SUPPORTING INFORMATION

Henry's Law Constant – A General-Purpose Fragment Model to Predict Log K_{aw} From Molecular Structure

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Example Calculations.

Manual application of the fragment scheme is now illustrated with three examples, thus providing insight into the mechanistic basis of the fragmentation scheme (with all model details being documented in scheme S2).

For 2,6-dimethoxyphenol (compound **1** in Scheme S1) used as smoke flavoring agent, the UFZ model proceeds as follows. First, the chemical structure of **1** contains six different model-defined fragments with the following occurrences and log K_{aw} contributions: (i) two sp^3-C (fragment #2, see SI) providing a log K_{aw} contribution of 2 • (–0.417) = –0.834; (ii) six aromatic C (#5) yielding 6 • (–0.575) = –3.45; (iii) six H attached to sp^3-C (#8) resulting in 6 • 0.275 = 1.650; (iv) three H attached to sp^2-C (#9) adding 3 • 0.405 = 1.215; (v) one OH (#14) contributing –4.581; and (vi) two O atoms summing up to 2 • (–2.85) = –5.7 log K_{aw} units.

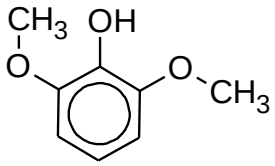
Second, the following three correction factors also contribute to the log K_{aw} of **1**: (i) one OH bonded to aromatic carbon (#46, aromatic alcohol) increasing log K_{aw} by 0.83; (ii) two O atoms bonded to aromatic carbon (#48, aromatically bonded alkoxy) adding 2 • 1.56 = 3.12; and (iii) one intramolecular H bond OH•••O yielding an increase by 2.12. These correction factors all yield preferences of the gas phase over water. Inclusion of the overall model regression constant of 0.455 leads to a total sum of –5.175 as predicted log Kaw, deviating the experimental value of –5.09 by –0.085.

The organosulfur compound 1,3-propane sultone (**2** in Scheme S1) is an alkylating agent and both mutagenic and carcinogenic, with industrial applications as precursor of polyether sulfones and as electrolyte in batteries. Its chemical structure contains the UFZ model fragments 3 x sp^3-C (fragment #2, yielding 3 • –0.417 = –1.251), 6 x H attached to sp^3-C (#8, 6 • 0.275 = 1.650), 1 x O (#15, –2.85), and 1 x SO_2 (#33, –4.32). Accordingly, SO_2 decreases log K_{aw} substantially. With the correction factors 3 x cyclic C (#76, 3 • (–0.064) = –0.192) and 2 x cyclic O or N or S or Si (#77, here 1 S and 1 O, 2 • (–0.15) = –0.30) and the regression constant (0.455), the predicted log K_{aw} of **2** is –6.718 and thus differs from the experimental value of –6.59 by –0.13. Here, all correction factors reduce the volatilization from water.

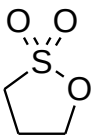
The carbamate insecticide aldicarb (**3** in Scheme 1) with an experimental log K_{aw} of –7.00 is an acetylcholine esterase inhibitor. Its UFZ fragment decomposition is as follows: 5 x sp^3-C (#2, 5 • (–0.417) = –2.085), 1 x C= (#3, non-aromatic sp^2-C, –0.547), 12 x H attached to sp^3-C (12 • 0.275 = 3.3), 1 x H attached to sp^2-C (#9, 0.405), 1 x O (#15, –2.85), 1 x O=C (#17, –3.995), 1 x NH/NH_2 (#19, here NH, –4.42), 1 x N= (#23, non-aromatic sp^2-N, –1.09), and 1 x S (#28, –2.60).

The three correction factors ester bond O–CO (#129, 3.19), amide bond N–CO (#130, 0.38), and carbamoyl oxime bonding pattern NCOON= (#113, carbamate with imine as ester function, 3.20) increase waterborne volatility. Final inclusion of the regression constant (0.455) yields a calculated value of –6.657 with a prediction error of +0.36. Note that for **1**, **2** and **3**, the HENRYWIN results are –7.096, –4.016 and –6.836 with prediction errors of –2.006, +2.574 and –0.085 log K_{aw} units, respectively.

Scheme S1. Chemical structures of the three calculation examples and of the discussed outlier



1



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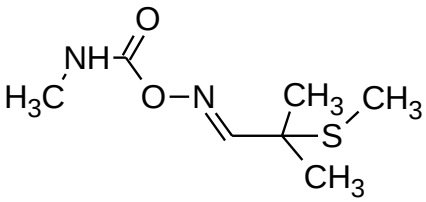

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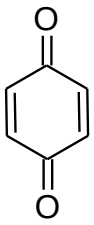

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2,6-dimethoxyphenol (1), 1,3-propane sultone (2), aldicarb (3), and 1,4-benzoquinone (4) as outlier example.

Table S1. Structural Complexity Impact on Model Performance.

Model and structural features	*n*	r^2	q^2	RMS	bias	MNE	MPE
UFZ model							
0 heteroatoms	265	0.989	0.989	0.191	-0.000	-0.72	0.54
1 heteroatom	451	0.976	0.976	0.220	0.003	-1.02	1.75
2 heteroatoms	386	0.960	0.960	0.432	-0.018	-2.12	1.76
3…4 heteroatoms	571	0.964	0.963	0.496	-0.018	-2.03	1.89
5…6 heteroatoms	506	0.968	0.967	0.587	-0.062	-2.63	2.25
7…8 heteroatoms	306	0.949	0.945	0.691	-0.114	-2.74	2.12
≥9 heteroatoms	151	0.965	0.963	0.791	-0.155	-2.59	2.01
w/o funct. group	265	0.989	0.989	0.191	-0.000	-0.72	0.54
1 funct. group	757	0.967	0.967	0.368	-0.008	-2.63	1.89
2 identical funct. groups	206	0.977	0.976	0.403	-0.079	-2.12	1.54
3…4 identical funct. groups	149	0.980	0.977	0.341	-0.091	-1.27	0.78
≥5 identical funct. groups	149	0.990	0.990	0.332	-0.031	-0.72	0.72
2 types of funct. groups	702	0.957	0.956	0.528	-0.050	-2.46	2.03
3 types of funct. groups	268	0.897	0.893	0.758	-0.016	-2.59	2.25
≥4 types of funct. groups	140	0.884	0.876	0.966	-0.186	-2.74	2.13
Non- and weakly polar	697	0.980	0.979	0.248	-0.024	-1.03	0.72
1 HB donor	597	0.950	0.949	0.562	-0.028	-2.46	2.25
≥2 HB donors	146	0.952	0.951	0.593	-0.019	-1.89	2.01
No HB donor, 1 acceptor	402	0.903	0.902	0.395	-0.008	-2.13	1.76
No HB donor, 2 acceptors	269	0.928	0.926	0.477	-0.043	-2.63	1.44
No HB donor, 3-5 acceptors	390	0.906	0.896	0.663	-0.098	-2.74	1.78
No HB donor, ≥6 acceptors	119	0.916	0.911	0.782	-0.144	-1.92	2.12
Polar w/o HB	16	0.967	0.931	0.755	0.028	-0.77	1.60
HENRYWIN							
0 heteroatoms	265	0.951	0.942	0.439	0.168	-0.69	1.95
1 heteroatom	451	0.942	0.940	0.348	0.016	-1.06	2.79
2 heteroatoms	385	0.817	0.794	0.976	0.160	-4.93	4.62
3…4 heteroatoms	569	0.767	0.745	1.310	-0.087	-5.69	8.27
5…6 heteroatoms	506	0.792	0.778	1.530	-0.263	-5.87	8.12
7…8 heteroatoms	306	0.820	0.731	1.520	-0.699	-6.70	2.93
≥9 heteroatoms	151	0.767	0.704	2.230	-0.756	-9.11	5.48
w/o funct. group	265	0.951	0.942	0.439	0.168	-0.69	1.95
1 funct. group	754	0.863	0.859	0.758	0.112	-4.93	7.98
2 identical funct. groups	206	0.860	0.852	1.000	0.147	-2.59	3.34
3…4 identical funct. groups	149	0.666	0.640	1.350	0.103	-4.47	8.27
≥5 identical funct. groups	149	0.879	0.787	1.520	0.497	-2.80	8.12
2 types of funct. groups	702	0.783	0.737	1.290	-0.476	-5.69	6.76
3 types of funct. groups	268	0.585	0.430	1.750	-0.586	-6.70	3.95
≥4 types of funct. groups	140	0.495	0.225	2.410	-1.100	-9.11	4.43
Non- and weakly polar	697	0.916	0.903	0.532	0.183	-3.12	2.49

1 HB donor	597	0.735	0.666	1.434	-0.282	-9.11	4.43
≥2 HB donors	146	0.369	0.260	2.320	0.186	-5.69	8.12
No HB donor, 1 acceptor	400	0.502	0.389	0.990	-0.270	-5.39	7.98
No HB donor, 2 acceptors	268	0.763	0.738	0.900	-0.160	-5.50	2.79
No HB donor, 3-5 acceptors	390	0.622	0.510	1.440	-0.257	-5.34	8.27
No HB donor, ≥6 acceptors	119	0.698	0.484	1.890	-1.090	-5.73	5.48
Polar w/o HB	16	0.722	0.561	1.900	-0.199	-4.93	4.04

Table S2. Permutation Test Statistics.

Degree of permutation [%]	q^2 (true vs scrambled)	r^2 (regression)	q^2_{cv}
0	1.000	0.974	0.966
10	0.808	0.795	0.684
20	0.589	0.616	0.518
30	0.427	0.501	0.337
40	0.172	0.341	0.157
50	-0.014	0.227	-0.013
60	-0.105	0.209	-0.029
70	-0.372	0.029	-0.776
80	-0.611	0.058	-0.278
90	-0.795	0.020	-0.313
100	-1.010	0.030	-0.471
100	-0.962	0.023	-0.403
100	-1.040	0.029	-0.420
100	-0.961	0.010	-0.667
100	-1.040	0.029	-0.359

Table S3. Calibration to the EPISuite HENRYWIN Data Set.

The procedure of curation and model calibration is explained in the main text. The statistical results are given here as *Calibration with experimental data from this study (UFZ).* The row Training set refers to the 80% primarily used for calibration, Prediction set to the application of the model obtained from the 80% set for the remaining 20%, and Total set to the recalibration with the 1602 compounds. The column HENRYWIN model gives the performance of the EPISuite for the total set.

In addition, similar calibrations were carried out with the HENRYWIN data for these 1602 compounds. There were equal data in 597 cases. For most of the remaining chemicals the data were only slightly differing, but there were also cases with substantial differences. The results are shown as *Calibration with experimental data from HENRYWIN.*

The third section *Prediction for disregarded experimental data* gives statistics for the 170 compounds with unreliable data in the HENRYWIN set. The predictions were carried out using the two calibrations explained here and applying the EPISuite, and

the results were compared to these unreliable experimental values from the HENRYWIN set.

Data set	*n*	r^2	q^2	RMS	bias	MNE	MPE
Calibration with experimental data from this study (UFZ)							
Training set	1282	0.977	0.976	0.439	-0.012	-2.41	2.25
Prediction set	320	0.968	0.967	0.520	0.010	-3.11	2.76
Total set	1602	0.976	0.975	0.449	-0.018	-3.11	2.32
HENRYWIN model	1601	0.856	0.832	1.185	-0.117	-8.42	8.50
Calibration with experimental data from HENRYWIN							
Training set	1282	0.937	0.936	0.733	-0.014	-4.85	4.22
Prediction set	320	0.905	0.898	0.915	0.005	-6.27	3.79
Total set	1602	0.934	0.933	0.750	-0.018	-5.33	4.21
HENRYWIN model	1601	0.877	0.854	1.095	-0.115	-9.11	8.27
Prediction for disregarded experimental data							
Calibration w. UFZ-data-trained-UFZ model [a)]	170	0.432	-1.100	3.912	-1.687	-16.48	5.91
Calibration w. HENRYWIN-data-trained UFZ model [b)]	170	0.436	-1.116	3.927	-1.684	-17.06	4.98
HENRYWIN model	170	0.468	-0.644	3.462	-1.531	-15.63	3.48

[a)] UFZ model trained with UFZ data for curated HENRYWIN data set with 1602 compounds

[b)] UFZ model trained with HENRYWIN data for curated HENRYWIN data set with 1602 compounds

Table S4. Data Set With Curated Experimental Log K_{aw}.

No.	**Compound name**	**CAS-RN**	**log K_{aw}**	**Data Type**	**Set**	**Group**	**Ref Type**
1	methane	74-82-8	1.43	1	T	2	D
2	ethane	74-84-0	1.33	1	T	1	D
3	propane	74-98-6	1.436	1	T	2	O
4	n-butane	106-97-8	1.58	1	T	1	D
5	n-pentane	109-66-0	1.71	1	T	2	O
6	n-hexane	110-54-3	1.845	1	T	1	O
7	n-heptane	142-82-5	1.92	1	T	2	D
8	n-octane	111-65-9	2.08	1	T	1	D
9	n-nonane	111-84-2	2.268	1	T	2	D
10	n-decane	124-18-5	2.32	1	P	1	D
11	undecane	1120-21-4	2.53	2	T	2	M
12	dodecane	112-40-3	2.52	2	P	1	D
13	tridecane	629-50-5	2.994	2	T	2	M
14	tetradecane	629-59-4	2.755	2	T	1	M

15	pentadecane	629-62-9	2.99	2	P	2	M
16	isobutane	75-28-5	1.64	1	T	1	D
17	isopentane	78-78-4	1.703	1	T	2	D
18	3-methylpentane	96-14-0	1.827	1	T	1	D
19	2-methylpentane	107-83-5	1.84	1	T	2	D
20	2,3-dimethylbutane	79-29-8	1.72	1	T	1	D
21	2-methylhexane	591-76-4	2.11	2	T	2	M
22	3-methylhexane	589-34-4	1.99	1	T	1	D
23	2,3-dimethylpentane	565-59-3	1.85	2	T	2	D
24	2,4-dimethylpentane	108-08-7	1.99	2	T	1	D
25	2-methylheptane	592-27-8	2.148	2	T	2	M
26	3-methylheptane	589-81-1	2.12	2	P	1	M
27	4-methylheptane	589-53-7	2.177	2	T	2	M
28	3-ethylhexane	619-99-8	2.445	2	T	1	M
29	2,4-dimethylhexane	589-43-5	2.16	2	T	2	M
30	2,5-dimethylhexane	592-13-2	2.17	1	P	1	D
31	3,4-dimethylhexane	583-48-2	2.22	2	T	2	M
32	2,3,4-trimethylpentane	565-75-3	1.88	1	T	1	D
33	4-methyloctane	2216-34-4	2.61	2	P	2	D
34	3-ethylheptane	15869-80-4	2.33	2	T	1	M
35	4-ethylheptane	2216-32-2	2.305	2	T	2	M
36	2,3-dimethylheptane	3074-71-3	2.34	2	P	1	M
37	2,4-dimethylheptane	2213-23-2	2.29	2	T	2	M
38	2,5-dimethylheptane	2216-30-0	2.3	2	T	1	M
39	2,6-dimethylheptane	1072-05-5	2.32	2	T	2	M
40	3,5-dimethylheptane	926-82-9	2.29	2	P	1	M
41	2-methyl-3-ethylhexane	16789-46-1	2.335	2	P	2	M
42	2-methyl-4-ethylhexane	3074-75-7	2.3	2	T	1	M
43	2,3,4-trimethylhexane	921-47-1	2.36	2	T	2	M
44	3-methylnonane	5911-04-6	2.39	2	T	1	M
45	4-methylnonane	17301-94-9	2.42	2	P	2	M
46	2,2-dimethylpropane	463-82-1	1.836	1	T	1	O
47	2,2-dimethylbutane	75-83-2	1.9	1	T	2	D
48	2,2-dimethylpentane	590-35-2	2.11	2	T	1	D
49	3,3-dimethylpentane	562-49-2	1.88	1	T	2	D
50	2,2-dimethylhexane	590-73-8	2.217	2	T	1	O
51	2,2,3,3-tetramethylbutane	594-82-1	1.99	2	T	2	M
52	2,2-dimethylheptane	1071-26-7	2.32	2	T	1	M
53	3,3-dimethylheptane	4032-86-4	2.335	2	T	2	M
54	4,4-dimethylheptane	1068-19-5	2.34	2	T	1	M
55	2,2-dimethyloctane	15869-87-1	2.42	2	P	2	M
56	2,2,3-trimethylbutane	464-06-2	2.1	2	T	1	M
57	2,2,3-trimethylpentane	564-02-3	1.915	2	P	2	D
58	2,2,4-trimethylpentane	540-84-1	2.12	1	T	1	D
59	2,2,3-trimethylhexane	16747-25-4	2.34	2	T	2	M
60	2,2,5-trimethylhexane	3522-94-9	2.33	1	P	1	D
61	cyclopropane	75-19-4	0.551	1	T	2	O
62	cyclopentane	287-92-3	0.88	1	T	1	D
63	cyclohexane	110-82-7	0.875	1	T	2	D
64	cycloheptane	291-64-5	0.65	2	T	1	D
65	cyclooctane	292-64-8	0.769	2	P	2	O
66	methylcyclopentane	96-37-7	1.134	1	T	1	D
67	methylcyclohexane	108-87-2	1.2	1	T	2	D
68	ethylcyclohexane	1678-91-7	1.297	2	T	1	O
69	propylcyclopentane	2040-96-2	1.56	2	T	2	D
70	cis-1,2-dimethylcyclohexane	2207-01-4	1.167	2	T	1	O

71	trans-1,2-dimethylcyclohexane	6876-23-9	1.394	2	T	2	O
72	trans-1,3-dimethylcyclohexane	2207-03-6	1.52	2	T	1	M
73	trans-1,4-dimethylcyclohexane	2207-04-7	1.55	2	P	2	D
74	decalin	91-17-8	0.68	1	T	1	O
75	pentylcyclopentane	3741-00-2	1.87	2	T	2	D
76	p-menthane	99-82-1	1.86	2	T	1	D
77	heptylcyclohexane	5617-41-4	1.815	2	P	2	M
78	n-octylcyclohexane	1795-15-9	2.02	2	P	1	M
79	1,1,3-trimethylcyclopentane	4516-69-2	1.81	2	T	2	D
80	1,1,3-trimethylcyclohexane	3073-66-3	1.635	2	P	1	D
81	tricyclene	508-32-7	0.918	2	T	2	D
82	ethylene	74-85-1	0.969	1	T	1	D
83	propene	115-07-1	0.904	1	T	2	D
84	1-butene	106-98-9	0.979	1	T	1	D
85	cis-2-butene	590-18-1	0.975	1	T	2	D
86	trans-2-butene	624-64-6	0.962	1	T	1	D
87	trans-2-pentene	646-04-8	0.98	1	T	2	D
88	1-pentene	109-67-1	1.22	1	T	1	D
89	cis-2-pentene	627-20-3	0.964	2	T	2	D
90	1-hexene	592-41-6	1.16	1	T	1	D
91	cis-2-hexene	7688-21-3	1.006	2	T	2	M
92	trans-2-hexene	4050-45-7	1.022	2	T	1	M
93	1-heptene	592-76-7	1.22	1	T	2	D
94	trans-2-heptene	14686-13-6	1.25	1	T	1	D
95	1-octene	111-66-0	1.41	1	T	2	D
96	trans-2-octene	13389-42-9	1.567	2	T	1	M
97	cis-2-octene	7642-04-8	1.54	2	P	2	M
98	1-nonene	124-11-8	1.51	1	P	1	D
99	1-decene	872-05-9	1.6	2	P	2	D
100	1-pentadecene	13360-61-7	2.25	2	P	1	M
101	isobutene	115-11-7	0.95	1	T	2	D
102	3-methyl-1-butene	563-45-1	1.34	1	T	1	D
103	trimethylethylene	513-35-9	0.98	1	T	2	D
104	2-methyl-1-butene	563-46-2	1.246	2	T	1	M
105	2-methyl-1-pentene	763-29-1	1.08	1	P	2	D
106	4-methyl-1-pentene	691-37-2	1.4	1	T	1	D
107	2,4,4-trimethyl-1-pentene	107-39-1	2	2	P	2	M
108	cyclopentene	142-29-0	0.246	1	T	1	O
109	cyclohexene	110-83-8	0.27	1	T	2	D
110	cycloheptene	628-92-2	0.28	2	T	1	M
111	cyclooctene	931-88-4	0.292	2	P	2	D
112	1-methylcylohexene	591-49-1	0.49	1	T	1	D
113	alpha-pinene	80-56-8	0.738	1	T	2	O
114	beta-pinene	127-91-3	0.444	1	T	1	O
115	camphene	79-92-5	0.23	2	P	2	D
116	delta-3-carene	13466-78-9	0.15	2	T	1	D
117	sabinene	3387-41-5	0.424	2	T	2	D
118	alpha-cedrene	469-61-4	0.15	1	T	1	O
119	alpha-longipinene	5989-08-2	0.08	1	P	2	O
120	isosativene	24959-83-9	0.01	1	P	1	O
121	alpha-neoclovene	4545-68-0	0.14	1	T	2	O
122	beta-neoclovene	56684-96-9	0.14	1	T	1	O
123	gamma-neoclovene		0.14	1	T	2	O
124	1,3-butadiene	106-99-0	0.41	1	T	1	D
125	1,4-pentadiene	591-93-5	0.68	1	T	2	D
126	1,5-hexadiene	592-42-7	0.74	1	T	1	D

