(3E)-4-methyl-3,5-hexadienal	-16.244	-16.458
O ₃	(E)-3-hexen-1-ol	-16.233	-15.864
O ₃	(Z)-3-hexenylpropanoate	-16.118	-16.323
O ₃	2-methyl-1-nitrooxy-but-3-en-2-ol	-15.975	-17.251
O ₃	(Z)-2-pentene	-15.893	-15.849

O ₃	alpha-copaene	-15.824	-15.940
O ₃	(E)-2-butene	-15.699	-15.788
O ₃	6-methyl-5-hepten-2-ol	-15.420	-15.482
O ₃	beta-ocimene	-15.292	-15.306
O ₃	1-methylcyclopentene	-15.174	-15.325
O ₃	terpinolene	-14.796	-14.928
NO ₃	propane	-17.036	-16.678
NO ₃	methyl vinyl ketone	-15.886	-14.269
NO ₃	cyclohexane	-15.870	-15.997
NO ₃	n-heptane	-15.854	-15.614
NO ₃	(Z)-1,2-dichloroethene	-15.824	-15.653
NO ₃	n-butyl acrylate	-15.721	-14.419
NO ₃	n-octane	-15.721	-15.362
NO ₃	n-decane	-15.585	-14.963
NO ₃	chloroethene	-15.409	-14.862
NO ₃	1-butyne	-15.328	-15.189
NO ₃	isopropyl methyl methylphosphonate	-15.319	-14.689
NO ₃	3-chloro-1-propene	-15.258	-14.411
NO ₃	divinyl sulfoxide	-15.215	-13.403
NO ₃	1-butanol	-14.728	-14.661
NO ₃	2-ethoxy-2-methylpropane	-14.068	-14.992
NO ₃	2-ethoxyethanol	-14.038	-13.980
NO ₃	2-methylpropanal	-13.903	-14.028
NO ₃	4,4-dimethyl-1-pentene	-13.886	-13.557
NO ₃	3,4-dimethyl-1-pentene	-13.854	-13.090
NO ₃	hexanal	-13.793	-13.599
NO ₃	4-methyl-1-hexene	-13.745	-13.483
NO ₃	(E)-2-heptenal	-13.699	-13.457
NO ₃	cyclobutanecarbaldehyde	-13.686	-13.785
NO ₃	2,2-dimethylpropanal	-13.620	-14.212
NO ₃	3-methylpentanal	-13.602	-13.615
NO ₃	(E)-2-formylcinnamaldehyde	-13.367	-13.227
NO ₃	1-methyl-2-pyrrolidone	-12.824	-14.174
NO ₃	isopropenyl-6-oxo-heptanal	-12.585	-12.383
NO ₃	diiodomethane	-12.398	-15.161
NO ₃	(Z)-2-hexene	-12.260	-12.097
NO ₃	9,10-dihydroanthracene	-11.921	-13.251
NO ₃	1-ethenoxybutane	-11.699	-11.400
NO ₃	phenol	-11.347	-11.201
NO ₃	alpha-cedrene	-11.086	-10.581

NO ₃	alpha-neoclovene	-11.084	-10.902
NO ₃	beta-caryophyllene	-10.721	-10.635
NO ₃	2-carene	-10.699	-10.557
NO ₃	2-methylfuran	-10.590	-10.682
NO ₃	guaiacol	-10.570	-10.845
NO ₃	pyrrole	-10.335	-9.321
NO ₃	alpha-terpinene	-9.745	-10.256
NO ₃	azulene	-9.409	-14.061

