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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.

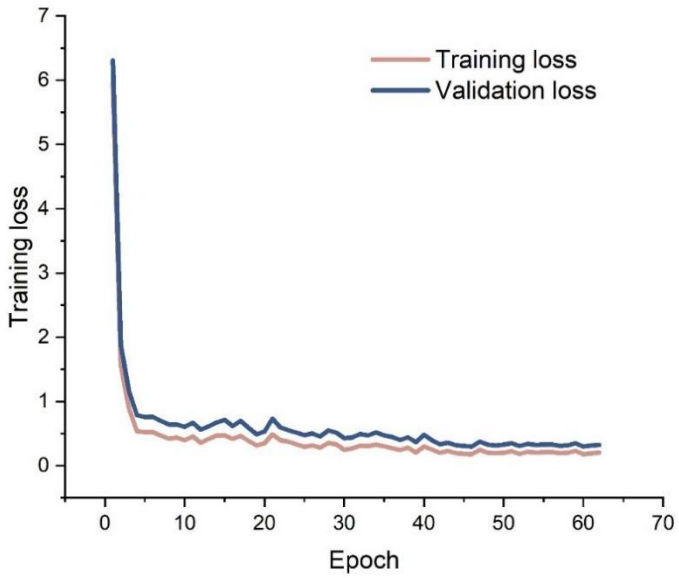


Figure S1 presents the learning curve of the model. The prediction loss on the training set decreases rapidly during the initial phase of training and stabilizes at a very low level. Similarly, the prediction loss on the validation set follows a comparable downward trend and, after a rapid decline, stabilizes 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. The chemical spatial distribution of VOCs in the OH, O_3, and NO_3 datasets used in this study and prior literature.

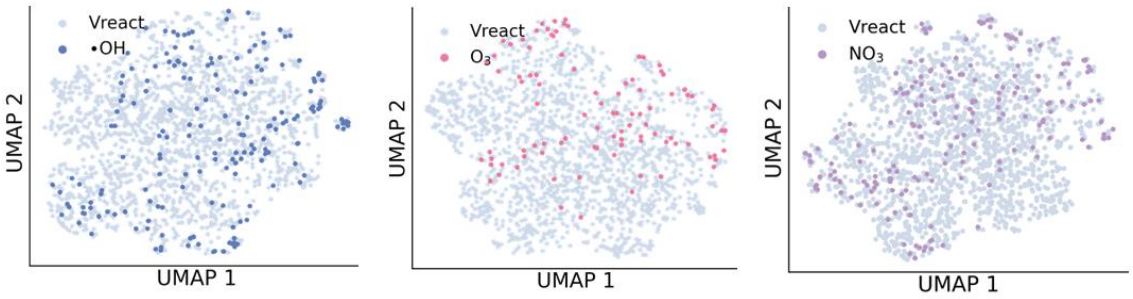
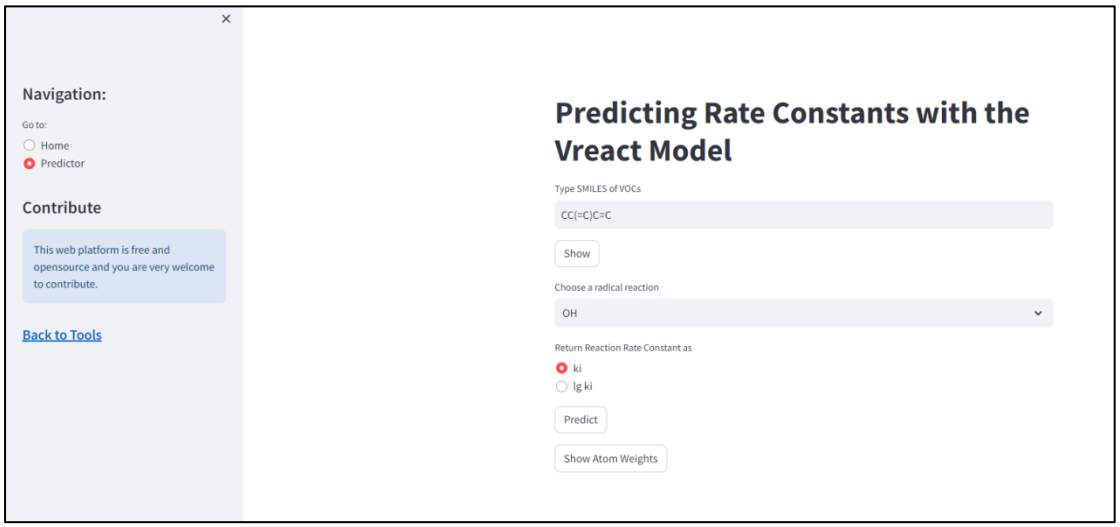


Figure S3. User interface of the web platform for predicting VOC reaction rate constants using the Vreact model.



This webpage is built using the Python open-source framework Streamlit, and the figure is sourced from the webpage constructed in this study: http://vreact.envwind.site:8001/.

S1. Graph representation of molecular structures.

The graph $\boldsymbol{G}$ *(V, E)* comprises a set of vertices (nodes) $i \in \boldsymbol{V}$ and a set of edges $e_{ij} \in \boldsymbol{E}$ that connect vertices *i* and *j*. Here, $\boldsymbol{V}$ represents the set of all atoms (nodes) in the molecule, and $\boldsymbol{E}$ 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 $\boldsymbol{X}$, 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 $\boldsymbol{Y}$, with dimensions $2m \times k$, where m is the number of chemical bonds and k is the feature dimension.

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 (S1). Then, the node embeddings are updated to obtain the hidden state h_i^{t+1} at time t+1, as shown in Equation (S2). 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 (S3). 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.

$$m_i^{t+1} = \sum_{j \in V} M_t\,(h_i^t, h_j^t,) \qquad \text{(S1)}$$

$$h_i^{t+1} = U_t(h_i^t, m_i^{t+1}) \qquad \text{(S2)}$$

$$F = R(h_i^T \mid i \in V) \qquad \text{(S3)}$$

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 (S4), where y_i represents the experimental value in the dataset and $\hat{y}_i$ represents the model's predicted value.

$$Loss = \begin{cases} 0.5(y_i - \hat{y}_i)^2, & |y_i - \hat{y}_i| < 1 \\ |y_i - \hat{y}_i| - 0.5, & |y_i - \hat{y}_i| \geq 1 \end{cases} \qquad \text{(S4)}$$

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.

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 (S1) to (S4), 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.

$$MSE = \frac{1}{m}\sum_{i=1}^{m}(y_i - \hat{y}_i)^2 \quad \text{(S1)}$$

$$RMSE = \sqrt{\frac{1}{m}\sum_{i=1}^{m}(y_i - \hat{y}_i)^2} \quad \text{(S2)}$$

$$MAE = \frac{1}{m}\sum_{i=1}^{m}|(y_i - \hat{y}_i)| \quad \text{(S3)}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{m}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{m}(y_i - \bar{y})^2} \quad \text{(S4)}$$

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^3d]	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	cyclobutanecarbaldehde	-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-Methylindane	874-35-1
Aromatic	4-Methylindane	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(CF2Cl2)	75-71-8
Halocarbon	Freon11(CFCl3)	75-69-4
Halocarbon	Chloroform	67-66-3
Halocarbon	Bromoform	75-25-2
Halocarbon	Freon22(CHClF2)	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(C2F3Cl3)	354-58-5
Halocarbon	Freon113(C2F3Cl3)	76-13-1
Halocarbon	Freon114(C2F4Cl2)	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-Pentenal	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	Proprylene 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