127	1,6-heptadiene	3070-53-9	0.858	2	T	2	D
128	2-methyl-1,3-butadiene	78-79-5	0.5	1	P	1	D
129	2,3-dimethyl-1,3-butadiene	513-81-5	0.29	1	T	2	D
130	2,5-dimethyl-2,4-hexadiene	764-13-6	0.28	2	T	1	M
131	cyclopentadiene	542-92-7	-0.07	2	T	2	D
132	1,4-cyclohexadiene	628-41-1	-0.392	2	P	1	D
133	4-vinylcyclohexene	100-40-3	0.263	1	T	2	D
134	ethylidenenorbornene	16219-75-3	-0.32	2	T	1	M
135	dicyclopentadiene	77-73-6	-0.36	2	T	2	M
136	alpha-terpinene	99-86-5	0.149	1	P	1	O
137	gamma-terpinene	99-85-4	0.023	1	T	2	O
138	limonene	138-86-3	0.063	1	T	1	O
139	terpinolene	586-62-9	0.031	1	P	2	O
140	alpha-phellandrene	99-83-2	0.352	1	T	1	O
141	beta-phellandrene	555-10-2	0.352	1	P	2	O
142	gamma-gurjunene	22567-17-5	0.09	1	T	1	O
143	beta-caryophyllene	87-44-5	0.04	1	T	2	O
144	valencene	4630-07-3	0.1	1	P	1	O
145	myrcene	123-35-3	0.421	2	T	2	D
146	cycloheptatriene	544-25-2	-0.73	1	T	1	D
147	1,5,9-cyclododecatriene, (E,E,Z)-	706-31-0	0.356	2	T	2	D
148	alpha-humulene	6753-98-6	0.14	1	T	1	O
149	alpha-farnesene	502-61-4	0.08	1	T	2	O
150	acetylene	74-86-2	-0.006	1	T	1	O
151	propyne	74-99-7	-0.223	1	T	2	O
152	1-butyne	107-00-6	-0.12	1	T	1	D
153	1-pentyne	627-19-0	0.01	1	T	2	D
154	1-hexyne	693-02-7	0.21	1	T	1	D
155	3-hexyne	928-49-4	-0.133	2	T	2	D
156	1-heptyne	628-71-7	0.44	1	T	1	D
157	2-heptyne	1119-65-9	0.363	2	T	2	D
158	1-octyne	629-05-0	0.52	1	P	1	D
159	1-nonyne	3452-09-3	0.77	1	P	2	D
160	2-methyl-3-hexyne	36566-80-0	0.27	2	T	1	D
161	2,2-dimethyl-3-hexyne	4911-60-8	0.445	2	P	2	D
162	2,2,5,5-tetramethyl-3-hexyne	17530-24-4	1.076	2	T	1	D
163	2,2,5-trimethyl-3-hexyne	17530-23-3	0.865	2	T	2	D
164	1-buten-3-yne	689-97-4	-0.004	1	T	1	D
165	diacetylene	460-12-8	-0.664	2	T	2	D
166	1,6-heptadiyne	2396-63-6	-1.062	2	T	1	D
167	1,8-nonadiyne	2396-65-8	-0.869	2	P	2	D
168	benzene	71-43-2	-0.636	1	T	1	O
169	toluene	108-88-3	-0.585	1	T	2	O
170	ethylbenzene	100-41-4	-0.419	1	T	1	D
171	o-xylene	95-47-6	-0.69	1	T	2	O
172	m-xylene	108-38-3	-0.572	1	T	1	O
173	p-xylene	106-42-3	-0.567	1	T	2	D
174	n-propylbenzene	103-65-1	-0.367	1	T	1	D
175	1-methyl-2-ethylbenzene	611-14-3	-0.642	1	T	2	D
176	1-ethyl-4-methylbenzene	622-96-8	-0.58	2	P	1	D
177	1,2,4-trimethylbenzene	95-63-6	-0.76	1	P	2	D
178	1,3,5-trimethylbenzene	108-67-8	-0.546	1	T	1	D
179	1,2,3-trimethylbenzene	526-73-8	-0.89	1	T	2	D
180	butylbenzene	104-51-8	-0.261	1	P	1	D
181	1,4-diethylbenzene	105-05-5	-0.41	2	T	2	M
182	m-diethylbenzene	141-93-5	-0.47	2	T	1	D

183	1,2,4,5-tetramethylbenzene	95-93-2	-1	2	T	2	M
184	1-methyl-3-propylbenzene	1074-43-7	-0.26	2	T	1	M
185	pentylbenzene	538-68-1	-0.17	1	T	2	M
186	pentamethylbenzene	700-12-9	-1.454	2	T	1	M
187	hexamethylbenzene	87-85-4	-1.325	2	T	2	M
188	1,3,5-triethylbenzene	102-25-0	-0.396	2	T	1	M
189	n-hexylbenzene	1077-16-3	-0.03	1	P	2	D
190	n-heptylbenzene	1078-71-3	0.09	2	P	1	M
191	n-octylbenzene	2189-60-8	0.296	2	T	2	M
192	n-decylbenzene	104-72-3	0.555	2	P	1	M
193	cumene	98-82-8	-0.328	1	P	2	D
194	isobutylbenzene	538-93-2	0.12	2	T	1	D
195	2-butylbenzene	135-98-8	-0.27	1	T	2	D
196	1-methyl-2-isopropylbenzene	527-84-4	-0.33	1	T	1	D
197	m-cymene	535-77-3	-0.534	2	T	2	D
198	p-isopropyltoluen	99-87-6	-0.39	1	T	1	D
199	1,3-diisopropylbenzene	99-62-7	-0.46	2	T	2	M
200	tert-butylbenzene	98-06-6	-0.37	1	T	1	D
201	tert-amylbenzene	2049-95-8	-0.13	1	P	2	D
202	p-tert-butyltoluene	98-51-1	0.16	2	T	1	M
203	indane	496-11-7	-1.07	1	T	2	D
204	1,2,3,4-tetrahydronaphthalene	119-64-2	-1.12	1	T	1	O
205	styrene	100-42-5	-0.806	1	T	2	D
206	m-methylstyrene	100-80-1	-0.911	2	T	1	D
207	p-methylstyrene	622-97-9	-0.89	2	P	2	M
208	alpha-methylstyrene	98-83-9	-0.91	1	T	1	D
209	4-phenylcyclohexene	4994-16-5	-1.29	2	T	2	D
210	ethynyl benzene	536-74-3	-1.6	2	T	1	D
211	diphenylmethane	101-81-5	-1.92	2	T	2	M
212	bibenzyl	103-29-7	-2.11	2	T	1	M
213	trans-stilbene	103-30-0	-2.717	2	T	2	M
214	biphenyl	92-52-4	-1.923	1	T	1	O
215	3-isopropylbiphenyl	20282-30-8	-1.155	1	T	2	D
216	4-isopropylbiphenyl	7116-95-2	-1.018	1	T	1	D
217	9H-fluorene	86-73-7	-2.57	1	T	2	O
218	1-methylfluorene	1730-37-6	-2.67	2	P	1	M
219	9,10-dihydrophenanthrene	776-35-2	-2.44	2	T	2	O
220	naphthalene	91-20-3	-1.769	1	T	1	O
221	2-methylnaphthalene	91-57-6	-1.89	1	T	2	O
222	1-methylnaphthalene	90-12-0	-1.79	1	T	1	D
223	1-ethylnaphthalene	1127-76-0	-1.72	1	T	2	D
224	2-ethylnaphthalene	939-27-5	-1.658	1	T	1	O
225	1,3-dimethylnaphthalene	575-41-7	-1.81	1	T	2	D
226	1,4-dimethylnaphthalene	571-58-4	-2.07	1	P	1	D
227	1,5-dimethylnaphthalene	571-61-9	-1.844	1	P	2	D
228	2,3-dimethylnaphthalene	581-40-8	-2.04	1	T	1	D
229	2,6-dimethylnaphthalene	581-42-0	-1.93	1	T	2	D
230	1,2-dimethylnaphtalene	573-98-8	-2.1	2	P	1	O
231	1,6-dimethylnaphthalene	575-43-9	-1.89	2	T	2	O
232	1,7-dimethylnaphthalene	575-37-1	-1.98	2	T	1	O
233	1,8-dimethylnaphthalene	569-41-5	-2.25	2	T	2	O
234	2,7-dimethylnaphthalene	582-16-1	-1.69	2	T	1	O
235	1,4,5-trimethylnaphthalene	2131-41-1	-2.02	2	T	2	D
236	1,2,4-trimethylnaphthalene	2717-42-2	-2.24	2	P	1	O
237	1,3,7-trimethylnaphthalene	2131-38-6	-2.17	2	T	2	O
238	1,4,6-trimethylnaphthalene	2131-42-2	-2.03	2	P	1	O

239	2,3,6-trimethylnaphthalene	829-26-5	-1.84	2	T	2	O
240	2,4,5-trimethylnaphthalene	17057-91-9	-2.22	2	P	1	O
241	1,2,5,6-tetramethylnaphthalene	2131-43-3	-2.26	2	P	2	O
242	1,4,6,7-tetramethylnaphthalene	13764-18-6	-2.33	2	T	1	O
243	2-isopropylnaphthalene	2027-17-0	-1.26	2	T	2	D
244	1,7-diisopropylnaphthalene	94133-80-9	-1.285	2	T	1	D
245	2,6-diisopropylnaphthalene	24157-81-1	-1.47	2	T	2	M
246	acenaphthene	83-32-9	-2.585	1	T	1	O
247	acenaphthylene	208-96-8	-2.67	2	T	2	D
248	benzo(b)fluorene	243-17-4	-3.49	2	T	1	M
249	fluoranthene	206-44-0	-3.35	1	T	2	O
250	anthracene	120-12-7	-3.1	1	T	1	O
251	benzo[k]fluoranthene	207-08-9	-4.622	1	T	2	O
252	phenanthrene	85-01-8	-2.762	1	T	1	O
253	1-methylphenanthrene	832-69-9	-2.695	1	T	2	O
254	benzo[b]fluoranthene	205-99-2	-4.55	1	T	1	O
255	benz(a)anthracene	56-55-3	-4.385	1	P	2	D
256	chrysene	218-01-9	-3.67	1	P	1	O
257	dibenz(a,h)anthracene	53-70-3	-4.76	2	T	2	M
258	dibenz(a,c)anthracene	215-58-7	-4.61	2	T	1	M
259	pyrene	129-00-0	-3.7	1	P	2	O
260	indeno-[1,2,3-cd]-pyrene	193-39-5	-4.847	1	T	1	D
261	benzo(a)pyrene	50-32-8	-4.729	1	T	2	D
262	benzo(e)pyrene	192-97-2	-4	1	P	1	D
263	perylene	198-55-0	-4.06	2	T	2	M
264	benzo[ghi]perylene	191-24-2	-5.23	1	T	1	D
265	coronene	191-07-1	-6.62	2	T	2	M
266	fluoromethane	593-53-3	-0.158	1	T	1	O
267	fluoroethane	353-36-6	-0.04	2	T	2	D
268	difluoromethane	75-10-5	-0.23	1	T	1	O
269	1,1-difluoroethane	75-37-6	-0.12	1	T	2	D
270	trifluoromethane	75-46-7	0.59	1	T	1	D
271	tetrafluoromethane	75-73-0	2.29	1	T	2	D
272	1,1,1,2-tetrafluoroethane	811-97-2	0.39	1	T	1	O
273	1,1,2,2-tetrafluoroethane	359-35-3	0.15	2	T	2	D
274	pentafluoroethane	354-33-6	1.05	1	P	1	O
275	hexafluoroethane	76-16-4	2.824	1	P	2	D
276	heptafluoropropane	431-89-0	1.46	1	T	1	O
277	perfluoropropane	76-19-7	3.14	1	T	2	D
278	chloromethane	74-87-3	-0.413	1	T	1	O
279	chloroethane	75-00-3	-0.325	1	T	2	D
280	1-chloropropane	540-54-5	-0.24	1	P	1	D
281	2-chloropropane	75-29-6	-0.13	1	T	2	D
282	1-chlorobutane	109-69-3	-0.12	1	P	1	D
283	2-chlorobutane	78-86-4	-0.01	1	T	2	D
284	tert-butylchloride	507-20-0	0.01	2	T	1	M
285	1-chloropentane	543-59-9	-0.012	1	P	2	D
286	2-chloropentane	625-29-6	0.05	1	T	1	D
287	3-chloropentane	616-20-6	0.05	1	T	2	D
288	2-chloro-2-methylbutane	594-36-5	0.12	2	T	1	M
289	1-chlorohexane	544-10-5	-0.005	1	T	2	D
290	1-chloroheptane	629-06-1	0.21	1	T	1	D
291	1-chlorooctane	111-85-3	0.37	2	T	2	M
292	dichloromethane	75-09-2	-0.978	1	T	1	O
293	1,2-dichloroethane	107-06-2	-1.398	1	T	2	D
294	1,1-dichloroethane	75-34-3	-0.686	1	T	1	O

295	1,3-dichloropropane	142-28-9	-1.44	1	P	2	D
296	1,1-dichloropropane	78-99-9	-0.813	2	T	1	D
297	1,2-dichloropropane	78-87-5	-0.951	1	T	2	O
298	2,2-dichloropropane	594-20-7	-0.315	1	T	1	O
299	1,4-dichlorobutane	110-56-5	-1.702	1	T	2	D
300	1,1-dichlorobutane	541-33-3	-0.51	1	T	1	D
301	2,3-dichlorobutane	7581-97-7	-0.57	2	T	2	D
302	1,5-dichloropentane	628-76-2	-1.642	1	T	1	D
303	1,8-dichlorooctane	2162-99-4	-1.25	2	T	2	O
304	1,10-dichlorodecane	2162-98-3	-0.69	1	T	1	O
305	1,12-dichlorododecane	3922-28-9	-0.58	1	P	2	O
306	chloroform	67-66-3	-0.66	1	T	1	O
307	1,1,2-trichloroethane	79-00-5	-1.473	1	T	2	D
308	1,1,1-trichloroethane	71-55-6	-0.186	1	T	1	O
309	1,2,3-trichloropropane	96-18-4	-1.998	1	T	2	D
310	1,1,1-trichloropropane	7789-89-1	-0.88	2	T	1	D
311	1,1,2-trichloropropane	598-77-6	-1.887	2	T	2	D
312	carbon tetrachloride	56-23-5	0.237	1	T	1	O
313	1,1,1,2-tetrachloroethane	630-20-6	-0.94	1	P	2	D
314	1,1,2,2-tetrachloroethane	79-34-5	-1.73	1	P	1	D
315	1,2,9,10-tetrachlorodecane	205646-11-3	-2.14	1	P	2	O
316	1,2,10,11-tetrachloroundecane	210049-49-3	-2.59	1	T	1	O
317	pentachloroethane	76-01-7	-1	1	P	2	D
318	hexachloroethane	67-72-1	-0.05	2	T	1	D
319	bromomethane	74-83-9	-0.594	1	T	2	O
320	bromoethane	74-96-4	-0.51	1	P	1	D
321	1-bromopropane	106-94-5	-0.41	1	T	2	D
322	2-bromopropane	75-26-3	-0.318	1	T	1	D
323	1-bromobutane	109-65-9	-0.29	1	P	2	D
324	2-bromobutane	78-76-2	-0.333	2	P	1	M
325	2-bromo-2-methylpropane	507-19-7	0.22	2	T	2	D
326	1-bromopentane	110-53-2	-0.07	1	T	1	D
327	1-bromohexane	111-25-1	0.13	1	T	2	D
328	1-bromoheptane	629-04-9	0.25	1	T	1	D
329	1-bromooctane	111-83-1	0.38	1	T	2	D
330	1-bromodecane	112-29-8	0.383	2	T	1	M
331	dibromomethane	74-95-3	-1.46	1	T	2	D
332	ethylene dibromide	106-93-4	-1.71	1	T	1	D
333	1,3-dibromopropane	109-64-8	-1.44	1	T	2	D
334	1,2-dibromopropane	78-75-1	-1.42	1	T	1	D
335	1,4-dibromobutane	110-52-1	-1.77	2	T	2	M
336	1,8-dibromooctane	4549-32-0	-1.514	2	T	1	O
337	bromoform	75-25-2	-1.56	1	T	2	D
338	1,1,2-tribromoethane	78-74-0	-1.77	2	P	1	M
339	tetrabromomethane	558-13-4	-0.154	2	T	2	M
340	1,1,2,2-tetrabromoethane	79-27-6	-1.39	1	P	1	M
341	methyl iodide	74-88-4	-0.66	1	T	2	O
342	iodoethane	75-03-6	-0.54	1	T	1	D
343	1-iodopropane	107-08-4	-0.39	1	P	2	D
344	2-iodopropane	75-30-9	-0.34	1	T	1	D
345	n-butyl iodide	542-69-8	-0.19	1	P	2	D
346	2-iodobutane	513-48-4	-0.094	2	T	1	D
347	1-iodopentane	628-17-1	-0.101	1	T	2	D
348	1-iodohexane	638-45-9	0.06	1	T	1	D
349	1-iodoheptane	4282-40-0	0.2	1	T	2	D
350	methylene iodide	75-11-6	-1.75	1	T	1	D

351	chlorofluoromethane	593-70-4	-0.57	1	T	2	D
352	chlorodifluoromethane	75-45-6	0.26	1	T	1	D
353	1-chloro-1,1-difluoroethane	75-68-3	0.43	1	T	2	D
354	chlorotrifluoromethane	75-72-9	1.751	1	T	1	D
355	1,1,1-trifluoro-2-chloroethane	75-88-7	0.04	1	T	2	D
356	1-chloro-1,1,2-trifluoroethane	421-04-5	0.04	1	T	1	O
357	1-chloro-1,2,2,2-tetrafluoroethane	2837-89-0	0.59	1	T	2	O
358	chloropentafluoroethane	76-15-3	2.11	1	T	1	O
359	dichlorofluoromethane	75-43-4	-0.355	2	T	2	D
360	1,1-dichloro-1-fluoroethane	1717-00-6	-0.006	1	P	1	D
361	dichlorodifluoromethane	75-71-8	1.24	1	T	2	D
362	1,2-dichloro-1,1-difluoroethane	1649-08-7	0.463	2	P	1	D
363	1,1,1-trifluoro-2,2-dichloroethane	306-83-2	0.45	1	T	2	D
364	1,2-dichlorotetrafluoroethane	76-14-2	1.65	1	T	1	O
365	1,1-dichloro-1,2,2,2-tetrafluoroethane	374-07-2	1.54	2	P	2	D
366	3,3-dichloro-1,1,1,2,2-pentafluoropro-pane	422-56-0	0.62	1	T	1	D
367	1,3-dichloro-1,1,2,2,3-pentafluoropro-pane	507-55-1	0.56	1	P	2	D
368	trichlorofluoromethane	75-69-4	0.6	1	T	1	O
369	1,1,2-trichlorotrifluoroethane	76-13-1	1.115	1	T	2	O
370	1,1,1,2-tetrachlorodifluoroethane	76-11-9	0.82	2	T	1	D
371	1,1,2,2-tetrachlorodifluoroethane	76-12-0	0.6	1	P	2	D
372	bromotrifluoromethane	75-63-8	1.31	1	T	1	D
373	tefluorane	124-72-1	0.37	1	T	2	D
374	bromochloromethane	74-97-5	-1.29	1	T	1	M
375	1-chloro-2-bromoethane	107-04-0	-1.43	1	T	2	D
376	1-bromo-3-chloropropane	109-70-6	-1.57	2	P	1	M
377	halothane	151-67-7	0.16	1	T	2	D
378	bromodichloromethane	75-27-4	-1.062	1	T	1	D
379	dibromochloromethane	124-48-1	-1.317	1	T	2	O
380	1,2-dibromo-3-chloropropane	96-12-8	-3.09	1	P	1	D
381	chloroiodomethane	593-71-5	-1.34	1	T	2	D
382	1-chloro-2-methylpropane	513-36-0	-0.094	2	T	1	D
383	3-(chloromethyl)-heptane	123-04-6	0.61	2	T	2	D
384	1-bromo-2-methylpropane	78-77-3	-0.02	1	T	1	D
385	1-bromo-2-methylbutane	10422-35-2	-0.02	1	T	2	D
386	1-bromo-3-methylbutane	107-82-4	0.15	1	P	1	D
387	1-bromo-3-methylpentane	51116-73-5	0.15	1	T	2	D
388	perfluorocyclobutane	115-25-3	2.54	1	T	1	D
389	chlorocyclohexane	542-18-7	-0.62	2	T	2	O
390	alpha-hexachlorocyclohexane	319-84-6	-3.634	1	T	1	O
391	beta-hexachlorocyclohexane	319-85-7	-4.13	2	T	2	M
392	gamma-hexachlorocyclohexane	58-89-9	-3.678	1	T	1	O
393	delta-hexachlorocyclohexane	319-86-8	-4.16	2	P	2	M
394	mirex	2385-85-5	-1.48	1	T	1	D
395	bromocyclohexane	108-85-0	-0.42	2	P	2	O
396	1,1-difluoroethene	75-38-7	1.163	2	T	1	D
397	tetrafluoroethylene	116-14-3	1.413	1	T	2	O
398	perfluoropropene	116-15-4	2.144	1	T	1	O
399	(E)-perfluoro(4-methyl-2-pentene)	3709-71-5	3.8	1	T	2	D
400	vinylchloride	75-01-4	-0.01	1	T	1	D
401	3-chloropropylene	107-05-1	-0.42	1	T	2	D
402	trans-1-chloro-2-butene	591-97-9	-0.37	2	T	1	D
403	cis-1,2-dichloroethene	156-59-2	-0.73	1	T	2	O
404	trans-1,2-dichloroethene	156-60-5	-0.66	1	T	1	D