Table S5. 447 real-world atmospheric VOCs

VOCs Group	VOCs chemical name	VOCs CAS
Alkane	Ethane	74-84-0
Alkane	Propane	74-98-6
Alkane	i-Butane	75-28-5
Alkane	n-Butane	106-97-8
Alkane	Cyclopentane	287-92-3
Alkane	i-Pentane	78-78-4
Alkane	n-Pentane	109-66-0
Alkane	2,2-Dimethylpropane	463-82-1
Alkane	Methylcyclopentane	96-37-7
Alkane	Cyclohexane	110-82-7
Alkane	2,2-Dimethylbutane	75-83-2
Alkane	2,3-Dimethylbutane	79-29-8
Alkane	2-Methylpentane	107-83-5
Alkane	3-Methylpentane	96-14-0
Alkane	n-Hexane	110-54-3
Alkane	n-Heptane	142-82-5
Alkane	Isoheptane	591-76-4
Alkane	3-Methylhexane	589-34-4
Alkane	2,3-DimethylPentane	565-59-3
Alkane	2,4-Dimethylpentane	108-08-7
Alkane	2-Methyl-2-pentene	625-27-4
Alkane	Ethylcyclohexane	1678-91-7
Alkane	3-Ethylhexane	619-99-8
Alkane	3,4-Dimethylhexane	583-48-2
Alkane	2,2,4-Trimethylpentane	540-84-1
Alkane	2,3,4-Trimethylpentane	565-75-3
Alkane	2,5-Dimethylhexane	592-13-2
Alkane	2,4-Dimethylhexane	589-43-5
Alkane	2,3-Dimethylhexane	584-94-1
Alkane	2-Methylheptane	592-27-8
Alkane	3-Methylheptane	589-81-1

Alkane	Methylcyclohexane	108-87-2
Alkane	Ethylcyclopentane	1640-89-7
Alkane	n-Octane	111-65-9
Alkane	n-Nonane	111-84-2
Alkane	2,2,4-Trimethylhexane	16747-26-5
Alkane	Methyl amyl, cyclopropane	6976-28-9
Alkane	n-Decane	124-18-5
Alkane	1,2-Dimethylcyclohexane	583-57-3
Alkane	1,1,3-Trimethylcyclohexane	3073-66-3
Alkane	1-Methyl-2-propyl cyclopentane	3728-57-2
Alkane	2,2-Dimethylhexane	590-73-8
Alkane	2-Methyl-3-ethylpentane	609-26-7
Alkane	4-Methylheptane	589-53-7
Alkane	trans-1-Ethyl-3-methyl cyclopentane	2613-65-2
Alkane	1-Ethyl-3-methyl cyclopentane	3726-47-4
Alkane	1-Ethyl-2-methyl cyclopentane	3726-46-3
Alkane	trans-1,2-Dimethylcyclohexane	6876-23-9
Alkane	1-Methyl ethyl cyclopentane	16747-50-5
Alkane	Isopropylcyclopentane	3875-51-2
Alkane	1,2,4-Trimethylcyclohexane	2234-75-5
Alkane	1,3,5-Trimethylcyclohexane	1795-27-3
Alkane	1-Ethyl-2-methylcyclohexane	3728-54-9
Alkane	1-Ethyl-2-methylcyclohexane, trans	4923-77-7
Alkane	2,6-Dimethyl heptadecane	54105-67-8
Alkane	2,6,10,14-Tetramethyl hexadecane	638-36-8
Alkane	1-Methyl-2-isopropylcyclohexane	16580-23-7
Alkane	Isobutylcyclohexane	1678-98-4
Alkane	2,5-Dimethyloctane	15869-89-3
Alkane	2,6-Dimethyloctane	2051-30-1
Alkane	4-Ethyloctane	15869-86-0
Alkane	3-MethylNonane	5911-04-6
Alkane	2,5-Dimethylnonane	17302-27-1
Alkane	2,2,4,4-Tetramethyloctane	62183-79-3

Alkane	4-Methyldecane	2847-72-5
Alkane	5-Methyldecane	13151-35-4
Alkane	2,2-Dimethyldecane	17302-37-3
Alkane	1,3-Dimethylcyclopentane	2451-00-1
Alkane	1,2,4-Trimethylcyclopentane	2815-58-9
Alkane	1-Ethyl-4-methylcyclohexane	3728-56-1
Alkane	Butyl cyclohexane	1678-93-9
Alkane	Pentyl cyclohexane	4292-92-6
Alkane	2-Methyldecane	6975-98-0
Alkane	n-Undecane	1120-21-4
Alkane	n-Dodecane	112-40-3
Alkane	Isododecane	13475-82-6
Alkane	Tridecane	629-50-5
Alkane	Tetradecane	629-59-4
Alkane	n-Pentadecane	629-62-9
Alkane	Hexadecane	544-76-3
Alkane	Heptadecane	629-78-7
Alkane	Octadecane	593-45-3
Alkane	Nonadecane	629-92-5
Alkane	Eicosane	112-95-8
Alkane	n-Heneicosane	629-94-7
Alkane	Docosane	629-97-0
Alkene	Ethene	74-85-1
Alkene	Propene	115-07-1
Alkene	1,2-Butadiene	590-19-2
Alkene	1,3-Butadiene	106-99-0
Alkene	1-Butene	106-98-9
Alkene	2-Butene	107-01-7
Alkene	i-butene	115-11-7
Alkene	cis-2-Butene	590-18-1
Alkene	trans-2-Butene	624-64-6
Alkene	1,3-Cyclopentadiene	542-92-7
Alkene	Isoprene	78-79-5