405	1,1-dichloroethene	75-35-4	0.18	1	T	2	D
406	cis-1,3-dichloropropene	10061-01-5	-0.87	1	P	1	D
407	trans-1,3-dichloropropene	10061-02-6	-1.34	1	T	2	D
408	1,1-dichloropropene	563-58-6	-0.13	1	P	1	D
409	1,2-dichloropropene	563-54-2	-0.59	2	T	2	M
410	2,3-dichloropropene	78-88-6	-0.77	2	P	1	D
411	cis-1,4-dichloro-2-butene	1476-11-5	-1.324	2	T	2	D
412	trans-1,4-dichloro-2-butene	110-57-6	-1.57	2	T	1	D
413	3,4-dichloro-1-butene	760-23-6	-1.15	2	T	2	M
414	trichloroethene	79-01-6	-0.397	1	P	1	O
415	tetrachloroethene	127-18-4	-0.12	1	T	2	D
416	perchloropropylene	1888-71-7	-0.67	2	T	1	M
417	vinyl bromide	593-60-2	-0.08	2	T	2	D
418	allylbromide	106-95-6	-0.63	1	P	1	D
419	1,2-dibromoethylene	540-49-8	-1.03	2	T	2	D
420	1-chloro-2,2-difluoroethene	359-10-4	0.39	1	T	1	O
421	3-chloro-2-methylpropene	563-47-3	-0.34	2	P	2	M
422	3-chloro-1-butene	563-52-0	-0.14	2	P	1	M
423	cis-chlordane	57-74-9	-2.654	1	P	2	O
424	trans-chlordane	5103-74-2	-2.62	1	T	1	O
425	gamma-chlordane	5566-34-7	-2.193	1	T	2	O
426	cis-nonachlor	5103-73-1	-3.54	1	T	1	D
427	trans-nonachlor	39765-80-5	-2.365	1	T	2	O
428	chloroprene	126-99-8	-0.24	2	P	1	M
429	hexachlorobutadiene	87-68-3	-0.76	1	T	2	D
430	hexachlorocyclopentadiene	77-47-4	-0.173	1	T	1	D
431	aldrin	309-00-2	-1.695	1	T	2	O
432	heptachlor	76-44-8	-1.67	1	P	1	D
433	dienochlor	2227-17-0	-2.62	2	T	2	M
434	propargyl bromide	106-96-7	-1.336	1	T	1	D
435	fluorobenzene	462-06-6	-0.57	1	T	2	O
436	1,2-difluorobenzene	367-11-3	-0.47	1	P	1	D
437	p-difluorobenzene	540-36-3	-0.47	2	T	2	M
438	1,3-difluorobenzene	372-18-9	-0.35	2	T	1	M
439	benzotrifluoride	98-08-8	-0.18	1	T	2	D
440	1,2,3,5-tetrafluorobenzene	2367-82-0	-0.098	2	T	1	M
441	1,2,4,5-tetrafluorobenzene	327-54-8	-0.14	2	P	2	M
442	hexafluorobenzene	392-56-3	0.13	2	T	1	M
443	chlorobenzene	108-90-7	-0.796	1	T	2	O
444	alpha-chlorotoluene	100-44-7	-1.46	1	T	1	O
445	2-chlorotoluene	95-49-8	-0.77	1	T	2	D
446	m-chlorotoluene	108-41-8	-0.83	2	P	1	M
447	p-chlorotoluene	106-43-4	-0.86	1	T	2	M
448	1,2-dichlorobenzene	95-50-1	-1.071	1	T	1	O
449	1,4-dichlorobenzene	106-46-7	-0.79	1	T	2	O
450	1,3-dichlorobenzene	541-73-1	-0.969	1	P	1	D
451	2,4-dichlorotoluene	95-73-8	-0.83	1	T	2	D
452	2,6-dichlorotoluene	118-69-4	-1.07	2	T	1	M
453	3,4-dichlorotoluene	95-75-0	-0.98	2	T	2	D
454	(dichloromethyl)benzene	98-87-3	-1.789	2	T	1	D
455	1,2,3-trichlorobenzene	87-61-6	-1.3	1	P	2	D
456	1,2,4-trichlorobenzene	120-82-1	-1.236	1	P	1	D
457	1,3,5-trichlorobenzene	108-70-3	-1.112	1	T	2	D
458	2,3,6-trichlorotoluene	2077-46-5	-1.21	1	T	1	D
459	2,4,5-trichlorotoluene	6639-30-1	-1.21	1	T	2	D
460	2,4,6-trichlorotoluene	23749-65-7	-1.21	1	T	1	D

461	benzotrichloride	98-07-7	-1.22	2	T	2	M
462	1,2,3,4-tetrachlorobenzene	634-66-2	-1.602	1	P	1	D
463	1,2,3,5-tetrachlorobenzene	634-90-2	-1.399	1	T	2	D
464	1,2,4,5-tetrachlorobenzene	95-94-3	-1.39	1	T	1	D
465	pentachlorobenzene	608-93-5	-1.62	1	T	2	D
466	2,3,4,5,6-pentachlorotoluene	877-11-2	-1.39	1	P	1	D
467	hexachlorobenzene	118-74-1	-1.91	1	T	2	D
468	bromobenzene	108-86-1	-1	1	T	1	O
469	benzyl bromide	100-39-0	-1.74	1	T	2	D
470	o-bromotoluene	95-46-5	-1.02	2	P	1	M
471	m-bromotoluene	591-17-3	-0.56	2	T	2	D
472	p-bromotoluene	106-38-7	-0.93	1	T	1	D
473	1-bromo-2-ethylbenzene	1973-22-4	-0.87	1	T	2	D
474	1,2-dibromobenzene	583-53-9	-1.53	2	T	1	M
475	1,3-dibromobenzene	108-36-1	-1.3	2	T	2	M
476	1,4-dibromobenzene	106-37-6	-1.37	2	P	1	M
477	1,3,5-tribromobenzene	626-39-1	-1.49	2	T	2	D
478	iodobenzene	591-50-4	-1.275	1	T	1	O
479	2-chlorofluorobenzene	348-51-6	-0.88	2	T	2	M
480	3-chlorofluorobenzene	625-98-9	-0.61	2	T	1	M
481	2-bromofluorobenzene	1072-85-1	-1.01	2	T	2	M
482	3-bromofluorobenzene	1073-06-9	-0.86	2	P	1	M
483	1-bromo-4-chlorobenzene	106-39-8	-1.23	1	T	2	D
484	4-iodofluorobenzene	352-34-1	-1.05	2	T	1	M
485	p-chloroiodobenzene	637-87-6	-1.23	2	T	2	M
486	p-bromoiodobenzene	589-87-7	-1.56	2	T	1	M
487	o-bromoisopropylbenzene	7073-94-1	-0.62	1	P	2	D
488	octachlorostyrene	29082-74-4	-2.11	1	T	1	D
489	p,p'-DDD	72-54-8	-3.57	1	T	2	D
490	o,p'-DDD	53-19-0	-3.53	2	P	1	M
491	p,p'-DDT	50-29-3	-3.468	1	T	2	D
492	o,p'-DDT	789-02-6	-3.47	2	T	1	D
493	p,p'-DDE	72-55-9	-2.77	1	P	2	D
494	o,p'-DDE	3424-82-6	-3.12	2	T	1	D
495	2-chlorobiphenyl	2051-60-7	-1.522	1	T	2	D
496	3-chlorobiphenyl	2051-61-8	-1.93	2	T	1	M
497	4-chlorobiphenyl	2051-62-9	-2.01	1	P	2	D
498	2,2'-dichlorobiphenyl	13029-08-8	-1.81	1	T	1	D
499	2,3-dichlorobiphenyl	16605-91-7	-2.027	1	T	2	D
500	2,3'-dichlorobiphenyl	25569-80-6	-1.87	1	T	1	D
501	2,4-dichlorobiphenyl	33284-50-3	-1.85	1	T	2	D
502	2,4'-dichlorobiphenyl	34883-43-7	-1.94	1	P	1	D
503	2,5-dichlorobiphenyl	34883-39-1	-1.8	1	T	2	O
504	2,6-dichlorobiphenyl	33146-45-1	-1.9	1	P	1	D
505	3,3'-dichlorobiphenyl	2050-67-1	-2.021	1	T	2	O
506	3,4-dichlorobiphenyl	2974-92-7	-2.242	1	T	1	O
507	3,4'-dichlorobiphenyl	2974-90-5	-2.17	1	T	2	O
508	3,5-dichlorobiphenyl	34883-41-5	-1.89	1	T	1	D
509	4,4'-dichlorobiphenyl	2050-68-2	-2.071	1	T	2	D
510	2',3,4-trichlorobiphenyl	38444-86-9	-2.184	1	T	1	D
511	2',3,5-trichlorobiphenyl	37680-68-5	-2.087	1	T	2	D
512	2,2',3-trichlorobiphenyl	38444-78-9	-2.09	1	T	1	D
513	2,2',4-trichlorobiphenyl	37680-66-3	-1.96	1	P	2	O
514	2,2',5-trichlorobiphenyl	37680-65-2	-1.991	1	T	1	O
515	2,2',6-trichlorobiphenyl	38444-73-4	-2.03	1	T	2	O
516	2,3,3'-trichlorobiphenyl	38444-84-7	-2.18	1	T	1	D

517	2,3',4-trichlorobiphenyl	55712-37-3	-1.84	1	T	2	O
518	2,3',5-trichlorobiphenyl	38444-81-4	-2.087	1	P	1	D
519	2,3',6-trichlorobiphenyl	38444-76-7	-1.83	1	T	2	O
520	2,3,4'-trichlorobiphenyl	38444-85-8	-2.242	1	T	1	O
521	2,3,6-trichlorobiphenyl	55702-45-9	-2.05	1	T	2	O
522	2,4,5-trichlorobiphenyl	15862-07-4	-2.087	1	T	1	O
523	2,4',5-trichlorobiphenyl	16606-02-3	-2.11	1	T	2	D
524	2,4,6-trichlorobiphenyl	35693-92-6	-1.89	1	T	1	M
525	2,4',6-trichlorobiphenyl	38444-77-8	-2.087	1	T	2	D
526	2,4,4'-trichlorobiphenyl	7012-37-5	-1.933	1	T	1	D
527	3,3',5-trichlorobiphenyl	38444-87-0	-2.16	1	T	2	O
528	3,4,4'-trichlorobiphenyl	38444-90-5	-2.39	1	T	1	D
529	2,3,4-trichlorobiphenyl	55702-46-0	-2.44	2	T	2	M
530	2,2',3,4-tetrachlorobiphenyl	52663-59-9	-2.242	1	T	1	D
531	2,2',3,4'-tetrachlorobiphenyl	36559-22-5	-2.242	1	T	2	D
532	2,2',3,5'-tetrachlorobiphenyl	41464-39-5	-2.242	1	T	1	D
533	2,2',3,6-tetrachlorobiphenyl	70362-45-7	-1.86	1	P	2	O
534	2,2',3,6'-tetrachlorobiphenyl	41464-47-5	-1.85	1	T	1	O
535	2,2',4,4'-tetrachlorobiphenyl	2437-79-8	-2.11	1	P	2	O
536	2,2',4,5-tetrachlorobiphenyl	70362-47-9	-1.73	1	T	1	M
537	2,2',4,5'-tetrachlorobiphenyl	41464-40-8	-2.07	1	T	2	D
538	2,2',4,6-tetrachlorobiphenyl	62796-65-0	-1.586	1	T	1	O
539	2,2',4,6'-tetrachlorobiphenyl	58194-04-7	-2.242	1	T	2	D
540	2,2',5,5'-tetrachlorobiphenyl	35693-99-3	-2.087	1	P	1	D
541	2,2',5,6'-tetrachlorobiphenyl	41464-41-9	-1.91	1	P	2	D
542	2,2',6,6'-tetrachlorobiphenyl	15968-05-5	-2.09	1	P	1	O
543	2,3,3',4'-tetrachlorobiphenyl	41464-43-1	-2.99	4	P	2	M
544	2,3,4,4'-tetrachlorobiphenyl	33025-41-1	-2.18	2	T	1	D
545	2,3,4',5-tetrachlorobiphenyl	74472-34-7	-1.75	1	T	2	M
546	2,3',4,4'-tetrachlorobiphenyl	32598-10-0	-2.309	1	T	1	D
547	2,3',4,5-tetrachlorobiphenyl	73575-53-8	-2.39	1	T	2	O
548	2,3',4',5-tetrachlorobiphenyl	32598-11-1	-2.389	1	P	1	D
549	2,3',4,6-tetrachlorobiphenyl	60233-24-1	-2.066	1	T	2	D
550	2,3,4,6-tetrachlorobiphenyl	54230-22-7	-2.07	1	P	1	O
551	2,3,4',6-tetrachlorobiphenyl	52663-58-8	-2.242	1	T	2	D
552	2,3,5,6-tetrachlorobiphenyl	33284-54-7	-1.97	1	T	1	O
553	2,4,4',5-tetrachlorobiphenyl	32690-93-0	-2.39	1	P	2	O
554	2,4,4',6-tetrachlorobiphenyl	32598-12-2	-1.77	1	T	1	D
555	3,3',4,4'-tetrachlorobiphenyl	32598-13-3	-2.754	1	T	2	O
556	3,3',4,5'-tetrachlorobiphenyl	41464-48-6	-2.434	1	T	1	D
557	3,3',5,5'-tetrachlorobiphenyl	33284-52-5	-1.99	1	T	2	O
558	3,4,4',5-tetrachlorobiphenyl	70362-50-4	-2.341	1	T	1	O
559	2,2',3,3'-tetrachlorobiphenyl	38444-93-8	-2.389	1	T	2	D
560	2,3',4',5-tetrachlorobiphenyl	70362-48-0	-2.39	1	T	1	O
561	2,3,4,5-tetrachlorobiphenyl	33284-53-6	-2.47	2	T	2	M
562	2,2',3,5-tetrachlorobiphenyl	70362-46-8	-2.07	2	P	1	M
563	2,2',3,3',4-pentachlorobiphenyl	52663-62-4	-2.09	1	T	2	D
564	2,2',3,4,4'-pentachlorobiphenyl	65510-45-4	-2.54	1	T	1	O
565	2,2',3,4',6-pentachlorobiphenyl	68194-05-8	-2.309	1	T	2	D
566	2,2',3',4,5-pentachlorobiphenyl	41464-51-1	-2.52	1	T	1	D
567	2,2',4,4',5-pentachlorobiphenyl	38380-01-7	-2.496	1	P	2	D
568	2,2',4,5,5'-pentachlorobiphenyl	37680-73-2	-2.434	1	P	1	D
569	2,2',4,5,6'-pentachlorobiphenyl	68194-06-9	-2.43	1	T	2	O
570	2,2',4,6,6'-pentachlorobiphenyl	56558-16-8	-1.6	1	T	1	O
571	2,3',4,4',5-pentachlorobiphenyl	31508-00-6	-2.423	1	T	2	O
572	2,3',4,4',6-pentachlorobiphenyl	56558-17-9	-2.519	1	T	1	D

573	2,3',4,5,5'-pentachlorobiphenyl	68194-12-7	-2.64	1	T	2	O
574	2,3,3',4,4'-pentachlorobiphenyl	32598-14-4	-2.64	1	T	1	O
575	2,3,3',4',5-pentachlorobiphenyl	70424-68-9	-2.4	1	T	2	O
576	2,3,3',4',6-pentachlorobiphenyl	38380-03-9	-2.84	4	T	1	M
577	2,3,4,4',5-pentachlorobiphenyl	74472-37-0	-2.24	2	T	2	M
578	2,3,4,5,6-pentachlorobiphenyl	18259-05-7	-2.45	2	T	1	M
579	2,2',3,4,5'-pentachlorobiphenyl	38380-02-8	-2.52	1	P	2	D
580	2,2',3,5',6-pentachlorobiphenyl	38379-99-6	-2.31	1	T	1	O
581	2',3,4,4',5-pentachlorobiphenyl	65510-44-3	-2.06	1	T	2	O
582	3,3',4,4',5-pentachlorobiphenyl	57465-28-8	-2.95	1	P	1	O
583	2,2',3,3',6-pentachlorobiphenyl	52663-60-2	-2.76	4	T	2	M
584	2',3,3',4,5-pentachlorobiphenyl	76842-07-4	-2.13	2	T	1	D
585	2',3,4,5,5'-pentachlorobiphenyl	70424-70-3	-2.075	2	P	2	M
586	2,2',3,3',4,4'-hexachlorobiphenyl	38380-07-3	-2.558	1	T	1	O
587	2,2',3,3',4,5'-hexachlorobiphenyl	52663-66-8	-2.82	1	T	2	O
588	2,2',3,3',4,6-hexachlorobiphenyl	61798-70-7	-2.797	1	T	1	D
589	2,2',3,3',4,6'-hexachlorobiphenyl	38380-05-1	-2.745	1	T	2	O
590	2,2',3,3',5,6-hexachlorobiphenyl	52704-70-8	-2.7	1	T	1	O
591	2,2',3,3',5,6'-hexachlorobiphenyl	52744-13-5	-2.64	1	T	2	O
592	2,2',3,3',6,6'-hexachlorobiphenyl	38411-22-2	-2.44	1	P	1	O
593	2,2',3,4',5',6'-hexachlorobiphenyl	38380-04-0	-2.47	4	T	2	D
594	2,2',3,4,4',5'-hexachlorobiphenyl	35065-28-2	-3.066	1	P	1	D
595	2,2',3,4,4',5-hexachlorobiphenyl	35694-06-5	-2.23	1	T	2	O
596	2,2',3,4,5',6-hexachlorobiphenyl	68194-14-9	-1.92	2	T	1	M
597	2,2',3,4,5,5'-hexachlorobiphenyl	52712-04-6	-3.03	1	T	2	O
598	2,2',3,4,5,6'-hexachlorobiphenyl	68194-15-0	-2.797	1	T	1	D
599	2,2',3,4',5,5'-hexachlorobiphenyl	51908-16-8	-2.99	1	T	2	O
600	2,2',3,4',5,6-hexachlorobiphenyl	68194-13-8	-2.68	1	P	1	O
601	2,2',4,4',5,5'-hexachlorobiphenyl	35065-27-1	-2.52	1	T	2	D
602	2,2',4,4',6,6'-hexachlorobiphenyl	33979-03-2	-2.33	1	P	1	D
603	2,3,3',4,4',6-hexachlorobiphenyl	74472-42-7	-2.25	2	P	2	M
604	2,2',3,3',4,5-hexachlorobiphenyl	55215-18-4	-2.93	1	T	1	O
605	2,2',3,5,5',6-hexachlorobiphenyl	52663-63-5	-2.62	1	T	2	O
606	2,3,3',4,4',5-hexachlorobiphenyl	38380-08-4	-2.75	1	T	1	O
607	2,3,3',4,4',5'-hexachlorobiphenyl	69782-90-7	-2.6	1	T	2	O
608	2,3,3',4,5,5'-hexachlorobiphenyl	39635-35-3	-3.087	1	T	1	D
609	2,3,3',4,5,6-hexachlorobiphenyl	41411-62-5	-3.087	1	T	2	D
610	2,3,3',4',5,6-hexachlorobiphenyl	74472-44-9	-3.212	1	T	1	D
611	2,3,3',5,5',6-hexachlorobiphenyl	74472-46-1	-2.926	1	T	2	D
612	2,3,4,4',5,5'-hexachlorobiphenyl	52663-72-6	-2.33	1	T	1	O
613	2,3,4,4',5,6-hexachlorobiphenyl	41411-63-6	-2.17	1	T	2	D
614	3,3',4,4',5,5'-hexachlorobiphenyl	32774-16-6	-2.99	1	T	1	O
615	2,2',3,4,4',6-hexachlorobiphenyl	56030-56-9	-2.22	2	T	2	M
616	2,2',3,3',4,4',5-heptachlorobiphenyl	35065-30-6	-3.434	1	P	1	O
617	2,2',3,3',4,4',6-heptachlorobiphenyl	52663-71-5	-3.5	4	T	2	M
618	2,2',3,3',4,5,5'-heptachlorobiphenyl	52663-74-8	-3.27	1	T	1	O
619	2,2',3,3',4,5,6-heptachlorobiphenyl	68194-16-1	-3.24	1	T	2	O
620	2,2',3,3',4,5,6'-heptachlorobiphenyl	38411-25-5	-3.24	1	T	1	O
621	2,2',3,3',4',5,6-heptachlorobiphenyl	52663-70-4	-2.65	1	T	2	O
622	2,2',3,3',5,5',6-heptachlorobiphenyl	52663-67-9	-3.03	1	T	1	O
623	2,2',3,3',5,6,6'-heptachlorobiphenyl	52663-64-6	-3.01	1	T	2	O
624	2,2',3,4,4',5,5'-heptachlorobiphenyl	35065-29-3	-3.389	1	T	1	O
625	2,2',3,4,4',5,6'-heptachlorobiphenyl	60145-23-5	-2.12	1	P	2	O
626	2,2',3,4,4',5',6-heptachlorobiphenyl	52663-69-1	-2.52	1	T	1	D
627	2,2',3,4,5,5',6-heptachlorobiphenyl	52712-05-7	-3.18	1	P	2	O
628	2,2',3,4',5,5',6-heptachlorobiphenyl	52663-68-0	-3.11	4	T	1	O