Alkene	1,3-Pentadiene	504-60-9
Alkene	1-Pentene	109-67-1
Alkene	cis-2-Pentene	627-20-3
Alkene	trans-2-Pentene	646-04-8
Alkene	2-Pentene	109-68-2
Alkene	Cyclopentene	142-29-0
Alkene	3-Methyl-1-butene	563-45-1
Alkene	2-Methyl-1-butene	563-46-2
Alkene	2-Methyl-2-butene	513-35-9
Alkene	1-Hexene	592-41-6
Alkene	trans-2-hexene	4050-45-7
Alkene	cis-2-Hexene	7688-21-3
Alkene	3-Methylcyclopentene	1120-62-3
Alkene	3-Methyl-1-pentene	760-20-3
Alkene	1-Methylcyclohexene	591-49-1
Alkene	4-Methyl-1-cyclohexene	591-47-9
Alkene	1-Heptene	592-76-7
Alkene	2-Methyl-1-pentene	763-29-1
Alkene	4-Methyl-1-pentene	691-37-2
Alkene	2,4-Dimethyl-2-pentene	625-65-0
Alkene	2,4,4-Trimethyl-1-pentene	107-39-1
Alkene	2,4,4-Trimethyl-2-pentene	107-40-4
Alkene	1-Octene	111-66-0
Alkene	1-Nonene	124-11-8
Alkene	1-Decene	872-05-9
Alkene	α -Pinene	80-56-8
Alkene	β -Pinene	127-91-3
Alkene	Endo-tetrahydrocyclopentadiene	2825-83-4
Alkene	1-Methoxy-1-propylene	7319-16-6
Alkene	3-Hexene	592-47-2
Alkene	2-Methylcyclopentene	639-89-0
Alkene	2,4-Hexadiene	592-46-1
Alkene	4-Methyl-1,4-hexadiene	1116-90-1

Alkene	4-Methyl-2-pentene	4461-48-7
Alkene	3-Methylcyclohexene	591-48-0
Alkene	1,4-Dimethylcyclohexene	70688-47-0
Alkene	1-Ethylcyclohexene	1453-24-3
Alkene	1-Methyl-1-cyclooctene	933-11-9
Alkene	1-Isobutyl-1-cyclohexene	3983-03-7
Alkene	3-Butylcyclohexene	3983-07-1
Alkene	1-Butylcyclohexene	3282-53-9
Alkene	3-Methyl-6-isopropylcyclohexene	5113-93-9
Alkene	2,6-Dimethyl-2,6-cyclooctadiene	3760-14-3
Alkyne	Ethyne	74-86-2
Alkyne	Allylene	74-99-7
Alkyne	Butenyne	689-97-4
Alkyne	2-Methyl,1- buten-3-yne	78-80-8
Alkyne	1-Pentene- 3-yne	645-05-9
Aromatic	Benzene	71-43-2
Aromatic	Toluene	108-88-3
Aromatic	Ethylbenzene	100-41-4
Aromatic	m-Xylene	108-38-3
Aromatic	p-Xylene	106-42-3
Aromatic	o-Xylene	95-47-6
Aromatic	m/p-Xylene	108-38-3/106-42-3
Aromatic	Xylene	1330-20-7
Aromatic	Styrene	100-42-5
Aromatic	Phenylethyne	536-74-3
Aromatic	1,2,3-Trimethylbenzene	526-73-8
Aromatic	1,2,4-Trimethylbenzene	95-63-6
Aromatic	1,3,5-Trimethylbenzene	108-67-8
Aromatic	1,3-Diisopropylbenzene	99-62-7
Aromatic	n-Propylbenzene	103-65-1
Aromatic	Isopropylbenzene	98-82-8
Aromatic	Allylbenzene	300-57-2

Aromatic	Cyclopropylbenzene	873-49-4
Aromatic	o-Ethyltoluene	611-14-3
Aromatic	m-Ethyltoluene	620-14-4
Aromatic	p-Ethyltoluene	622-96-8
Aromatic	o-Diethylbenzene	135-01-3
Aromatic	m-Diethylbenzene	141-93-5
Aromatic	p-Diethylbenzene	105-05-5
Aromatic	1-Methyl-3-propylbenzene	1074-43-7
Aromatic	1-Methyl-4-propylbenzene	1074-55-1
Aromatic	1,2,3,4-Tetramethylbenzene	488-23-3
Aromatic	1,2,3,5-Tetramethylbenzene	527-53-7
Aromatic	1,2,4,5-Tetramethylbenzene	95-93-2
Aromatic	2-Ethyl-1,3-dimethyl-benzene	2870-04-4
Aromatic	2-Ethyl-1,4-dimethyl-benzene	1758-88-9
Aromatic	1-Ethyl-2,3-dimethyl benzene	933-98-2
Aromatic	1-Ethyl-2,4-dimethylbenzene	874-41-9
Aromatic	1,2-Dimethyl-4-ethylbenzene	934-80-5
Aromatic	5-Ethyl-m-xylene	934-74-7
Aromatic	Tert-butylbenzene	98-06-6
Aromatic	sec-Butylbenzene	135-98-8
Aromatic	p-Isopropyltoluene	99-87-6
Aromatic	n-Butylbenzene	104-51-8
Aromatic	(2-Methylpropyl)benzene	538-93-2
Aromatic	1-Methyl-2-(1-methyl ethyl) benzene	527-84-4
Aromatic	3,5-Diethyltoluene	2050-24-0
Aromatic	sec-Pentylbenzene	2719-52-0
Aromatic	1,2,4-Triethylbenzene	877-44-1
Aromatic	1,2,5-Triethylbenzene	102-25-0
Aromatic	cis-Hydrindane	4551-51-3
Aromatic	Indene	95-13-6
Aromatic	Indane	496-11-7
Aromatic	5-Methyldane	874-35-1
Aromatic	4-Methyldane	824-22-6

Aromatic	Naphthalene	91-20-3
Aromatic	2-Methyl naphthalene	91-57-6
Aromatic	1-Methyl naphthalene	90-12-0
Aromatic	Octahydronaphthalene	1194-95-2
Aromatic	Decahydronaphthalene	91-17-8
Aromatic	1-Methyldecalin	2958-75-0
Aromatic	Acenaphthene	83-32-9
Aromatic	Dihydroanthracene	208-96-8
Aromatic	Fluorene	86-73-7
Aromatic	Phenanthrene	85-01-8
Aromatic	Anthracene	120-12-7
Aromatic	Fluoranthene	206-44-0
Aromatic	Pyrene	129-00-0
Halocarbon	Tetrachloromethane	56-23-5
Halocarbon	Freon12(CF ₂ Cl ₂)	75-71-8
Halocarbon	Freon11(CFCl ₃)	75-69-4
Halocarbon	Chloroform	67-66-3
Halocarbon	Bromoform	75-25-2
Halocarbon	Freon22(CHClF ₂)	75-45-6
Halocarbon	Dichloromethane	75-09-2
Halocarbon	Chloromethane	74-87-3
Halocarbon	Methyl bromide	74-83-9
Halocarbon	Iodomethane	74-88-4
Halocarbon	Tetrachloroethylene	127-18-4
Halocarbon	Freon113a(C ₂ F ₃ Cl ₃)	354-58-5
Halocarbon	Freon113(C ₂ F ₃ Cl ₃)	76-13-1
Halocarbon	Freon114(C ₂ F ₄ Cl ₂)	76-14-2
Halocarbon	Trichloroethylene	79-01-6
Halocarbon	1,1-Dichloroethylene	75-35-4
Halocarbon	1,2-Dichloroethylene	540-59-0
Halocarbon	cis-1,2-Dichloroethylene	156-59-2
Halocarbon	1,1,2,2-Tetrachloroethane	79-34-5
Halocarbon	1,1,1-Trichloroethane	71-55-6