629	2,2',3,4',5,6,6'-heptachlorobiphenyl	74487-85-7	-2.25	1	T	2	O
630	2,3,3',4',5,5',6-heptachlorobiphenyl	69782-91-8	-2.71	1	P	1	O
631	2,2',3,3',4,6,6'-heptachlorobiphenyl	52663-65-7	-3.11	2	T	2	D
632	2,2',3,3',4,4',5,5'-octachlorobiphenyl	35694-08-7	-3.39	1	T	1	O
633	2,2',3,3',4,4',5,6-octachlorobiphenyl	52663-78-2	-3.35	1	T	2	O
634	2,2',3,3',4,5,5',6'-octachlorobiphenyl	52663-75-9	-3.39	1	T	1	O
635	2,2',3,3',4,5',6,6'-octachlorobiphenyl	40186-71-8	-3.16	1	T	2	O
636	2,2',3,3',5,5',6,6'-octachlorobiphenyl	2136-99-4	-3.13	1	T	1	O
637	2,2',3,3',4,4',5,6'-octachlorobiphenyl	42740-50-1	-3.39	1	T	2	O
638	2,2',3,3',4,5,5',6-octachlorobiphenyl	68194-17-2	-3.24	1	T	1	O
639	2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl	52663-77-1	-2.78	2	P	2	M
640	decachlorobiphenyl	2051-24-3	-3.13	2	T	1	M
641	4-bromobiphenyl	92-66-0	-2.14	2	P	2	M
642	1-chloronaphthalene	90-13-1	-1.84	1	T	1	D
643	2-chloronaphthalene	91-58-7	-1.88	1	T	2	D
644	1,2-dichloronaphthalene	2050-69-3	-2.47	4	T	1	M
645	1,4-dichloronaphthalene	1825-31-6	-2.27	4	P	2	M
646	1,5-dichloronaphthalene	1825-30-5	-2	4	P	1	M
647	2,7-dichloronaphthalene	2198-77-8	-1.89	4	P	2	D
648	1,3,5-trichloronaphthalene	51570-43-5	-2.247	1	P	1	D
649	1,4,6-trichloronaphthalene	2437-54-9	-2.315	1	T	2	D
650	1,2,4-trichloronaphthalene	50402-51-2	-2.315	1	T	1	D
651	1,2,5-trichloronaphthalene	55720-33-7	-2.435	1	T	2	D
652	1,2,6-trichloronaphthalene	51570-44-6	-2.619	1	T	1	D
653	1,2,7-trichloronaphthalene	55720-34-8	-2.562	1	P	2	D
654	1,6,7-trichloronaphthalene	55720-39-3	-2.562	1	P	1	D
655	1,4,5-trichloronaphthalene	2437-55-0	-2.745	1	T	2	D
656	1,2,3,4-tetrachloronaphthalene	20020-02-4	-2.58	4	T	1	M
657	1,2,3,5-tetrachloronaphthalene	53555-63-8	-2.51	4	T	2	M
658	1,3,5,7-tetrachloronaphthalene	53555-64-9	-2.19	1	P	1	D
659	1,3,5,8-tetrachloronaphthalene	31604-28-1	-2.52	4	P	2	D
660	1,4,6,7-tetrachloronaphthalene	55720-43-9	-2.44	4	T	1	M
661	1,2,4,6-tetrachloronaphthalene	51570-45-7	-2.287	1	T	2	D
662	1,2,4,7-tetrachloronaphthalene	67922-21-8	-2.287	1	T	1	D
663	1,2,5,7-tetrachloronaphthalene	67922-23-0	-2.287	1	T	2	D
664	1,2,5,6-tetrachloronaphthalene	67922-22-9	-2.393	1	P	1	D
665	1,3,6,8-tetrachloronaphthalene	150224-15-0	-2.393	1	T	2	D
666	1,2,4,5-tetrachloronaphthalene	6733-54-6	-2.574	1	T	1	D
667	1,2,4,8-tetrachloronaphthalene	6529-87-9	-2.652	1	T	2	D
668	1,2,5,8-tetrachloronaphthalene	149864-80-2	-2.744	1	T	1	D
669	1,2,6,8-tetrachloronaphthalene	67922-24-1	-2.744	1	P	2	D
670	1,4,5,8-tetrachloronaphthalene	3432-57-3	-2.944	1	P	1	D
671	1,2,3,4,6-pentachloronaphthalene	67922-26-3	-2.38	1	T	2	D
672	1,2,3,5,8-pentachloronaphthalene	150224-24-1	-2.67	1	T	1	M
673	1,2,3,5,7-pentachloronaphthalene	53555-65-0	-2.233	1	T	2	D
674	1,2,4,6,7-pentachloronaphthalene	150224-17-2	-2.233	1	T	1	D
675	1,2,4,5,7-pentachloronaphthalene	150224-19-4	-2.344	1	T	2	D
676	1,2,4,6,8-pentachloronaphthalene	150224-22-9	-2.400	1	T	1	D
677	1,2,4,5,6-pentachloronaphthalene	150224-20-7	-2.537	1	T	2	D
678	1,2,4,7,8-pentachloronaphthalene	150224-21-8	-2.632	1	P	1	D
679	1,2,4,5,8-pentachloronaphthalene	150224-25-2	-2.814	1	T	2	D
680	1,2,3,4,6,7-hexachloronaphthalene	103426-96-6	-3.03	4	T	1	M
681	1,2,3,5,7,8-hexachloronaphthalene	103426-94-4	-3.02	1	T	2	D
682	1,2,3,5,6,7-hexachloronaphthalene	103426-97-7	-2.798	1	T	1	D
683	1,2,3,4,5,7-hexachloronaphthalene	67922-27-4	-2.968	1	T	2	D
684	1,2,3,5,6,8-hexachloronaphthalene	103426-95-5	-2.968	1	T	1	D

685	1,2,4,5,6,8-hexachloronaphthalene	90948-28-0	-3.044	1	T	2	D
686	1,2,4,5,7,8-hexachloronaphthalene	103426-92-2	-3.044	1	T	1	D
687	1,2,3,4,5,6-hexachloronaphthalene	58877-88-6	-3.284	1	T	2	D
688	1,2,3,4,5,8-hexachloronaphthalene	103426-93-3	-3.365	1	T	1	D
689	1,2,3,4,5,6,7-heptachloronaphthalene	58863-14-2	-3.95	1	T	2	D
690	1,2,3,4,5,6,8-heptachloronaphthalene	58863-15-3	-3.77	1	T	1	D
691	octachloronaphthalene	2234-13-1	-3.48	1	T	2	D
692	1-bromonaphthalene	90-11-9	-1.93	2	T	1	D
693	2-bromonaphthalene	580-13-2	-2.03	2	T	2	D
694	1,4-dibromonaphthalene	83-53-4	-2.16	2	T	1	M
695	methanol	67-56-1	-3.747	1	T	2	O
696	ethanol	64-17-5	-3.62	1	T	1	D
697	1-propanol	71-23-8	-3.519	1	P	2	D
698	1-butanol	71-36-3	-3.394	1	T	1	D
699	1-pentanol	71-41-0	-3.27	1	T	2	D
700	1-hexanol	111-27-3	-3.155	1	P	1	O
701	1-heptanol	111-70-6	-3.09	1	T	2	D
702	1-octanol	111-87-5	-3	1	T	1	O
703	1-nonanol	143-08-8	-2.85	1	T	2	D
704	1-decanol	112-30-1	-2.67	1	T	1	D
705	1-undecanol	112-42-5	-2.466	2	P	2	M
706	1-dodecanol	112-53-8	-2.576	2	T	1	M
707	1-tridecanol	112-70-9	-2.12	2	T	2	M
708	1-tetradecanol	112-72-1	-2.184	2	P	1	M
709	1-hexadecanol	36653-82-4	-2.06	2	T	2	M
710	1-octadecanol	112-92-5	-1.44	2	T	1	D
711	isobutyl alcohol	78-83-1	-3.315	1	P	2	D
712	2-methyl-1-butanol	137-32-6	-3.239	1	P	1	D
713	isopentanol	123-51-3	-3.24	1	T	2	D
714	2-methyl-1-pentanol	105-30-6	-2.88	1	T	1	D
715	2-ethyl-1-butanol	97-95-0	-3.07	2	T	2	M
716	2,3-dimethylbutanol	54206-54-1	-2.87	1	T	1	D
717	2-ethyl-1-hexanol	104-76-7	-2.73	2	T	2	M
718	2,2-dimethyl-1-propanol	75-84-3	-2.854	2	T	1	M
719	3,5,5-trimethylhexanol	3452-97-9	-2.1	2	T	2	M
720	allyl alcohol	107-18-6	-3.69	1	T	1	D
721	citronellol	106-22-9	-3.14	2	P	2	M
722	trans-phytol	150-86-7	-1.404	1	T	1	D
723	codlemone	33956-49-9	-3.62	2	T	2	M
724	(E,Z)-octadeca-3,13-dien-1-ol	66410-28-4	-2.77	2	P	1	D
725	geraniol	106-24-1	-3.82	2	T	2	M
726	isopropanol	67-63-0	-3.48	1	T	1	D
727	2-butanol	78-92-2	-3.37	1	P	2	O
728	2-pentanol	6032-29-7	-3.218	1	T	1	D
729	3-pentanol	584-02-1	-3.19	1	P	2	D
730	3-methyl-2-butanol	598-75-4	-3.13	2	T	1	D
731	2-hexanol	626-93-7	-3.06	2	T	2	M
732	3-hexanol	623-37-0	-2.98	1	T	1	D
733	4-methyl-2-pentanol	108-11-2	-2.74	1	T	2	D
734	2-methyl-3-pentanol	565-67-3	-2.85	1	T	1	D
735	2-heptanol	543-49-7	-2.863	2	T	2	M
736	3-heptanol	589-82-2	-2.91	2	P	1	D
737	4-heptanol	589-55-9	-2.94	1	T	2	D
738	2,4-dimethyl-3-pentanol	600-36-2	-2.61	2	T	1	M
739	2-octanol	123-96-6	-2.82	2	T	2	D
740	3-octanol	589-98-0	-2.78	2	T	1	M

741	4-octanol	589-62-8	-2.743	2	T	2	D
742	2-nonanol	628-99-9	-2.7	2	T	1	D
743	3-nonanol	624-51-1	-2.56	2	P	2	M
744	2,6-dimethyl-4-heptanol	108-82-7	-2.63	2	T	1	D
745	cyclopentanol	96-41-3	-4.03	1	T	2	D
746	cyclohexanol	108-93-0	-4.01	1	T	1	D
747	cycloheptanol	502-41-0	-4	1	T	2	D
748	2-methylcyclohexanol	583-59-5	-3.51	1	P	1	D
749	3-methylcyclohexanol	591-23-1	-3.82	1	T	2	D
750	4-methylcyclohexanol	589-91-3	-3.8	2	T	1	D
751	menthol	1490-04-6	-2.89	2	T	2	D
752	cyclododecanol	1724-39-6	-3.92	1	P	1	D
753	borneol	507-70-0	-3.04	2	T	2	M
754	fenchyl alcohol	1632-73-1	-2.94	2	T	1	O
755	1-octene-3-ol	3391-86-4	-2.9	1	T	2	D
756	tert-butanol	75-65-0	-3.3	1	T	1	O
757	2-methyl-2-butanol	75-85-4	-3.249	1	P	2	D
758	2-methyl-2-pentanol	590-36-3	-2.88	1	P	1	D
759	3-methyl-3-pentanol	77-74-7	-3.076	1	T	2	D
760	2-methyl-2-hexanol	625-23-0	-2.855	2	T	1	M
761	3-ethyl-3-pentanol	597-49-9	-2.873	2	T	2	D
762	2-methyl-2-heptanol	625-25-2	-2.694	2	T	1	M
763	2,3-dimethyl-2-butanol	594-60-5	-2.97	2	T	2	M
764	2-methylisoborneol	2371-42-8	-2.377	1	T	1	O
765	geosmin	19700-21-1	-2.268	1	T	2	O
766	2-methyl-3-butene-2-ol	115-18-4	-3.39	1	T	1	O
767	alpha-terpineol	98-55-5	-4.04	1	T	2	O
768	plinol	11039-70-6	-3.076	2	T	1	O
769	linalool	78-70-6	-3.06	1	P	2	D
770	nerolidol	7212-44-4	-2.76	2	T	1	D
771	2-methyl-3-butyn-2-ol	115-19-5	-3.8	1	T	2	D
772	methyl pentynol	77-75-8	-3.51	2	T	1	D
773	ethylene glycol	107-21-1	-7.21	3	T	2	O
774	1,3-propanediol	504-63-2	-7.09	1	T	1	O
775	1,4-butanediol	110-63-4	-7.94	2	T	2	D
776	1,5-pentanediol	111-29-5	-8.24	2	T	1	D
777	2,3-butanediol	513-85-9	-6.44	2	P	2	D
778	2,4-pentanediol	625-69-4	-6.97	2	P	1	D
779	2,5-hexanediol	2935-44-6	-7.54	2	T	2	D
780	1,2-propanediol	57-55-6	-6.83	2	T	1	D
781	1,2-butanediol	584-03-2	-6.72	2	T	2	D
782	1,3-butanediol	107-88-0	-7.24	2	T	1	D
783	1,2-pentanediol	5343-92-0	-6.54	2	T	2	D
784	1,4-pentanediol	626-95-9	-7.76	2	T	1	D
785	1,2-hexanediol	6920-22-5	-6.62	2	T	2	D
786	2-ethyl-1,3-hexanediol	94-96-2	-5.6	2	T	1	M
787	glycerol	56-81-5	-10.07	2	T	2	D
788	erithrytol	149-32-6	-13.44	2	T	1	D
789	xylitol	87-99-0	-14.98	2	P	2	D
790	ribitol	488-81-3	-15.06	2	P	1	D
791	arabitol	2152-56-9	-15.22	2	T	2	D
792	sorbitol	50-70-4	-18.21	2	T	1	D
793	mannitol	69-65-8	-18.65	2	T	2	D
794	galacticol	608-66-2	-18.35	2	P	1	D
795	phenylmethanol	100-51-6	-4.86	1	T	2	D
796	2-phenylethanol	60-12-8	-4.98	1	P	1	D

797	3-phenylpropanol	122-97-4	-5.08	1	T	2	D
798	benzhydrol	91-01-0	-5.97	2	T	1	D
799	phenol	108-95-2	-4.77	1	P	2	O
800	m-cresol	108-39-4	-4.46	1	T	1	O
801	p-cresol	106-44-5	-4.5	1	P	2	D
802	o-cresol	95-48-7	-4.3	1	T	1	D
803	2,3-dimethylphenol	526-75-0	-4.52	1	T	2	D
804	2,4-dimethylphenol	105-67-9	-4.41	1	P	1	D
805	2,5-dimethylphenol	95-87-4	-4.34	1	P	2	D
806	2,6-dimethylphenol	576-26-1	-3.86	1	T	1	D
807	3,4-dimethylphenol	95-65-8	-4.77	1	T	2	D
808	3,5-dimethylphenol	108-68-9	-4.6	1	T	1	D
809	o-ethylphenol	90-00-6	-4.14	2	T	2	M
810	p-ethylphenol	123-07-9	-4.5	1	T	1	D
811	m-ethylphenol	620-17-7	-4.59	1	T	2	D
812	p-propylphenol	645-56-7	-4.33	1	T	1	D
813	p-nonylphenol[1]	104-40-5	-3.8	2	T	2	D
814	thymol	89-83-8	-3.82	2	T	1	M
815	2-sec-butylphenol	89-72-5	-3.47	2	T	2	D
816	carvacrol	499-75-2	-3.775	2	T	1	M
817	m-tert-butylphenol	585-34-2	-4.105	2	T	2	D
818	p-tert-butylphenol	98-54-4	-4.31	1	T	1	D
819	p-tert-octylphenol	140-66-9	-3.76	1	T	2	D
820	4-(3',5'-dimethyl-3'-heptyl)-phenol (+)		-3.86	1	T	1	D
821	4-(3',5'-dimethyl-3'-heptyl)-phenol (-)		-3.91	1	P	2	D
822	2-naphthol	135-19-3	-5.95	1	T	1	D
823	1,2-benzenediol	120-80-9	-7.01	2	T	2	M
824	1,3-benzenediol	108-46-3	-8.79	2	T	1	M
825	1,4-benzenediol	123-31-9	-8.8	2	T	2	M
826	2,3-dihydroxynaphthalene	92-44-4	-8.695	2	T	1	M
827	dimethyl ether	115-10-6	-1.4	1	T	2	D
828	methyl ethyl ether	540-67-0	-1.54	1	T	1	D
829	diethyl ether	60-29-7	-1.36	1	P	2	D
830	methyl propyl ether	557-17-5	-1.33	1	T	1	D
831	methyl n-butyl ether	628-28-4	-1.136	2	T	2	D
832	ethyl propyl ether	628-32-0	-1.33	1	T	1	D
833	di(n-propyl) ether	111-43-3	-1.022	1	P	2	O
834	ethyl butyl ether	628-81-9	-1.14	1	T	1	O
835	di-n-butyl ether	142-96-1	-0.735	1	T	2	O
836	methyl isopropyl ether	598-53-8	-1.47	1	T	1	D
837	sec-butyl methyl ether	6795-87-5	-1.22	2	T	2	D
838	methyl isobutyl ether	625-44-5	-1.044	2	P	1	D
839	diisopropyl ether	108-20-3	-1.143	1	T	2	O
840	diisobutyl ether	628-55-7	-0.62	4	P	1	M
841	diisopentyl ether	544-01-4	-0.2	2	T	2	D
842	methyl tert-butyl ether	1634-04-4	-1.256	1	T	1	O
843	ethyl tert-butyl ether	637-92-3	-1.174	1	T	2	D
844	methyl tert-amyl ether	994-05-8	-1.05	1	T	1	O
845	ethyl tert-amyl ether	919-94-8	-1.075	3	T	2	M
846	methyl tert-octyl ether	62108-41-2	-0.673	3	P	1	O
847	ethyl tert-octyl ether		-0.284	3	T	2	O
848	methyl vinyl ether	107-25-5	-0.71	2	T	1	M
849	ethyl vinyl ether	109-92-2	-0.7	2	T	2	M
850	butyl vinyl ether	111-34-2	-0.22	2	P	1	M
851	isobutyl vinyl ether	109-53-5	-0.82	2	T	2	M
852	divinyl ether	109-93-3	-0.483	2	T	1	M