Halocarbon	Vinyl chloride	75-01-4
Halocarbon	1,1,2-Trichloroethane	79-00-5
Halocarbon	1,1-Dichloroethane	75-34-3
Halocarbon	1,2-Dichloroethane	107-06-2
Halocarbon	1,2,3-Trichloropropane	96-18-4
Halocarbon	Chloroethane	75-00-3
Halocarbon	cis-1,3-Dichloropropene	10061-01-5
Halocarbon	trans-1,3-Dichloropropene	10061-02-6
Halocarbon	1,3-Dichloropropene	542-75-6
Halocarbon	1,2-Dichloropropene	563-54-2
Halocarbon	1,2-Dichloropropane	78-87-5
Halocarbon	1,2,4-Trichlorobenzene	120-82-1
Halocarbon	1,2-Dichlorobenzene	95-50-1
Halocarbon	1,3-Dichlorobenzene	541-73-1
Halocarbon	1,4-Dichlorobenzene	106-46-7
Halocarbon	Chlorobenzene	108-90-7
Halocarbon	Chlorotoluene	25168-05-2
Halocarbon	Dichlorotoluene	98-87-3
Halocarbon	Benzyl chloride	100-44-7
Halocarbon	Monobromo-dichloro-methane	75-27-4
Halocarbon	Dibromo-monochloro-methane	124-48-1
Halocarbon	Monofluorotrichloromethane	62185-70-0
Halocarbon	Vinyl bromide	593-60-2
Halocarbon	Dibromoethane	106-93-4
Halocarbon	Trans-1,2-Dichloroethylene	156-60-5
Halocarbon	Allyl chloride	107-05-1
Halocarbon	Hexachlorobutadiene	87-68-3
OVOC	Formic acid	64-18-6
OVOC	Acetic acid	64-19-7
OVOC	2-Methylpropanoic acid	79-31-2
OVOC	Benzoic acid	65-85-0
OVOC	Methanol	67-56-1
OVOC	Ethanol	64-17-5

OVOC	Ethylene glycol	107-21-1
OVOC	Propylene glycol	57-55-6
OVOC	Isopropanol	67-63-0
OVOC	n-Propanol	71-23-8
OVOC	n-Butanol	71-36-3
OVOC	sec-Butanol	78-92-2
OVOC	Cyclobutanol	2919-23-5
OVOC	Diethylene glycol	111-46-6
OVOC	3-Methoxy-1-propanol	1589-49-7
OVOC	Glycolaldehyde dimethyl acetal	30934-97-5
OVOC	1,3-Butanediol	107-88-0
OVOC	1,2-Dimethoxyethane	110-71-4
OVOC	2-Isopropoxyethanol	109-59-1
OVOC	3-Methoxy-1-butanol	2517-43-3
OVOC	2-(2-Hydroxypropoxy)-1-propanol	106-62-7
OVOC	Polypropylene glycol	110-98-5
OVOC	Benzyl alcohol	100-51-6
OVOC	1-Butoxy-2-propanol	5131-66-8
OVOC	2-Ethyl-1-hexanol	104-76-7
OVOC	2-Ethylhexane-1,3-diol	94-96-2
OVOC	2-Ethylhexanol	123-05-7
OVOC	2-Propoxyethanol	2807-30-9
OVOC	2-Methyl-2-propanol	75-65-0
OVOC	Neopentyl glycol	126-30-7
OVOC	2-Propen-1-ol	107-18-6
OVOC	Glycidol	556-52-5
OVOC	Isobutanol	78-83-1
OVOC	3-Methyl-2-butanol	75-85-4
OVOC	1-Pentanol	71-41-0
OVOC	1,3-Dimethoxy-2-propanol	623-69-8
OVOC	Cyclohexaneethanol	4442-79-9
OVOC	3,4-Dimethylcyclohexanol	5715-23-1
OVOC	2-Propyl-1-pentanol	58175-57-8

OVOC	Isopropyl alcohol	1344575-38-7
OVOC	3-Cyclohexyl-1-propanol	1124-63-6
OVOC	1-Phenoxypropan-2-ol	770-35-4
OVOC	2-Phenyl-2-propanol	617-94-7
OVOC	Formaldehyde	50-00-0
OVOC	Glyoxal	107-22-2
OVOC	Acetaldehyde	75-07-0
OVOC	Acrolein	107-02-8
OVOC	Methylglyoxal	78-98-8
OVOC	Propionaldehyde/Propanal	123-38-6
OVOC	Isobutyraldehyde	78-84-2
OVOC	Crotonaldehyde	4170-30-3
OVOC	Methacrolein	78-85-3
OVOC	Butyraldehyde/n-Butanal	123-72-8
OVOC	3-Hydroxybutyraldehyde	107-89-1
OVOC	Valeraldehyde	110-62-3
OVOC	Isovaleraldehyde	590-86-3
OVOC	Hexanaldehyde	66-25-1
OVOC	Heptaldehyde	111-71-7
OVOC	Benzaldehyde	100-52-7
OVOC	Octanal	124-13-0
OVOC	o-Tolualdehyde	529-20-4
OVOC	m-Tolualdehyde	620-23-5
OVOC	p-Tolualdehyde	104-87-0
OVOC	2,5-Dimethylbenzaldehyde	5779-94-2
OVOC	Nonanal	124-19-6
OVOC	Decanal	112-31-2
OVOC	Furfural	98-01-1
OVOC	3-Furaldehyde	498-60-2
OVOC	Tolualdehyde	1334-78-7
OVOC	Crotonaldehyde	123-73-9
OVOC	Dimethylbenzaldehyde	5973-71-7
OVOC	2-Crotonaldehyde	123-72-9

OVOC	trans-2-Pentalenal	1576-87-0
OVOC	Acetone	67-64-1
OVOC	Methylethylketone	78-93-3
OVOC	Diacetyl	431-03-8
OVOC	1-Methoxy-2-propanon	5878-19-3
OVOC	2-pentanone	107-87-9
OVOC	3-Pentanone	96-22-0
OVOC	3-Methyl,3-buten-2-one	814-78-8
OVOC	Cyclopentanone	120-92-3
OVOC	Cyclohexanone	108-94-1
OVOC	4-Methyl-2-Pentanone	108-10-1
OVOC	Methyl Vinyl ketone	78-94-4
OVOC	2,4-Dimethyl-3-pentanone	565-80-0
OVOC	Acetylbenzene	98-86-2
OVOC	Benzofuranone	533-86-6
OVOC	7-Methyl benzofuranone	669-04-5
OVOC	2-Methyl benzofuranone	35567-59-0
OVOC	Methyl n-butyl ketone	563-80-4
OVOC	2,6-Dimethyl-4-heptanone	108-83-8
OVOC	2-Hexanone	591-78-6
OVOC	4-Methyl-4-penten-2-one	3744-02-3
OVOC	4-Methyl-3-penten-2-one	141-79-7
OVOC	3-Hydroxy-3-M-2-butanone	115-22-0
OVOC	4-Hydroxy-2-pentanone	4161-60-8
OVOC	3-Heptanone	106-35-4
OVOC	4,6-Dimethyl-2-heptanone	19549-80-5
OVOC	3,5,5-Trimethyl-2-cyclohexen-1-one	78-59-1
OVOC	Ethyl vinyl ketone	1629-58-9
OVOC	5-Methyl-3-hexene-2-one	5166-53-0
OVOC	2-Methylcyclopentanone	1120-72-5
OVOC	3-Methylcyclopentanone	6195-92-2
OVOC	Pinacolone	75-97-8
OVOC	2-Methyl-2-cyclohexen-1-one	1121-18-2