853	dimethoxymethane	109-87-5	-2.35	1	T	2	D
854	dimethoxyethane	110-71-4	-3.55	1	T	1	D
855	diethoxymethane	462-95-3	-2.564	2	P	2	M
856	1,2-diethoxyethane	629-14-1	-2.59	1	P	1	D
857	1,2-dibutoxyethane	112-48-1	-2.8	2	T	2	M
858	1,1-diethoxyethane	105-57-7	-2.4	1	T	1	D
859	2,2-dimethoxypropane	77-76-9	-2.534	2	T	2	M
860	diethylene glycol dibutyl ether	112-73-2	-3.99	2	T	1	D
861	methoxybenzene	100-66-3	-1.86	1	T	2	D
862	ethoxybenzene	103-73-1	-1.63	1	T	1	D
863	benzyl methyl ether	538-86-3	-2.44	2	T	2	M
864	anethole	104-46-1	-2.4	2	P	1	M
865	diphenyl ether	101-84-8	-2.01	2	T	2	M
866	dibenzyl ether	103-50-4	-3.57	2	T	1	D
867	1,2-dimethoxybenzene	91-16-7	-3.287	2	T	2	M
868	etofenprox	80844-07-1	-5.26	2	T	1	D
869	ethylene oxide	75-21-8	-2.31	1	T	2	D
870	tetrahydrofuran	109-99-9	-2.54	1	T	1	D
871	tetrahydropyran	142-68-7	-2.29	1	P	2	D
872	propylene oxide	75-56-9	-2.38	2	T	1	M
873	1,2-butylene oxide	106-88-7	-2.13	2	P	2	M
874	2-methyltetrahydrofuran	96-47-9	-2.42	1	T	1	D
875	3-methyltetrahydropyran	26093-63-0	-2.09	2	T	2	M
876	2,5-dimethyltetrahydrofuran	1003-38-9	-2.14	1	T	1	D
877	1,2-epoxy-2-methylpropane	558-30-5	-1.85	2	T	2	M
878	alpha-pinene oxide	1686-14-2	-2.08	2	T	1	M
879	1,4-cineole	470-67-7	-2.11	1	P	2	O
880	1,8-cineole	470-82-6	-2.16	1	T	1	D
881	3,4-dihydropyran	110-87-2	-1.455	2	T	2	M
882	(+)-limonene oxide	1195-92-2	-2.58	2	T	1	M
883	1,3-dioxalane	646-06-0	-3	1	T	2	D
884	1,3-dioxane	505-22-6	-3.5	1	T	1	O
885	1,4-dioxane	123-91-1	-3.707	1	T	2	D
886	2-methyl-1,3-dioxolane	497-26-7	-3.293	2	T	1	M
887	2,2-dimethyl-1,3-dioxolane	2916-31-6	-3.073	2	P	2	M
888	1,3,5-trioxane	110-88-3	-3.3	2	T	1	M
889	paraldehyde	123-63-7	-2.54	2	P	2	M
890	metaldehyde	108-62-3	-2.68	2	T	1	D
891	furan	110-00-9	-0.62	3	T	2	M
892	2-methylfuran	534-22-5	-0.58	2	P	1	M
893	styrene oxide	96-09-3	-3.03	2	T	2	D
894	galaxolide	1222-05-5	-2.48	2	T	1	D
895	dibenzofuran	132-64-9	-2.44	2	T	2	M
896	dibenzo-p-dioxine	262-12-4	-2.34	2	T	1	D
897	glycidyl n-butyl ether	2426-08-6	-2.95	2	T	2	D
898	2-methoxy-2,3-dihydro-4H-pyran	4454-05-1	-2.38	2	T	1	M
899	allyl glycidyl ether	106-92-3	-3.71	2	P	2	M
900	(phenoxymethyl)-oxirane	122-60-1	-4.473	2	T	1	D
901	cinmethylin	87818-31-3	-4.5	2	T	2	D
902	diofenolan	63837-33-2	-5.57	2	T	1	D
903	bis(1,1-dimethylethyl)peroxide	110-05-4	0.08	2	T	2	M
904	methylhydroperoxide	3031-73-0	-3.88	1	T	1	O
905	ethylhydroperoxide	3031-74-1	-3.915	1	T	2	O
906	cumene hydroperoxide	80-15-9	-5.72	2	T	1	D
907	formaldehyde	50-00-0	-1.786	1	T	2	O

908	acetaldehyde	75-07-0	-2.56	1	T	1	O
909	propionaldehyde	123-38-6	-2.35	1	T	2	D
910	butyraldehyde	123-72-8	-2.328	1	T	1	O
911	pentanal	110-62-3	-2.222	1	P	2	O
912	hexanal	66-25-1	-2.06	1	T	1	O
913	heptanal	111-71-7	-1.959	1	T	2	O
914	octanal	124-13-0	-1.715	1	T	1	O
915	nonanal	124-19-6	-1.523	1	T	2	O
916	decanal	112-31-2	-1.3	1	P	1	D
917	isobutyraldehyde	78-84-2	-2.1	1	T	2	D
918	2-methylbutanal	96-17-3	-1.76	1	T	1	D
919	3-methyl-1-butanal	590-86-3	-1.94	2	T	2	M
920	2-ethylbutyraldehyde	97-96-1	-1.67	2	P	1	M
921	2-methylvaleraldehyde	123-15-9	-1.67	2	T	2	M
922	2-ethylhexanealdehyde	123-05-7	-1.38	2	T	1	M
923	acrolein	107-02-8	-2.79	1	T	2	D
924	trans-crotonaldehyde	123-73-9	-2.8	1	T	1	D
925	trans-2-hexenal	505-57-7	-2.54	1	T	2	D
926	cis-4-heptenal	6728-31-0	-2.336	1	T	1	O
927	2-heptenal	2463-63-0	-2.56	1	T	2	O
928	2-octenal	2363-89-5	-2.36	1	P	1	O
929	trans-2-nonenal	18829-56-6	-2.16	1	T	2	D
930	alpha-methylacrolein	78-85-3	-2.202	1	T	1	O
931	2-ethyl-2-hexenal	645-62-5	-2.04	2	T	2	M
932	2,4-hexadienal	142-83-6	-3.4	1	P	1	O
933	trans-2,cis-6-nonadienal	557-48-2	-2.357	1	P	2	O
934	citral	5392-40-5	-2.72	2	T	1	M
935	glyoxal	107-22-2	-6.866	1	T	2	D
936	glutaraldehyde	111-30-8	-5.87	1	T	1	D
937	benzaldehyde	100-52-7	-3.036	1	P	2	D
938	2-methylbenzaldehyde	529-20-4	-2.866	1	T	1	O
939	3-methylbenzaldehyde	620-23-5	-2.9	1	T	2	O
940	p-methylbenzaldehyde	104-87-0	-3.081	1	T	1	O
941	acetone	67-64-1	-2.77	1	T	2	O
942	2-butanone	78-93-3	-2.633	1	P	1	O
943	2-pentanone	107-87-9	-2.466	1	P	2	O
944	diethyl ketone	96-22-0	-2.5	1	T	1	D
945	methyl butyl ketone	591-78-6	-2.41	1	T	2	D
946	3-hexanone	589-38-8	-2.29	1	P	1	D
947	2-heptanone	110-43-0	-2.229	1	T	2	O
948	3-heptanone	106-35-4	-2.314	2	T	1	M
949	4-heptanone	123-19-3	-2.14	1	T	2	D
950	2-octanone	111-13-7	-2.114	1	T	1	O
951	3-octanone	106-68-3	-2.06	1	T	2	D
952	dibutyl ketone	502-56-7	-1.94	1	P	1	D
953	2-nonanone	821-55-6	-1.9	1	T	2	O
954	2-decanone	693-54-9	-1.72	1	T	1	D
955	2-undecanone	112-12-9	-1.585	1	T	2	O
956	6-undecanone	927-49-1	-1.85	2	T	1	D
957	methyl isopropyl ketone	563-80-4	-2.38	1	T	2	D
958	methyl isobutyl ketone	108-10-1	-2.39	1	T	1	D
959	3-methylpentan-2-one	565-61-7	-2.277	1	P	2	M
960	2-methyl-3-pentanone	565-69-5	-2.2	2	T	1	D
961	5-methyl-2-hexanone	110-12-3	-2.15	2	P	2	M
962	diisopropyl ketone	565-80-0	-2.01	1	T	1	D
963	5-methyl-3-heptanone	541-85-5	-2.09	2	T	2	M

964	2,6-dimethyl-4-heptanone	108-83-8	-1.873	2	T	1	M
965	3,3-dimethyl-2-butanone	75-97-8	-2.12	1	T	2	D
966	cyclopentanone	120-92-3	-3.315	1	T	1	O
967	cyclohexanone	108-94-1	-3.315	1	T	2	O
968	methyl cyclopropyl ketone	765-43-5	-3.38	1	P	1	D
969	2-methylcyclohexanone	583-60-8	-3	2	T	2	M
970	3-methylcyclohexanone	591-24-2	-3.22	2	P	1	M
971	4-methylcyclohexanone	589-92-4	-3.25	2	T	2	M
972	methyl cyclohexyl ketone	823-76-7	-2.86	1	T	1	D
973	menthone	89-80-5	-2.15	1	T	2	D
974	camphor	76-22-2	-2.9	2	T	1	M
975	methyl vinyl ketone	78-94-4	-3.002	1	T	2	O
976	mesityl oxide	141-79-7	-2.82	2	T	1	M
977	(R)-(+)-pulegone	89-82-7	-2.835	2	T	2	M
978	isophorone	78-59-1	-3.567	2	T	1	D
979	carvone	99-49-0	-3.08	1	P	2	D
980	beta-ionone	79-77-6	-2.47	2	T	1	O
981	2,3-butanedione	431-03-8	-3.39	1	T	2	D
982	acetylacetone	123-54-6	-3.85	2	T	1	D
983	acetophenone	98-86-2	-3.456	1	T	2	O
984	2'-methylacetophenone	577-16-2	-3.252	1	T	1	O
985	3'-methylacetophenone	585-74-0	-3.553	1	T	2	O
986	4-methylacetophenone	122-00-9	-3.45	1	P	1	D
987	propiophenone	93-55-0	-3.367	1	T	2	O
988	tonalide	1506-02-1	-2.29	2	P	1	D
989	9-fluorenone	486-25-9	-4.43	2	T	2	M
990	anthraquinone	84-65-1	-5	2	T	1	D
991	diphacinone	82-66-6	-8.2	2	T	2	D
992	1,4-benzoquinone	106-51-4	-4.71	2	T	1	M
993	methylglyoxal	78-98-8	-4.93	1	T	2	D
994	formic acid	64-18-6	-4.91	1	T	1	D
995	acetic acid	64-19-7	-5	1	T	2	O
996	propionic acid	79-09-4	-4.74	1	T	1	D
997	butyric acid	107-92-6	-4.66	1	T	2	D
998	n-valeric acid	109-52-4	-4.715	1	T	1	D
999	n-hexanoic acid	142-62-1	-4.531	1	P	2	O
1000	n-heptanoic acid	111-14-8	-4.52	1	P	1	D
1001	caprylic acid	124-07-2	-4.44	1	T	2	D
1002	pelargonic acid	112-05-0	-4.18	2	T	1	D
1003	decanoic acid	334-48-5	-4.26	2	T	2	D
1004	isobutyric acid	79-31-2	-4.442	1	T	1	O
1005	isovaleric acid	503-74-2	-4.468	1	T	2	O
1006	2-methylbutanoic acid	116-53-0	-4.22	2	P	1	D
1007	2-ethylbutyric acid	88-09-5	-4.18	2	T	2	D
1008	2-ethylhexanoic acid	149-57-5	-3.736	2	T	1	D
1009	2,2-dimethylpropionic acid	75-98-9	-3.944	1	T	2	D
1010	acrylic acid	79-10-7	-4.89	1	T	1	D
1011	trans-crotonic acid	107-93-7	-4.757	2	T	2	M
1012	methacrylic acid	79-41-4	-4.8	1	P	1	O
1013	sorbic acid	110-44-1	-6	2	T	2	D
1014	oxalic acid	144-62-7	-8.23	1	T	1	D
1015	malonic acid	141-82-2	-10.16	2	T	2	M
1016	succinic acid	110-15-6	-10.67	2	T	1	M
1017	glutaric acid	110-94-1	-10.67	1	P	2	D
1018	adipic acid	124-04-9	-11.15	2	T	1	M
1019	pimelic acid	111-16-0	-10.5	2	T	2	O

1020	suberic acid	505-48-6	-10.35	2	P	1	O
1021	dodecanedioic acid	693-23-2	-9.39	2	T	2	M
1022	benzoic acid	65-85-0	-5.54	1	T	1	D
1023	1-naphthylacetic acid	86-87-3	-6.95	2	T	2	M
1024	peroxyformic acid	107-32-4	-4.45	1	T	1	D
1025	peroxyacetic acid	79-21-0	-4.4	1	T	2	O
1026	methyl formate	107-31-3	-2.04	1	T	1	D
1027	ethyl formate	109-94-4	-1.94	1	T	2	D
1028	methyl acetate	79-20-9	-2.328	1	P	1	O
1029	propyl formate	110-74-7	-1.82	1	P	2	D
1030	ethyl acetate	141-78-6	-2.19	1	T	1	D
1031	methyl propionate	554-12-1	-2.18	1	T	2	D
1032	butyl formate	592-84-7	-1.68	2	P	1	M
1033	methyl butyrate	623-42-7	-2.076	1	T	2	O
1034	n-propyl acetate	109-60-4	-2.05	1	P	1	O
1035	ethyl propionate	105-37-3	-2.05	1	T	2	D
1036	n-butyl acetate	123-86-4	-1.94	1	T	1	O
1037	propyl propionate	106-36-5	-1.86	1	T	2	D
1038	methyl valerate	624-24-8	-1.886	1	T	1	O
1039	ethyl butyrate	105-54-4	-1.86	1	T	2	D
1040	methyl hexanoate	106-70-7	-1.824	1	T	1	O
1041	n-amyl acetate	628-63-7	-1.838	1	T	2	O
1042	n-butyl propionate	590-01-2	-1.7	2	T	1	M
1043	ethyl valerate	539-82-2	-1.85	1	P	2	D
1044	n-propyl butyrate	105-66-8	-1.67	1	T	1	D
1045	n-hexyl acetate	142-92-7	-1.664	1	T	2	D
1046	butyl butyrate	109-21-7	-1.55	2	P	1	D
1047	amyl propionate	624-54-4	-1.55	1	T	2	D
1048	ethyl hexanoate	123-66-0	-1.64	1	T	1	D
1049	methyl octanoate	111-11-5	-1.495	1	T	2	O
1050	ethyl heptanoate	106-30-9	-1.69	1	T	1	D
1051	ethyl octanoate	106-32-1	-1.44	1	P	2	D
1052	methyl decanoate	110-42-9	-1.44	1	T	1	D
1053	ethyl decanoate	110-38-3	-1.54	1	T	2	D
1054	methyl laurate	111-82-0	-1.215	2	T	1	M
1055	isopropyl formate	625-55-8	-1.48	1	T	2	D
1056	isobutyl formate	542-55-2	-1.63	1	T	1	D
1057	isopropyl acetate	108-21-4	-1.944	1	T	2	D
1058	isoamyl formate	110-45-2	-1.56	1	T	1	D
1059	sec-butyl acetate	105-46-4	-1.64	2	T	2	M
1060	isopropyl propionate	637-78-5	-1.63	1	P	1	D
1061	isobutyl acetate	110-19-0	-1.73	1	T	2	D
1062	2-pentanol acetate	626-38-0	-1.5	2	T	1	M
1063	3-methylbutanoic acid ethyl ester	108-64-5	-1.69	2	T	2	D
1064	isoamyl acetate	123-92-2	-1.62	1	T	1	D
1065	2-methylpropyl propanoate	540-42-1	-1.574	2	T	2	D
1066	2-methylbutanoic acid ethyl ester	7452-79-1	-1.34	1	T	1	D
1067	isobutyl isobutyrate	97-85-8	-1.47	2	P	2	D
1068	4-methyl-2-pentyl acetate	108-84-9	-1.5	2	P	1	M
1069	2-ethylhexyl acetate	103-09-3	-1.93	2	T	2	D
1070	tert-butyl formate	762-75-4	-1.55	1	T	1	O
1071	tert-butyl acetate	540-88-5	-1.54	2	T	2	M
1072	methyl trimethylacetate	598-98-1	-1.76	1	T	1	D
1073	tert-amyl ethanoate	625-16-1	-1.31	2	P	2	M
1074	tert-butyl propionate	20487-40-5	-1.27	1	T	1	D
1075	beta-propiolactone	57-57-8	-4.51	2	T	2	M

1076	pentadecalactone	106-02-5	-1.56	2	T	1	D
1077	methyl cyclopropylcarboxylate	2868-37-3	-3.01	1	T	2	D
1078	methyl cyclohexylcarboxylate	4630-82-4	-2.42	1	T	1	D
1079	cyclohexyl acetate	622-45-7	-2.42	2	P	2	M
1080	gamma-nonalactone	104-61-0	-4.54	2	P	1	M
1081	cyclohexyl butyrate	1551-44-6	-2.82	2	T	2	M
1082	methyl acrylate	96-33-3	-2.09	2	T	1	D
1083	vinyl acetate	108-05-4	-1.685	1	T	2	O
1084	ethyl acrylate	140-88-5	-1.86	2	P	1	D
1085	allyl acetate	591-87-7	-2.15	2	T	2	D
1086	butyl acrylate	141-32-2	-1.72	2	T	1	D
1087	(E)-3-hexenyl ethanoate	3681-82-1	-1.91	1	T	2	D
1088	(Z)-3-hexenyl ethanoate	3681-71-8	-1.89	1	T	1	D
1089	methyl oleate	112-62-9	-1.56	2	P	2	M
1090	methyl methacrylate	80-62-6	-1.88	2	P	1	M
1091	ethyl methacrylate	97-63-2	-1.78	2	T	2	M
1092	isobutyl acrylate	106-63-8	-1.51	2	T	1	D
1093	butyl methacrylate	97-88-1	-1.53	2	T	2	M
1094	isobutyl methacrylate	97-86-9	-1.67	2	T	1	D
1095	2-ethylhexyl acrylate	103-11-7	-1.3	2	T	2	M
1096	dodeca-7,9-dienyl acetate	54364-62-4	-1.47	2	T	1	D
1097	(Z,E)-tetradeca-9,12-dienyl acetate	30507-70-1	-2.62	2	T	2	D
1098	gossyplure	50933-33-0	-1.9	2	T	1	D
1099	allyl methacrylate	96-05-9	-2.008	2	P	2	M
1100	hydroprene	41096-46-2	-2.1	2	T	1	M
1101	kinoprene	42588-37-4	-2.65	2	P	2	M
1102	empenthrin	54406-48-3	-1.85	2	T	1	M
1103	methyl oxalate	553-90-2	-3.92	2	T	2	D
1104	dimethyl malonate	108-59-8	-4.991	1	T	1	O
1105	ethyl oxalate	95-92-1	-4.03	2	T	2	M
1106	dimethyl succinate	106-65-0	-4.866	1	T	1	O
1107	ethylene glycol diacetate	111-55-7	-4.78	2	T	2	M
1108	malonic acid diethyl ester	105-53-3	-4.22	2	T	1	M
1109	dimethyl adipate	627-93-0	-5.03	2	T	2	M
1110	ethyl succinate	123-25-1	-4.66	2	T	1	M
1111	diethyl glutarate	818-38-2	-4.62	2	P	2	M
1112	diethyl adipate	141-28-6	-4.65	2	P	1	M
1113	diethyl pimelate	2050-20-6	-4.73	2	P	2	D
1114	dimethyl sebacate	106-79-6	-4.64	2	T	1	M
1115	dioctyl adipate	123-79-5	-4.29	2	T	2	D
1116	methyl maleate	624-48-6	-4.54	2	T	1	D
1117	dibutyl maleate	105-76-0	-4.355	2	P	2	M
1118	glyceryl triacetate	102-76-1	-6.47	2	T	1	M
1119	benzyl formate	104-57-4	-3.08	2	T	2	M
1120	methyl benzoate	93-58-3	-2.88	1	P	1	D
1121	ethyl benzoate	93-89-0	-2.67	1	T	2	D
1122	benzyl acetate	140-11-4	-3.34	2	T	1	D
1123	butyl benzoate	136-60-7	-2.4	2	T	2	M
1124	ethyl cinnamate	103-36-6	-3.76	2	T	1	M
1125	coumarin	91-64-5	-5.34	2	T	2	M
1126	benzyl benzoate	120-51-4	-4.01	2	P	1	D
1127	dimethyl terephthalate	120-61-6	-4.75	2	T	2	M
1128	dimethyl phthalate	131-11-3	-5.3	2	T	1	D
1129	diethyl phthalate	84-66-2	-5.13	2	T	2	M
1130	dipropyl phthalate	131-16-8	-4.74	2	T	1	M
1131	dibutyl phthalate	84-74-2	-4.36	1	P	2	D

1132	dihexyl phthalate	84-75-3	-3.87	2	T	1	M
1133	dioctyl phthalate	117-84-0	-3.63	2	T	2	M
1134	diisooctyl phthalate	27554-26-3	-3.84	2	T	1	M
1135	di(2-ethylhexyl) phthalate	117-81-7	-3.57	2	T	2	M
1136	di(2-ethylhexyl) terephthalate	6422-86-2	-2.67	2	T	1	M
1137	diisodecyl phthalate	26761-40-0	-2.14	2	P	2	M
1138	dicyclohexyl phthalate	84-61-7	-5.41	2	T	1	M
1139	spiromesifen	283594-90-1	-4.94	2	T	2	D
1140	diallyl phthalate	131-17-9	-4.803	1	T	1	D
1141	benzyl butyl phthalate	85-68-7	-5.39	1	P	2	M
1142	dimethyl carbonate	616-38-6	-2.7	2	T	1	M
1143	diethyl carbonate	105-58-8	-2.43	2	P	2	M
1144	propylene carbonate	108-32-7	-5.54	1	T	1	D
1145	diphenyl carbonate	102-09-0	-3.72	2	T	2	M
1146	acetic anhydride	108-24-7	-3.63	2	T	1	D
1147	maleic anhydride	108-31-6	-5.71	2	T	2	M
1148	phthalic anhydride	85-44-9	-6.16	2	T	1	M
1149	benzoyl peroxide	94-36-0	-4.17	2	T	2	M
1150	acetylsalicylic acid	50-78-2	-7.275	2	T	1	D
1151	hydroxymethyl hydroperoxide	15932-89-5	-6.96	1	T	2	O
1152	bis(hydroxymethyl)peroxide	17088-73-2	-7.03	1	T	1	O
1153	2-methoxyethanol	109-86-4	-4.87	1	T	2	D
1154	2-ethoxyethanol	110-80-5	-4.716	1	T	1	D
1155	2-propoxyethanol	2807-30-9	-4.7	1	T	2	D
1156	2-butoxyethanol	111-76-2	-4.184	1	T	1	D
1157	2-hexyloxyethanol	112-25-4	-3.91	2	T	2	D
1158	2-isopropoxyethanol	109-59-1	-4.425	1	P	1	D
1159	arbanol	7070-15-7	-3.43	2	T	2	O
1160	diethylene glycol mono-n-butylether	112-34-5	-6.531	1	P	1	D
1161	2-2-(hexyloxy)ethoxyethanol	112-59-4	-5.09	2	T	2	D
1162	1-methoxy-2-propanol	107-98-2	-4.425	1	T	1	D
1163	1-butoxy-2-propanol	5131-66-8	-3.73	2	P	2	M
1164	2-phenoxyethanol	122-99-6	-4.88	2	P	1	M
1165	ethylene glycol monobenzyl ether	622-08-2	-5.306	2	T	2	D
1166	2-methoxyphenol	90-05-1	-4.09	1	P	1	D
1167	3-methoxyphenol	150-19-6	-5.625	1	T	2	D
1168	4-methyl-2-methoxyphenol	93-51-6	-4.25	1	T	1	D
1169	eugenol	97-53-0	-4.1	2	T	2	M
1170	2,6-dimethoxyphenol	91-10-1	-5.09	1	T	1	D
1171	glycolaldehyde	141-46-8	-5.001	1	T	2	O
1172	salicylaldehyde	90-02-8	-3.14	2	T	1	M
1173	3-hydroxybenzaldehyde	100-83-4	-6.99	1	T	2	D
1174	4-hydroxybenzaldehyde	123-08-0	-7.68	1	T	1	D
1175	vanillin	121-33-5	-6.4	2	T	2	M
1176	ethylvanillin	121-32-4	-6.12	2	T	1	M
1177	hydroxyacetone	116-09-6	-5.287	1	T	2	D
1178	2'-hydroxyacetophenone	118-93-4	-3.387	1	T	1	O
1179	2-hydroxyanthraquinone	605-32-3	-9.05	2	T	2	D
1180	1-hydroxyanthraquinone	129-43-1	-6.52	2	P	1	D
1181	1,4-dihydroxyanthraquinone	81-64-1	-5.486	2	T	2	D
1182	glycolic acid	79-14-1	-7.68	2	T	1	M
1183	malic acid	6915-15-7	-11.83	2	T	2	D
1184	salicylic acid	69-72-7	-6.27	2	T	1	M
1185	trinexapac	104273-73-6	-9.79	2	T	2	M
1186	2-hydroxy-1-methylethyl laurate	107328-11-0	-4.81	2	T	1	D
1187	2-hydroxyethyl methacrylate	868-77-9	-5.055	2	T	2	D

1188	butyl lactate	138-22-7	-4	2	T	1	M
1189	2-hydroxypropyl laurate	142-55-2	-2.37	2	P	2	D
1190	coumatetralyl	5836-29-3	-10.19	1	T	1	D
1191	methyl salicylate	119-36-8	-3.39	2	T	2	M
1192	4-hydroxy methyl benzoate	99-76-3	-6.98	2	P	1	M
1193	ethylparaben	120-47-8	-6.64	2	T	2	M
1194	propylparaben	94-13-3	-6.63	2	T	1	M
1195	butylparaben	94-26-8	-6.21	2	T	2	M
1196	milbemectin A3	51596-10-2	-12.06	2	T	1	M
1197	milbemectin A4	51596-11-3	-10.281	2	P	2	D
1198	trinexapac-ethyl	95266-40-3	-6.66	1	P	1	D
1199	warfarin	81-81-2	-8	2	T	2	D
1200	gibberelic acid	77-06-5	-10.53	2	T	1	M
1201	2-methoxybenzaldehyde	135-02-4	-4.367	1	T	2	O
1202	3-methoxybenzaldehyde	591-31-1	-4.066	1	T	1	O
1203	4-methoxybenzaldehyde	123-11-5	-4.77	1	T	2	O
1204	furfural	98-01-1	-3.61	2	T	1	M
1205	5-methylfurfural	620-02-0	-4.07	2	P	2	M
1206	4-methoxy-4-methylpentan-2-one	107-70-0	-4.13	2	P	1	D
1207	2'-methoxyacetophenone	579-74-8	-4.602	1	T	2	O
1208	3'-methoxyacetophenone	586-37-8	-4.638	1	T	1	O
1209	4-methoxyacetophenone	100-06-1	-4.68	1	T	2	O
1210	2-naphthyloxyacetic acid	120-23-0	-8.935	2	T	1	D
1211	endothal	145-73-3	-13.72	2	T	2	D
1212	methyl methoxy acetate	6290-49-9	-3.9	1	T	1	O
1213	2-methoxyethyl acetate	110-49-6	-4.05	1	T	2	O
1214	2-ethoxyethanol acetate	111-15-9	-3.883	1	P	1	D
1215	(2-butoxyethyl)acetate	112-07-2	-3.651	1	P	2	D
1216	propylene glycol methyl ether acetate	108-65-6	-3.77	2	T	1	D
1217	methoprene	40596-69-8	-3.56	2	P	2	D
1218	S-methoprene	65733-16-6	-3.58	2	T	1	D
1219	2-(2-butoxyethoxy)ethanol acetate	124-17-4	-4.97	2	T	2	D
1220	phenothrin	26002-80-2	-5.54	1	T	1	D
1221	dipropylene glycol dibenzoate	27138-31-4	-6.25	2	T	2	D
1222	resmethrin	10453-86-8	-4.86	2	T	1	D
1223	glyoxylic acid	298-12-4	-5.44	1	T	2	D
1224	pyruvic acid	127-17-3	-6.881	1	T	1	O
1225	methyl acetoacetate	105-45-3	-4.35	1	T	2	O
1226	ethyl acetoacetate	141-97-9	-4.32	1	T	1	O
1227	n-propyl dihydrojasmonate	158474-72-7	-4.54	2	T	2	D
1228	allyl acetoacetate	1118-84-9	-4.49	2	P	1	D
1229	allethrin	584-79-2	-5.17	2	T	2	D
1230	acequinocyl	57960-19-7	-4.45	2	T	1	D
1231	2-fluoroethanol	371-62-0	-2.9	1	T	2	O
1232	2,2-difluoroethanol	359-13-7	-3.19	1	T	1	O
1233	2,2,2-trifluoroethanol	75-89-8	-3.07	1	T	2	O
1234	2,2,3,3-tetrafluoropropanol	76-37-9	-3.535	1	T	1	O
1235	pentafluoro-1-propanol	422-05-9	-2.555	1	P	2	O
1236	2-(perfluorobutyl)ethanol	2043-47-2	-1.52	1	T	1	O
1237	2-(perfluorohexyl)ethanol	647-42-7	-0.84	2	T	2	M
1238	2-(perfluorooctyl)ethanol	678-39-7	-0.53	1	T	1	O
1239	2-chloroethanol	107-07-3	-4.27	4	P	2	M
1240	3-chloro-1-propanol	627-30-5	-4.51	2	T	1	M
1241	2,2-dichloroethanol	598-38-9	-2.79	1	T	2	O
1242	2,2,2-trichloroethanol	115-20-8	-3.86	2	T	1	M

1243	3-bromopropanol	627-18-9	-5.08	2	P	2	M
1244	1,1,1-trifluoro-2-propanol	374-01-6	-3.05	1	P	1	D
1245	1,1,1,3,3,3-hexafluoropropan-2-ol	920-66-1	-2.76	1	T	2	D
1246	1,3-dichloro-2-propanol	96-23-1	-4.33	2	T	1	M
1247	chloral hydrate	302-17-0	-6.93	1	T	2	M
1248	dicofol	115-32-2	-5.22	2	T	1	M
1249	2-fluorophenol	367-12-4	-3.88	1	P	2	D
1250	4-fluorophenol	371-41-5	-4.54	1	T	1	D
1251	2-chlorophenol	95-57-8	-3.34	1	T	2	D
1252	3-chlorophenol	108-43-0	-4.85	1	T	1	D
1253	4-chlorophenol	106-48-9	-5.16	1	T	2	D
1254	2-methyl-4-chlorophenol	1570-64-5	-4.35	2	T	1	D
1255	3-methyl-4-chlorophenol	59-50-7	-4.98	1	T	2	D
1256	2,4-dichlorophenol	120-83-2	-3.74	1	T	1	D
1257	2,6-dichlorophenol	87-65-0	-3.36	2	T	2	D
1258	3,5-dichlorophenol	591-35-5	-4.86	2	T	1	D
1259	2,3-dichlorophenol	576-24-9	-3.39	2	P	2	M
1260	2,3,5-trichlorophenol	933-78-8	-3.52	2	T	1	M
1261	2,4,5-trichlorophenol	95-95-4	-3.21	1	T	2	D
1262	2,4,6-trichlorophenol	88-06-2	-3.3	2	T	1	D
1263	2,3,4,6-tetrachlorophenol	58-90-2	-3.54	2	P	2	M
1264	pentachlorophenol	87-86-5	-3.809	2	P	1	D
1265	p-bromophenol	106-41-2	-5.23	1	T	2	D
1266	2-iodophenol	533-58-4	-4.55	1	T	1	D
1267	4-iodophenol	540-38-5	-5.33	2	T	2	M
1268	4,5-dichlorocatechol	3428-24-8	-6.5	2	T	1	D
1269	3,4,5-trichlorocatechol	56961-20-7	-5.78	2	P	2	O
1270	tetrachlorocatechol	1198-55-6	-4.85	2	T	1	D
1271	dichlorophen	97-23-4	-10.33	2	T	2	M
1272	tetrabromobisphenol A	79-94-7	-8.16	2	T	1	M
1273	1,1-difluoro-2-methoxyethane	461-57-4	-1.507	2	P	2	M
1274	3-ethoxyperfluoro(2-methylhexane)	297730-93-9	4.33	1	T	1	D
1275	bis(chloromethyl)ether	542-88-1	-2	2	P	2	M
1276	2,2'-dichloroethylether	111-44-4	-2.29	1	T	1	D
1277	ethrane	13838-16-9	-0.36	1	T	2	D
1278	isofluorane	26675-46-7	0.07	1	T	1	D
1279	2-(chlorofluoromethoxy)-1,1,1,2-tetrafluoroethane	56885-28-0	0.27	1	T	2	D
1280	2-[chloro(difluoro)methoxy]-1,1,1-trifluoroethane	33018-78-9	1.37	1	T	1	D
1281	methoxyfluorane	76-38-0	-0.82	1	T	2	D
1282	sevoflurane	28523-86-6	0.44	1	T	1	D
1283	dichloroisopropyl ether	108-60-1	-2.21	1	P	2	O
1284	fluoroxene	406-90-6	-0.1	1	T	1	D
1285	2-chloroethyl vinyl ether	110-75-8	-1.48	2	T	2	M
1286	1,2-bis(2-chloroethoxy)ethane	112-26-5	-4.32	2	T	1	D
1287	ethane, 2-chloro-1,1-dimethoxy-	97-97-2	-2.9	2	T	2	D
1288	2-chloroanisole	766-51-8	-2.42	2	T	1	M
1289	3-chloroanisole	2845-89-8	-2.06	2	T	2	O
1290	4-chloroanisole	623-12-1	-2.13	2	T	1	O
1291	2,3-dichloroanisole	1984-59-4	-1.75	2	P	2	O
1292	2,4-dichloroanisole	553-82-2	-1.48	2	P	1	O
1293	2,5-dichloroanisole	1984-58-3	-1.72	2	T	2	O
1294	2,6-dichloroanisole	1984-65-2	-1.34	2	T	1	O
1295	3,4-dichloroanisole	36404-30-5	-1.53	2	T	2	O
1296	3,5-dichloroanisole	33719-74-3	-0.97	2	T	1	O

1297	2,3,4-trichloroanisole	54135-80-7	-1.52	2	T	2	O
1298	2,3,5-trichloroanisole	54135-81-8	-1.27	2	T	1	O
1299	2,4,5-trichloroanisole	6130-75-2	-1.42	2	P	2	O
1300	2,4,6-trichloroanisole	87-40-1	-1.05	1	T	1	O
1301	2,3,6-trichloroanisole	50375-10-5	-1.42	1	T	2	O
1302	3,4,5-trichloroanisole	54135-82-9	-1.28	2	T	1	O
1303	2,3,4,5-tetrachloroanisole	938-86-3	-1.21	2	T	2	O
1304	2,3,4,6-tetrachloroanisole	938-22-7	-1.13	2	P	1	O
1305	2,3,5,6-tetrachloroanisole	6936-40-9	-0.89	2	T	2	O
1306	pentachloroanisole	1825-21-4	-0.97	2	T	1	O
1307	2-bromoanisole	578-57-4	-1.86	2	T	2	O
1308	3-bromoanisole	2398-37-0	-1.39	2	T	1	O
1309	4-bromoanisole	104-92-7	-1.42	2	T	2	O
1310	2,4-dibromoanisole	21702-84-1	-2.29	2	T	1	O
1311	2,6-dibromoanisole	38603-09-7	-1.95	2	T	2	O
1312	2,3,4-tribromoanisole	95970-13-1	-1.39	4	T	1	O
1313	2,3,6-tribromoanisole	95970-19-7	-1.37	4	T	2	O
1314	2,4,6-tribromoanisole	607-99-8	-1.68	1	T	1	O
1315	pentabromoanisole	1825-26-9	-3.44	2	P	2	O
1316	2-bromo-4-chloroanisole	60633-25-2	-1.65	2	P	1	O
1317	2-bromo-6-chloroanisole	174913-10-1	-1.53	4	T	2	O
1318	4-bromo-2-chloroanisole	50438-47-6	-1.5	4	T	1	O
1319	2-bromo-3,5-dichloroanisole		-1.44	4	T	2	O
1320	2-bromo-3,6-dichloroanisole		-1.25	1	P	1	O
1321	2-bromo-4,6-dichloroanisole	60633-26-3	-1.28	1	T	2	O
1322	3-bromo-2,4-dichloroanisole	174913-16-7	-1.47	4	T	1	O
1323	3-bromo-2,6-dichloroanisole	174913-18-9	-1.45	4	T	2	O
1324	4-bromo-2,3-dichloroanisole		-1.43	4	T	1	O
1325	4-bromo-2,6-dichloroanisole	19240-91-6	-1.47	4	T	2	O
1326	4-bromo-3,5-dichloroanisole	174913-20-3	-1.44	4	T	1	O
1327	5-bromo-2,4-dichloroanisole	174913-22-5	-1.43	4	T	2	O
1328	6-bromo-2,3-dichloroanisole	174913-23-6	-1.43	4	T	1	O
1329	2-bromo-3,4,5-trichloroanisole		-1.39	4	P	2	O
1330	3-bromo-2,4,6-trichloroanisole		-1.41	4	P	1	O
1331	3-bromo-2,5,6-trichloroanisole		-1.41	4	T	2	O
1332	4-bromo-2,3,6-trichloroanisole		-1.41	4	T	1	O
1333	6-bromo-2,3,4-trichloroanisole		-1.42	4	P	2	O
1334	4-bromo-2,3,5,6-tetrachloroanisole		-1.36	4	P	1	O
1335	2,4-dibromo-3-chloroanisole		-1.41	4	T	2	O
1336	2,4-dibromo-5-chloroanisole	174913-38-3	-1.4	4	T	1	O
1337	2,6-dibromo-3-chloroanisole		-1.29	1	T	2	O
1338	2,6-dibromo-4-chloroanisole	174913-44-1	-1.44	4	T	1	O
1339	2,4-dibromo-3,5-dichloroanisole		-1.35	4	T	2	O
1340	2,4-dibromo-5,6-dichloroanisole		-1.38	4	P	1	O
1341	2,3-dibromo-5,6-dichloroanisole		-1.35	4	T	2	O
1342	2,6-dibromo-3,4,5-trichloroanisole		-1.33	4	P	1	O
1343	2,4,6-tribromo-3-chloroanisole		-1.35	4	T	2	O
1344	2-chlorophenyl phenyl ether	2689-07-8	-1.89	2	T	1	O
1345	4-chlorophenyl phenyl ether	7005-72-3	-2.04	1	T	2	D
1346	2,4-dichlorodiphenylether	51892-26-3	-2.67	2	T	1	D
1347	2,6-dichlorodiphenylether	28419-69-4	-2.09	2	T	2	D
1348	3,4-dichlorodiphenylether	55538-69-7	-2.434	2	T	1	D
1349	3,4'-dichlorodiphenylether	6842-62-2	-2.484	2	T	2	D
1350	3,5-dichlorodiphenylether	24910-68-7	-2.21	2	T	1	D
1351	2,2',4-trichlorodiphenylether	68914-97-6	-3.044	2	T	2	D
1352	2,3,4'-trichlorodiphenyl ether	157683-71-1	-2.904	2	T	1	D