OVOC	2-Cyclohexene-1-one	930-68-7
OVOC	cis-1-Methyl-4-ethyl cyclohexanone	4926-78-7
OVOC	trans-1-Methyl-4-ethyl cyclohexanone	6236-88-0
OVOC	2,3-Dimethylcyclohexanone	1551-88-8
OVOC	2-Methyl-5-(1-methyl vinyl) cyclohexanone	3792-53-8
OVOC	Methyl acetate	79-20-9
OVOC	Vinyl acetate	108-05-4
OVOC	Ethyl acetate	141-78-6
OVOC	Methyl methacrylate	80-62-6
OVOC	Ethyl acrylate	140-88-5
OVOC	2-Methoxyethyl acetate	110-49-6
OVOC	Butyl acrylate	141-32-2
OVOC	1-Methoxy-2-propylacetate	108-65-6
OVOC	Isobutyl acetate	110-19-0
OVOC	2-Ethoxyethyl acetate	817-95-8
OVOC	sec-Butyl acetate	105-46-4
OVOC	n-Butyl acetate	123-86-4
OVOC	Vinyl methacrylate	4245-37-8
OVOC	2-Pentanol acetate	626-38-0
OVOC	n-Propyl acetate	109-60-4
OVOC	2-Ethoxyethyl acetate	111-15-9
OVOC	Carbonic acid , dimethyl ester	616-38-6
OVOC	Aceticacid,1-methylethylester	108-21-4
OVOC	Carbonicacid,ethyl-,methylester	623-53-0
OVOC	Propanoicacid,ethylester	105-37-3
OVOC	Formicacid,butylester	592-84-7
OVOC	Carbonicacid,diethylester	105-58-8
OVOC	Propanoicacid,propylester	106-36-5
OVOC	1-Methylethyl ester	617-51-6
OVOC	3-Methyl-2-Butanol,acetate	123-92-2
OVOC	2-Pentanol,acetate	628-63-7

OVOC	Butyl isobutyrate	97-87-0
OVOC	Butyl Methacrylate	97-88-1
OVOC	Octyl acetate	112-14-1
OVOC	MTBE/methyl tertiary butyl ether	1634-04-4
OVOC	Propylene glycol monomethyl ether	107-98-2
OVOC	Ethylene glycol monoethyl ether	110-80-5
OVOC	2-Butoxyethanol	111-76-2
OVOC	2-(2-Methoxyethoxy)ethanol	111-77-3
OVOC	1-Methylthiobutane	628-29-5
OVOC	1,4-Dioxane	123-91-1
OVOC	Ethylene oxide	75-21-8
OVOC	Propylene oxide	75-56-9
OVOC	Methylene dimethyl ether	/
OVOC	Dimethoxymethane	109-87-5
OVOC	Methyl Ether	115-10-6
OVOC	Methyl n-pnopyl ether	557-17-5
OVOC	2-Methoxypropane	116-11-0
OVOC	1-Methoxybutane	628-28-4
OVOC	Ethyl Isopropyl Ether	625-54-7
OVOC	1,3-Dimethoxypropane	17081-21-9
OVOC	2-Methyl-1,3-dioxolane	497-26-7
OVOC	Ethylene glycol monobutyl ether	111-46-2
OVOC	Isopropyl ether	108-20-3
OVOC	(Chloromethyl)-oxirane	106-89-8
OVOC	1,1,3,3-Tetramethoxypropane	102-52-3
OVOC	Dipropylene glycol monomethyl ether	34590-94-8
OVOC	Di-tertbutylperoxide	110-05-4
OVOC	2-(2-Butoxyethoxy)ethanol	112-34-5
OVOC	1-(1-Methylpropoxy)-butane	999-65-5
OVOC	Di-n-butyl ether	142-96-1
OVOC	(2-Methoxyethoxy)benzene	41532-81-4
OVOC	Diethylene glycol dibutyl ether	112-73-2
OVOC	Tetrahydrofuran	109-99-9

OVOC	Furan	110-00-9
OVOC	2-Methyl-furan	534-22-5
OVOC	3-Methyl,furan	930-27-8
OVOC	2,3-Benzofuran	271-89-6
OVOC	Tetrahydropyran	142-68-7
OVOC	2-Ethyl furan	3208-16-0
OVOC	2,5-Dimethylfuran	625-86-5
OVOC	Phenol	108-95-2
OVOC	o-Cresol	95-48-7
Others	Hydroxyurea	127-07-1
Others	Formamide	75-12-7
Others	Acetonitrile	75-05-8
Others	12AP	78-90-0
Others	Acrylonitrile	107-13-1
Others	n,n-Dimethylformamide	68-12-2
Others	1-Methoxypropan-2-amine	37143-54-7
Others	Caprolactam	105-62-2
Others	Triethylamine	121-44-8
Others	Benzonitrile	100-47-0
Others	2-Cyclohexylethylamine	4442-85-7
Others	C2S	15596-07-3
Others	DMS	75-18-3
Others	Carbon disulfide	75-15-0