1353	2,3,5-trichlorodiphenyl ether	162853-24-9	-2.735	2	T	2	D
1354	2,3,6-trichlorodiphenyl ether	162853-25-0	-1.865	2	T	1	D
1355	2,3',4-trichlorodiphenyl ether	155999-93-2	-2.574	2	T	2	D
1356	2,4,4'-trichlorodiphenylether	59039-21-3	-1.865	2	P	1	D
1357	2,4,5-trichlorodiphenylether	52322-80-2	-1.34	2	T	2	D
1358	2,4',5-trichlorodiphenylether	65075-00-5	-2.595	2	P	1	D
1359	2,4',6-trichlorodiphenylether	157683-72-2	-2.014	2	P	2	D
1360	2',3,4-trichlorodiphenylether	61328-44-7	-2.925	2	T	1	D
1361	3,3',4-trichlorodiphenylether	66794-60-3	-2.744	2	P	2	D
1362	3,4,4'-trichlorodiphenylether	63646-51-5	-2.594	2	P	1	D
1363	3,4',5-trichlorodiphenylether	24910-73-4	-2.514	2	P	2	D
1364	2,2',4,4'-tetrachlorodiphenylether	28076-73-5	-1.85	2	T	1	M
1365	2,3',4,4'-tetrachlorodiphenylether	61328-46-9	-1.78	2	P	2	M
1366	2,4,4',5-tetrachlorodiphenylether	61328-45-8	-1.67	2	T	1	M
1367	3,3',4,4'-tetrachlorodiphenylether	56348-72-2	-2	2	T	2	M
1368	2,2',3,4,4'-pentachlorodiphenylether	71585-37-0	-2.11	2	P	1	M
1369	2,2',4,4',5-pentachlorodiphenylether	60123-64-0	-1.65	2	T	2	M
1370	2,2',4,4',6-pentachlorodiphenylether	104294-16-8	-1.72	2	T	1	M
1371	2,2',4,5,5'-pentachlorodiphenylether	131138-21-1	-1.59	2	T	2	M
1372	2,3,3',4,4'-pentachlorodiphenylether	85918-31-6	-2.01	2	T	1	M
1373	3,3',4,4',5-pentachlorodiphenylether	94339-59-0	-1.39	2	T	2	M
1374	2,2',3,3',4,4'-hexachlorodiphenylether	71585-39-2	-2.31	2	P	1	M
1375	2,2',3,4,4',5-hexachlorodiphenylether	71585-36-9	-1.65	2	T	2	M
1376	2,2',3,4,4',5'-hexachlorodiphenylether	71585-38-1	-1.85	2	T	1	M
1377	2,2',3,4,4',6'-hexachlorodiphenylether	106220-82-0	-1.86	2	T	2	M
1378	2,2',4,4',5,5'-hexachlorodiphenylether	71859-30-8	-1.49	2	T	1	M
1379	2,2',4,4',5,6'-hexachlorodiphenylether	106220-81-9	-1.54	2	P	2	M
1380	2,3',4,4',5,5'-hexachlorodiphenylether	131138-20-0	-1.31	2	T	1	M
1381	2,2',3,4,4',5,5'-heptachlorodiphe-nylether	83992-69-2	-1.09	2	T	2	M
1382	2,2',3,3',4,4',5,5'-octachlorodiphe-nylether	57379-40-5	-1.02	2	T	1	M
1383	2,2',3,3',4,4',5,5',6-nonachlorodiphe-nylether	83992-73-8	-1	2	T	2	M
1384	decachlorodiphenylether	31710-30-2	0.75	2	T	1	M
1385	4-bromodiphenylether	101-55-3	-2.09	1	T	2	O
1386	4,4'-dibromodiphenylether	2050-47-7	-2.78	1	T	1	O
1387	2,2',4-tribromodiphenylether	147217-75-2	-3.53	4	T	2	M
1388	2,4,4'-tribromodiphenylether	41318-75-6	-3.11	1	P	1	D
1389	2,2',4,4'-tetrabromodiphenylether	5436-43-1	-3.35	1	T	2	D
1390	2,3',4,4'-tetrabromodiphenylether	189084-61-5	-3.7	2	T	1	D
1391	3,3',4,4'-pentabromodiphenylether	93703-48-1	-3.31	2	T	2	D
1392	2,2',3,4,4'-pentabromodiphenylether	182346-21-0	-4.26	4	T	1	M
1393	2,2',4,4',5-pentabromodiphenylether	60348-60-9	-3.67	1	T	2	D
1394	2,2',4,4',6-pentabromodiphenylether	189084-64-8	-3.81	1	P	1	D
1395	2,3‘,4,4‘,5-pentabromodiphenylether		-3.28	1	T	2	O
1396	2,2',4,4',5,5'-hexabromodiphenylether	68631-49-2	-3.93	1	T	1	D
1397	2,2',4,4',5,6'-hexabromodiphenylether	207122-15-4	-4.01	2	P	2	O
1398	2,2',3,4,4',5',6-heptabromodiphe-nylether	207122-16-5	-5.52	2	T	1	O
1399	decabromodiphenylether	1163-19-5	-5.09	1	T	2	D
1400	chloroneb	2675-77-6	-2.38	2	T	1	M
1401	3,4,5-trichloroveratrole	16766-29-3	-2.82	2	T	2	O
1402	tetrachloroveratrole	944-61-6	-2.35	2	P	1	O
1403	methoxychlor	72-43-5	-5.08	1	T	2	D
1404	flufenprox	107713-58-6	-4.72	2	T	1	D

1405	halfenprox	111872-58-3	-4.67	2	T	2	D
1406	trifluoro(trifluoromethyl)oxirane	428-59-1	5	1	T	1	D
1407	epichlorohydrin	106-89-8	-2.906	2	T	2	M
1408	dieldrin	60-57-1	-3.398	1	T	1	O
1409	endrin	72-20-8	-4.7	1	P	2	D
1410	heptachlor epoxide	1024-57-3	-3.45	2	T	1	M
1411	tridiphane	58138-08-2	-2.71	2	T	2	M
1412	2-chlorodibenzofuran	51230-49-0	-2.38	1	T	1	D
1413	3-chlorodibenzofuran	25074-67-3	-2.38	1	T	2	D
1414	2,3-dichlorodibenzofuran	64126-86-9	-2.71	1	P	1	D
1415	2,7-dichlorodibenzofuran	74992-98-6	-2.7	1	T	2	D
1416	2,8-dichlorodibenzofuran	5409-83-6	-2.71	1	T	1	D
1417	3,6-dichlorodibenzofuran	74918-40-4	-2.72	1	T	2	D
1418	2,3,8-trichlorodibenzofuran	57117-32-5	-2.98	1	P	1	D
1419	2,4,6-trichlorodibenzofuran	58802-14-5	-2.94	1	T	2	D
1420	2,4,8-trichlorodibenzofuran	54589-71-8	-2.94	1	P	1	D
1421	1,2,3,4-tetrachlorodibenzofuran	24478-72-6	-3.15	1	T	2	D
1422	1,2,3,7-tetrachlorodibenzofuran	83704-22-7	-3.14	1	T	1	D
1423	1,2,7,8-tetrachlorodibenzofuran	58802-20-3	-3.16	1	T	2	D
1424	1,3,6,8-tetrachlorodibenzofuran	71998-72-6	-3.08	1	P	1	D
1425	1,3,7,8-tetrachlorodibenzofuran	57117-35-8	-3.11	1	T	2	D
1426	1,3,7,9-tetrachlorodibenzofuran	64560-17-4	-3.12	1	T	1	D
1427	2,3,7,8-tetrachlorodibenzofuran	51207-31-9	-3.17	1	T	2	D
1428	1,2,3,4,7-pentachlorodibenzofuran	83704-48-7	-3.26	1	T	1	D
1429	1,2,3,7,8-pentachlorodibenzofuran	57117-41-6	-3.26	1	T	2	D
1430	1,2,4,7,8-pentachlorodibenzofuran	58802-15-6	-3.26	1	T	1	D
1431	2,3,4,7,8-pentachlorodibenzofuran	57117-31-4	-3.28	1	T	2	D
1432	1,2,3,4,6,8-hexachlorodibenzofuran	69698-60-8	-3.29	1	T	1	D
1433	1,2,3,4,7,8-hexachlorodibenzofuran	70648-26-9	-3.29	1	T	2	D
1434	1,2,3,6,7,8-hexachlorodibenzofuran	57117-44-9	-3.29	1	T	1	D
1435	1,2,3,7,8,9-hexachlorodibenzofuran	72918-21-9	-3.28	1	T	2	D
1436	1,2,4,6,7,8-hexachlorodibenzofuran	67562-40-7	-3.29	1	T	1	D
1437	1,2,4,6,8,9-hexachlorodibenzofuran	69698-59-5	-3.29	1	P	2	D
1438	2,3,4,6,7,8-hexachlorodibenzofuran	60851-34-5	-3.29	1	P	1	D
1439	1,2,3,4,6,7,8-heptachlorodibenzofuran	67562-39-4	-3.24	1	T	2	M
1440	1,2,3,4,6,8,9-heptachlorodibenzofuran	69698-58-4	-3.23	1	P	1	D
1441	1,2,3,4,7,8,9-heptachlorodibenzofuran	55673-89-7	-3.19	1	T	2	D
1442	octachlorodibenzofuran	39001-02-0	-4.11	2	T	1	M
1443	1-chlorodibenzo-p-dioxin	39227-53-7	-2.5	1	T	2	D
1444	2-chlorodibenzo-p-dioxin	39227-54-8	-2.51	1	T	1	D
1445	2,3-dichlorodibenzo-p-dioxin	29446-15-9	-2.815	1	T	2	D
1446	2,7-dichlorodibenzo-p-dioxin	33857-26-0	-2.8	1	P	1	D
1447	2,8-dichlorodibenzo-p-dioxin	38964-22-6	-2.804	1	T	2	D
1448	1,2,4-trichlorodibenzo-p-dioxin	39227-58-2	-3.035	1	T	1	D
1449	1,3,7-trichlorodibenzo-p-dioxin	67028-17-5	-3.025	1	T	2	D
1450	2,3,7-trichlorodibenzo-p-dioxin	33857-28-2	-3.085	1	P	1	D
1451	1,2,3,4-tetrachlorodibenzo-p-dioxin	30746-58-8	-3.33	1	T	2	D
1452	1,2,3,7-tetrachlorodibenzo-p-dioxin	67028-18-6	-3.33	1	T	1	D
1453	1,2,7,8-tetrachlorodibenzo-p-dioxin	34816-53-0	-3.28	1	T	2	D
1454	1,3,6,8-tetrachlorodibenzo-p-dioxin	33423-92-6	-3.22	1	P	1	D
1455	1,3,7,8-tetrachlorodibenzo-p-dioxin	50585-46-1	-3.28	1	T	2	D
1456	1,3,7,9-tetrachlorodibenzo-p-dioxin	62470-53-5	-3.24	1	T	1	D
1457	2,3,7,8-tetrachlorodibenzo-p-dioxin	1746-01-6	-3.345	1	T	2	D
1458	1,2,3,4,7-pentachlorodibenzo-p-dioxin	39227-61-7	-3.555	1	T	1	D
1459	1,2,3,7,8-pentachlorodibenzo-p-dioxin	40321-76-4	-3.57	1	T	2	D
1460	1,2,4,7,8-pentachlorodibenzo-p-dioxin	58802-08-7	-3.79	2	T	1	D

1461	1,2,3,4,7,8-hexachlorodibenzo-p-dioxin	39227-28-6	-3.76	1	T	2	D
1462	1,2,3,6,7,8-hexachlorodibenzo-p-dioxin	57653-85-7	-3.78	1	P	1	D
1463	1,2,3,7,8,9-hexachlorodibenzo-p-dioxin	19408-74-3	-3.78	1	P	2	D
1464	1,2,4,6,7,9-hexachlorodibenzo-p-dioxin	39227-62-8	-3.71	1	P	1	D
1465	1,2,3,4,6,7,8-heptachlorodibenzo-p-dioxin	35822-46-9	-3.955	1	T	2	D
1466	1,2,3,4,6,7,9-heptachlorodibenzo-p-dioxin	58200-70-7	-3.92	1	T	1	D
1467	octachlorodibenzo-p-dioxin	3268-87-9	-4.11	1	T	2	D
1468	2,3,7,8-tetrabromdibenzo-p-dioxin	50585-41-6	-3.867	2	T	1	D
1469	octabromdibenzo-p-dioxin	2170-45-8	-5.104	2	T	2	D
1470	2,3-dibromo-7,8-dichlorodibenzo-p-dioxin	50585-40-5	-3.9	2	T	1	D
1471	2-methoxyperfluoro(2,5-di(propan-2-yl)-oxolane)	957209-18-6	4.606	1	T	2	D
1472	chloroacetaldehyde	107-20-0	-3.214	2	T	1	M
1473	trichloroacetaldehyde	75-87-6	-1.88	2	T	2	O
1474	endrin aldehyde	7421-93-4	-3.767	2	T	1	D
1475	fluoroacetone	430-51-3	-2.96	1	T	2	O
1476	1,1,1-trifluoroacetone	421-50-1	-3.496	1	T	1	D
1477	chloroacetone	78-95-5	-3.17	1	T	2	D
1478	3-chloro-2-butanone	4091-39-8	-2.37	2	P	1	M
1479	1,1-dichloroacetone	513-88-2	-2.83	1	T	2	O
1480	kepone	143-50-0	-5.4	2	T	1	M
1481	2,3-dichloro-1.4-naphthoquinone	117-80-6	-5.03	2	T	2	D
1482	chlorophacinone	3691-35-8	-9.87	2	T	1	M
1483	fluoroacetic acid	144-49-0	-6.3	1	T	2	O
1484	difluoroacetic acid	381-73-7	-5.87	1	T	1	O
1485	trifluoroacetic acid	76-05-1	-5.34	1	P	2	O
1486	perfluorooctanoic acid	335-67-1	-2.08	1	T	1	D
1487	chloroacetic acid	79-11-8	-6.42	1	T	2	O
1488	dichloroacetic acid	79-43-6	-6.47	1	P	1	O
1489	2,2-dichloropropionic acid	75-99-0	-5.99	2	T	2	M
1490	trichloroacetic acid	76-03-9	-6.26	1	T	1	O
1491	bromoacetic acid	79-08-3	-6.57	1	P	2	O
1492	dibromoacetic acid	631-64-1	-6.74	1	T	1	O
1493	tribromoacetic acid	75-96-7	-6.86	1	T	2	O
1494	chlorodifluoroacetic acid	76-04-0	-5.78	1	T	1	O
1495	2,3,6-trichlorobenzoic acid	50-31-7	-6.06	2	T	2	M
1496	2,2,2-trifluoroethyl formate	32042-38-9	-1.137	1	T	1	O
1497	methyl trifluoroacetate	431-47-0	-1.05	1	P	2	O
1498	ethyl trifluoroacetate	383-63-1	-0.389	1	T	1	O
1499	2,2,2-trifluoroethyl acetate	406-95-1	-1.159	1	P	2	O
1500	chloroacetic acid methyl ester	96-34-4	-3.02	2	T	1	D
1501	ethyl chloroacetate	105-39-5	-2.79	2	T	2	M
1502	chlorfenprop-methyl	14437-17-3	-4.04	1	T	1	D
1503	plifenate	21757-82-4	-4.03	2	T	2	M
1504	tetrachlorophthalide	27355-22-2	-4.66	1	T	1	O
1505	profluthrin	223419-20-3	-1.789	2	P	2	D
1506	tefluthrin	79538-32-2	-1	2	T	1	O
1507	transfluthrin	118712-89-3	-2.73	2	T	2	D
1508	bifenthrin	82657-04-3	-4.39	2	T	1	M
1509	dimethyl tetrachloroterephthalate	1861-32-1	-4.25	2	T	2	M

1510	trifluoroacetyl fluoride	354-34-7	-1.866	1	T	1	D
1511	trichloroacetyl chloride	76-02-8	-1.684	1	T	2	D
1512	trifluoroacetyl chloride	354-32-5	-1.735	1	T	1	D
1513	tritac	1861-44-5	-4.702	1	T	2	D
1514	4,5-dichloroguaiacol	2460-49-3	-3.75	2	P	1	O
1515	3,4,5-trichloroguaiacol	57057-83-7	-4.32	2	T	2	O
1516	4,5,6-trichloroguaiacol	2668-24-8	-2.96	2	T	1	M
1517	3,4,5,6-tetrachloroguaiacol	2539-17-5	-3.39	1	T	2	D
1518	3-chlorosyringol	18113-22-9	-5.01	2	P	1	O
1519	3,5-dichlorosyringol	78782-46-4	-4.56	2	T	2	O
1520	trichlorosyringol	2539-26-6	-5.05	2	T	1	O
1521	2-chlorosyringaldehyde	76341-69-0	-5.35	2	T	2	O
1522	2,6-dichlorosyringaldehyde	76330-06-8	-5.83	2	P	1	O
1523	cloxyfenac	6386-63-6	-8.26	2	T	2	M
1524	chlorobenzilate	510-15-6	-5.74	2	P	1	M
1525	chloropropylate	5836-10-2	-6.21	2	T	2	D
1526	bromopropylate	18181-80-1	-6.31	2	T	1	M
1527	chlorfurenol-methyl	2536-31-4	-6.5	1	T	2	D
1528	indanofan	133220-30-1	-7.67	2	T	1	M
1529	(4-chlorophenoxy)acetic acid	122-88-3	-8.41	2	T	2	M
1530	(4-chloro-2-methylphenoxy)acetic acid	94-74-6	-7.78	2	P	1	D
1531	(4-chloro-*o*-tolyloxy)butyric acid	94-81-5	-7.95	2	T	2	M
1532	dicamba	1918-00-9	-6.85	2	T	1	M
1533	2,4-dichlorophenoxyacetic acid	94-75-7	-7.58	2	P	2	M
1534	4-(2,4-dichlorophenoxy)butyric acid	94-82-6	-6.83	2	T	1	M
1535	2,4,5-trichlorophenoxyacetic acid	93-76-5	-6.45	1	T	2	D
1536	mecoprop	93-65-2	-6.8	2	T	1	M
1537	mecoprop-P	16484-77-8	-7.74	2	T	2	D
1538	D(+)-dichlorprop	15165-67-0	-7.37	2	T	1	D
1539	a-(2,4-dichlorophenoxy)propionic acid	120-36-5	-7.46	2	T	2	D
1540	diclofop	40843-25-2	-9.36	2	P	1	M
1541	ethyl 4-[(4-chloro-*o*-tolyl)oxy]butyrate	10443-70-6	-4.94	2	T	2	D
1542	methyl (2,4-dichlorophenoxy)acetate	1928-38-7	-3.93	2	P	1	D
1543	ethyl (2,4-dichlorophenoxy)acetate	533-23-3	-3.88	2	T	2	D
1544	butyl (2,4-dichlorophenoxy)acetate	94-80-4	-4.22	2	T	1	M
1545	MCPA-2-ethylhexyl ester	29450-45-1	-2.75	2	P	2	D
1546	2,4-D isopropyl ester	94-11-1	-3.92	2	T	1	M
1547	2,4-D-2-ethylhexyl ester	1928-43-4	-3.14	2	T	2	D
1548	2,4-D isooctyl ester	25168-26-7	-2.62	2	T	1	D
1549	metofluthrin	240494-70-6	-3.46	2	T	2	D
1550	permethrin	52645-53-1	-5.45	2	P	1	D
1551	2,4-D butoxyethyl ester	1929-73-3	-5.19	2	T	2	D
1552	mecoprop-P-etotyl	97659-39-7	-4.09	2	T	1	D
1553	diclofop-methyl	51338-27-3	-4.9	2	T	2	D
1554	methyl 2-chloroacetoacetate	4755-81-1	-3.76	2	T	1	D
1555	carbonic difluoride	353-50-4	-0.92	1	T	2	D
1556	phosgene	75-44-5	-0.166	1	T	1	D
1557	methylamine	74-89-5	-3.374	1	T	2	D
1558	ethylamine	75-04-7	-3.3	1	P	1	D
1559	propylamine	107-10-8	-3.29	1	T	2	D
1560	n-butylamine	109-73-9	-3.11	1	P	1	D
1561	n-pentylamine	110-58-7	-3	1	T	2	D
1562	n-hexylamine	111-26-2	-2.9	1	T	1	D
1563	heptylamine	111-68-2	-2.78	1	T	2	D
1564	octylamine	111-86-4	-2.68	1	T	1	D

1565	decylamine	2016-57-1	-2.68	2	T	2	D
1566	tridecylamine	2869-34-3	-2.35	1	T	1	D
1567	sec-butylamine	13952-84-6	-3	2	T	2	D
1568	2-ethylhexylamine	104-75-6	-2.41	2	T	1	D
1569	cyclohexylamine	108-91-8	-3.77	1	T	2	D
1570	allylamine	107-11-9	-3.4	1	T	1	O
1571	1,2-diaminoethane	107-15-3	-7.15	1	T	2	D
1572	dimethylamine	124-40-3	-3.14	1	T	1	D
1573	diethylamine	109-89-7	-2.98	1	T	2	D
1574	dipropylamine	142-84-7	-2.68	1	T	1	D
1575	dibutylamine	111-92-2	-2.38	1	T	2	D
1576	dipentylamine	2050-92-2	-2.19	2	P	1	M
1577	diisopropylamine	108-18-9	-2.36	1	T	2	D
1578	diisobutylamine	110-96-3	-2	2	P	1	M
1579	azetidine	503-29-7	-4.08	1	T	2	D
1580	pyrrolidine	123-75-1	-4.01	1	P	1	D
1581	piperidine	110-89-4	-3.74	1	T	2	D
1582	hexamethyleneimine	111-49-9	-3.6	1	T	1	D
1583	diallylamine	124-02-7	-3	2	T	2	M
1584	piperazine	110-85-0	-5.43	1	P	1	D
1585	trimethylamine	75-50-3	-2.35	1	T	2	D
1586	triethylamine	121-44-8	-2.215	1	T	1	D
1587	tripropylamine	102-69-2	-1.56	2	T	2	M
1588	N,N-dimethyloctylamine	7378-99-6	-1.7	2	P	1	M
1589	tributylamine	102-82-9	-1.3	2	T	2	M
1590	1-methyl-pyrrolidine	120-94-5	-2.91	1	T	1	D
1591	N-methylpiperidine	626-67-5	-2.85	1	T	2	D
1592	N,N-dimethylcyclohexylamine	98-94-2	-2.74	1	T	1	D
1593	triallylamine	102-70-5	-1.97	2	T	2	D
1594	hexamethylenetetramine	100-97-0	-7.45	2	T	1	M
1595	N-methylpiperazine	109-01-3	-5.43	1	T	2	D
1596	aniline	62-53-3	-4.03	1	T	1	D
1597	m-methylaniline	108-44-1	-4.17	1	T	2	D
1598	4-methylaniline	106-49-0	-4.04	1	T	1	D
1599	o-methylaniline	95-53-4	-4.06	1	T	2	D
1600	o-ethylaniline	578-54-1	-3.81	2	T	1	M
1601	4-ethylaniline	589-16-2	-3.8	2	T	2	M
1602	2,3-dimethylaniline	87-59-2	-4.06	2	T	1	M
1603	2,4-dimethylaniline	95-68-1	-3.81	2	P	2	M
1604	2,5-dimethylaniline	95-78-3	-3.79	2	T	1	M
1605	2,6-dimethylaniline	87-62-7	-3.82	1	T	2	D
1606	3,4-dimethylaniline	95-64-7	-4.12	1	P	1	D
1607	2,4,5-trimethylaniline	137-17-7	-3.994	1	P	2	D
1608	2-methyl-6-ethylaniline	24549-06-2	-3.62	2	P	1	D
1609	2,6-diethylaniline	579-66-8	-3.5	2	T	2	M
1610	2-isopropylaniline	643-28-7	-3.574	2	T	1	D
1611	1-naphthylamine	134-32-7	-5.34	1	T	2	D
1612	2-naphthylamine	91-59-8	-5.48	1	T	1	D
1613	o-phenylenediamine	95-54-5	-5.77	2	T	2	M
1614	m-phenylenediamine	108-45-2	-7.35	2	T	1	M
1615	benzidine	92-87-5	-9.29	2	T	2	D
1616	N-methylaniline	100-61-8	-3.44	1	T	1	D
1617	N-ethylaniline	103-69-5	-3.398	1	T	2	D
1618	diphenylamine	122-39-4	-3.96	2	T	1	M
1619	N,N-dimethylaniline	121-69-7	-2.53	1	T	2	D
1620	N,N,4-trimethylaniline	99-97-8	-2.701	2	T	1	D

1621	N,N-dimethylbenzylamine	103-83-3	-3.107	2	T	2	M
1622	N,N-diethylaniline	91-66-7	-2.26	2	P	1	M
1623	fenpropidin	67306-00-7	-3.52	2	T	2	D
1624	1-pyrroline	5724-81-2	-3.6	1	T	1	D
1625	hydrocyanic acid	74-90-8	-2.26	1	T	2	D
1626	acetonitrile	75-05-8	-2.85	1	T	1	D
1627	propionitrile	107-12-0	-2.67	1	P	2	D
1628	butyronitrile	109-74-0	-2.56	1	T	1	D
1629	valeronitrile	110-59-8	-2.547	1	T	2	O
1630	hexanenitrile	628-73-9	-2.42	2	T	1	M
1631	nonanenitrile	2243-27-8	-2	2	P	2	M
1632	isobutyronitrile	78-82-0	-2.4	1	T	1	O
1633	acrylonitrile	107-13-1	-2.35	1	T	2	D
1634	2-butenenitrile	4786-20-3	-2.34	2	T	1	D
1635	3-butenenitrile	109-75-1	-2.69	2	P	2	M
1636	methacrylonitrile	126-98-7	-2.06	2	T	1	M
1637	geranyl nitrile	5146-66-7	-2	1	T	2	O
1638	succinonitrile	110-61-2	-6.58	2	T	1	D
1639	adiponitrile	111-69-3	-6.3	2	T	2	M
1640	benzonitrile	100-47-0	-2.86	1	T	1	D
1641	benzyl cyanide	140-29-4	-3.55	2	T	2	M
1642	o-tolunitrile	529-19-1	-2.54	2	T	1	M
1643	phenylhydrazine	100-63-0	-6.71	2	T	2	D
1644	azobenzene	103-33-3	-3.26	2	T	1	D
1645	n-propylguanidine	462-25-9	-8.01	1	T	2	D
1646	pyrrole	109-97-7	-3.154	1	T	1	D
1647	N-methylpyrrole	96-54-8	-2.15	2	T	2	M
1648	indole	120-72-9	-4.97	2	T	1	M
1649	N-methylindole	603-76-9	-4.335	1	T	2	D
1650	carbazole	86-74-8	-5.324	1	P	1	O
1651	1H-benzotriazole	95-14-7	-4.72	2	T	2	M
1652	pyridine	110-86-1	-3.44	1	T	1	O
1653	2-methylpyridine	109-06-8	-3.39	1	T	2	D
1654	3-methylpyridine	108-99-6	-3.498	1	P	1	D
1655	4-methylpyridine	108-89-4	-3.615	1	T	2	D
1656	2-ethylpyridine	100-71-0	-3.173	1	T	1	D
1657	3-ethylpyridine	536-78-7	-3.373	1	P	2	D
1658	4-ethylpyridine	536-75-4	-3.46	1	P	1	D
1659	2,3-dimethylpyridine	583-61-9	-3.535	1	P	2	D
1660	2,4-dimethylpyridine	108-47-4	-3.56	1	T	1	D
1661	3,4-dimethylpyridine	583-58-4	-3.826	1	T	2	D
1662	3,5-dimethylpyridine	591-22-0	-3.547	1	T	1	O
1663	2,5-dimethylpyridine	589-93-5	-3.456	1	T	2	D
1664	2,6- dimethylpyridine	108-48-5	-3.37	1	T	1	D
1665	2,4,6-trimethylpyridine	108-75-8	-3.37	2	T	2	M
1666	5-ethyl-2-methylpyridine	104-90-5	-3.11	2	T	1	D
1667	4-tert-butylpyridine	3978-81-2	-3.27	1	T	2	D
1668	4-vinylpyridine	100-43-6	-3.4	2	T	1	M
1669	2-methyl-5-vinylpyridine	140-76-1	-3.75	2	T	2	M
1670	quinoline	91-22-5	-4.2	1	P	1	D
1671	isoquinoline	119-65-3	-4.21	2	T	2	M
1672	2-methylquinoline	91-63-4	-4.53	2	T	1	M
1673	acridine	260-94-6	-5.07	2	T	2	D
1674	benzo(f)quinoline	85-02-9	-5.15	2	T	1	D
1675	phenanthridine	229-87-8	-6.23	2	T	2	M
1676	2-methylpyrazine	109-08-0	-4.046	1	T	1	D

1677	2-ethylpyrazine	13925-00-3	-4	1	T	2	D
1678	2,5-dimethylpyrazine	123-32-0	-4.25	1	P	1	D
1679	2,6-dimethylpyrazine	108-50-9	-3.38	1	T	2	D
1680	2,3-diethyl-5-methylpyrazine	18138-04-0	-3.3	1	T	1	D
1681	2-isobutylpyrazine	29460-93-3	-3.7	1	T	2	D
1682	4,4'-dipyridyl	553-26-4	-6.75	2	T	1	D
1683	diquat	2764-72-9	-8.844	2	T	2	D
1684	amitraz	33089-61-1	-4.5	2	T	1	D
1685	4-aminopyridine	504-24-5	-8.0195	2	P	2	D
1686	3-amino-1,2,4-triazole	61-82-5	-9.6	2	T	1	M
1687	ametoctradin	865318-97-4	-9.55	2	T	2	D
1688	phenazopyridine	94-78-0	-11.37	2	T	1	M
1689	9-methyladenine	700-00-5	-9.98	1	T	2	D
1690	pyrimethanil	53112-28-0	-5.75	2	T	1	D
1691	cyprodinil	121552-61-2	-5.46	2	P	2	M
1692	mepanipyrim	110235-47-7	-6.13	2	T	1	D
1693	6-benzyladenine	1214-39-7	-11.15	2	T	2	M
1694	N,N-bis(2-ethylhexyl)-1,2,4-triazol-1-ylmethanamine	91273-04-0	-4.863	1	P	1	D
1695	cyromazine	66215-27-8	-11.56	2	T	2	M
1696	2,2'-azobis(2-methylpropionitrile)	78-67-1	-3.73	2	T	1	M
1697	3-cyanopyridine	100-54-9	-4.95	1	T	2	D
1698	4-cyanopyridine	100-48-1	-4.42	1	T	1	D
1699	ferimzone	89269-64-7	-8.25	2	T	2	D
1700	ethanolamine	141-43-5	-8.17	1	T	1	O
1701	2-(bis(1-methylethyl)amino)ethanol	96-80-0	-5.07	2	T	2	M
1702	3-cyanophenol	873-62-1	-6.97	1	T	1	D
1703	4-cyanophenol	767-00-0	-7.46	1	T	2	D
1704	p-phenylazophenol	1689-82-3	-7.56	2	T	1	D
1705	triapenthenol	76608-88-3	-8	2	T	2	D
1706	8-quinolinol	148-24-3	-4.7	2	T	1	M
1707	ethirimol	23947-60-6	-6.86	2	T	2	M
1708	dimethirimol	5221-53-4	-7.15	2	T	1	M
1709	2-methoxyethanamine	109-85-3	-4.8	1	T	2	D
1710	2-methoxyaniline	90-04-0	-4.24	1	T	1	D
1711	3-methoxyaniline	536-90-3	-5.35	1	P	2	D
1712	4-methoxyaniline	104-94-9	-5.49	1	P	1	D
1713	2,4-dimethoxyaniline	2735-04-8	-4.6	2	T	2	D
1714	ethoxyquin	91-53-2	-4.296	2	T	1	D
1715	morpholine	110-91-8	-5.26	1	T	2	D
1716	n-methylmorpholine	109-02-4	-4.367	1	T	1	O
1717	tridemorph	24602-86-6	-2.16	2	T	2	D
1718	spiroxamine A (cis)		-3.77	2	T	1	D
1719	spiroxamine B (trans)		-3.39	2	T	2	D
1720	fenpropimorph	67564-91-4	-3.7	2	P	1	M
1721	fuberidazole	3878-19-1	-8.68	2	T	2	D
1722	2-ethyl-3-methoxypyrazine	25680-58-4	-3.22	1	P	1	D
1723	2-isobutyl-3-methoxypyrazine	24168-70-5	-2.7	1	T	2	D
1724	fenazaquin	120928-09-8	-4.68	2	T	1	D
1725	isoxazole	288-14-2	-2.994	2	T	2	D
1726	simeton	673-04-1	-7.8	2	T	1	D
1727	atratone	1610-17-9	-7.41	2	T	2	M
1728	secbumeton	26259-45-0	-6.55	2	P	1	M
1729	prometon	1610-18-0	-6.92	2	T	2	M
1730	terbumeton	33693-04-8	-6.43	2	T	1	M
1731	2-aminoanthraquinone	117-79-3	-8.425	2	T	2	D

1732	1-aminoanthraquinone	82-45-1	-6.7	2	T	1	D
1733	1,4-diaminoanthraquinone	128-95-0	-8.1	2	P	2	D
1734	1,4-bis(methylamino)anthraquinone	2475-44-7	-8.11	2	T	1	D
1735	3-formylpyridine	500-22-1	-5.21	1	T	2	D
1736	4-formylpyridine	872-85-5	-5.14	1	P	1	D
1737	3-acetylpyridine	350-03-8	-6.06	1	T	2	D
1738	4-acetylpyridine	1122-54-9	-5.59	1	T	1	D
1739	o-aminobenzoic acid	118-92-3	-7.17	2	T	2	M
1740	m-aminobenzoic acid	99-05-8	-9.968	2	P	1	M
1741	p-aminobenzoic acid	150-13-0	-8.983	2	T	2	M
1742	cocaine	50-36-2	-8.79	2	T	1	D
1743	methyl cyanoacetate	105-34-0	-4.94	2	T	2	M
1744	ethyl cyanoacetate	105-56-6	-4.93	2	T	1	M
1745	cyenopyrafen	560121-52-0	-6.6	2	T	2	D
1746	1-amino-4-hydroxyanthraquinone	116-85-8	-6.87	2	T	1	M
1747	heroin	561-27-3	-10.6	2	T	2	D
1748	fenpropathrin	39515-41-8	-3.5	2	T	1	D
1749	bitertanol A	70585-36-3	-10.47	2	P	2	D
1750	bitertanol B	70585-38-5	-9	2	P	1	D
1751	ancymidol	12771-68-5	-9.78	1	T	2	D
1752	hymexazole	10004-44-1	-6.95	2	T	1	D
1753	azoxystrobin	131860-33-8	-11.01	2	T	2	D
1754	mechlorethamine	51-75-2	-3.52	2	T	1	M
1755	bis(2-chloroethyl)ethylamine	538-07-8	-3.72	2	T	2	M
1756	N,N,N-tris(2-chloroethyl)amine	555-77-1	-4.12	2	T	1	D
1757	2-fluoroaniline	348-54-9	-3.53	2	T	2	D
1758	4-fluoroaniline	371-40-4	-3.76	2	T	1	D
1759	3-trifluoromethylaniline	98-16-8	-2.98	2	P	2	M
1760	o-chloroaniline	95-51-2	-3.6	1	T	1	D
1761	m-chloroaniline	108-42-9	-4.27	1	T	2	D
1762	p-chloroaniline	106-47-8	-4.33	1	T	1	D
1763	3-chloro-p-toluidine	95-74-9	-4.139	1	P	2	D
1764	3,4-dichloroaniline	95-76-1	-4.48	2	T	1	D
1765	2,3,3,3-tetrafluoro-2-(trifluoromethyl)-propanenitrile	42532-60-5	4.4	1	T	2	D
1766	chloroacetonitrile	107-14-2	-3.13	2	T	1	M
1767	trichloroacetonitrile	545-06-2	-0.23	2	T	2	M
1768	2,6-dichlorobenzonitrile	1194-65-6	-3.08	1	T	1	O
1769	chlorothanonil	1897-45-6	-5.1	1	T	2	O
1770	4-chloroazobenzene	4340-77-6	-4.26	2	T	1	D
1771	chlordimeform	6164-98-3	-4.44	2	T	2	M
1772	1,1'-dimethyl-3,3',4,4',5,5'-hexabromo-2,2'-bipyrrole	253798-63-9	-6.09	2	P	1	O
1773	1,1'-dimethyl-3,3',4-tribromo-4',5,5'-trichloro-2,2'-bipyrrole		-4.25	2	T	2	O
1774	1,1'-dimethyl-3,4,4'-tribromo-3',5,5'-trichloro-2,2'-bipyrrole		-4.92	2	T	1	O
1775	1,1'-dimethyl-3,3',4,4'-tetrabromo-5,5'-dichloro-2,2'-bipyrrole		-4.84	2	T	2	O
1776	1,1'-dimethyl-3,3',4,4',5-pentabromo-5'-chloro-2,2'-bipyrrole		-5.56	2	T	1	O
1777	penconazole	66246-88-6	-6.236	2	T	2	M
1778	3-chloropyridine	626-60-8	-2.94	1	T	1	D
1779	2-chloropyridine	109-09-1	-3.22	1	T	2	D
1780	2,3,5,6-tetrachloropyridine	2402-79-1	-2.1	2	P	1	D
1781	nitrapyrin	1929-82-4	-3.25	2	T	2	M
1782	3-bromopyridine	626-55-1	-3.315	2	P	1	M

1783	fenclorim	3740-92-9	-3.14	2	T	2	D
1784	clofentezine	74115-24-5	-7.8	2	T	1	M
1785	anilazine	101-05-3	-4.6	2	T	2	M
1786	simazine	122-34-9	-6.855	2	P	1	D
1787	atrazine	1912-24-9	-6.54	1	T	2	D
1788	sebuthylazine	7286-69-3	-6.32	2	T	1	D
1789	propazine	139-40-2	-6.27	2	T	2	M
1790	terbuthylazine	5915-41-3	-6.03	2	P	1	D
1791	cyprazine	22936-86-3	-7.27	2	T	2	D
1792	cyanazine	21725-46-2	-7.98	2	T	1	M
1793	indaziflam A	730979-19-8	-8.66	2	T	2	D
1794	indaziflam B	730979-32-5	-9.12	2	P	1	D
1795	fenpiclonil	74738-17-3	-6.66	2	T	2	D
1796	tolprocarb	911499-62-2	-8.21	2	T	1	D
1797	myclobutanil	88671-89-0	-6.77	2	T	2	D
1798	fenbuconazole	114369-43-6	-7.91	2	T	1	M
1799	bromoxynil	1689-84-5	-6.38	2	T	2	D
1800	ioxynil	1689-83-4	-8.11	1	P	1	D
1801	paclobutrazol	76738-62-0	-7.88	2	T	2	D
1802	diclobutrazol	75736-33-3	-7.38	2	P	1	D
1803	tebuconazole	107534-96-3	-7.92	2	T	2	M
1804	hexaconazole	79983-71-4	-7.05	2	P	1	M
1805	cyproconazole	94361-06-5	-7.66	2	T	2	M
1806	metconazole	125116-23-6	-6.79	2	T	1	D
1807	ipconazole	125225-28-7	-6.99	2	T	2	M
1808	flutriafol	76674-21-0	-8.59	2	T	1	D
1809	nuarimol	63284-71-9	-8.01	2	T	2	M
1810	perfluoro-N-methylmorpholine	382-28-5	3.8	1	T	1	D
1811	imazalil	35554-44-0	-6.71	2	T	2	M
1812	tetraconazole	112281-77-3	-6.58	2	P	1	D
1813	(±)-(2R*,4R*)-bromuconazole	114544-81-9	-8.37	1	P	2	D
1814	(±)-(2R*,4S*)-bromuconazole	114544-80-8	-8.2	1	T	1	D
1815	azaconazole	60207-31-0	-8.1	2	T	2	D
1816	etaconazole	60207-93-4	-7.26	2	T	1	M
1817	cis-propiconazole	112721-87-6	-7.47	2	T	2	D
1818	trans-propiconazole	120523-07-1	-7.285	2	T	1	D
1819	furconazole-cis	112839-32-4	-6.96	2	P	2	D
1820	difenoconazole	119446-68-3	-8.95	2	T	1	M
1821	quinoxyfen	124495-18-7	-4.21	2	T	2	D
1822	pyridalyl	179101-81-6	-3.9	2	T	1	D
1823	benzpyrimoxan	1449021-97-9	-6.422	2	P	2	D
1824	diflumetorim	130339-07-0	-5.88	2	T	1	D
1825	pyrimidifen	105779-78-0	-7.95	2	T	2	D
1826	triflumizole	68694-11-1	-5.77	2	T	1	M
1827	fludioxonil	131341-86-1	-7.66	2	T	2	D
1828	quinoclamine	2797-51-5	-7.52	2	T	1	D
1829	fluridone	59756-60-4	-6.84	2	P	2	D
1830	bromoxynil butyrate	3861-41-4	-4.75	2	T	1	D
1831	bromoxynil heptanoate	56634-95-8	-3.778	2	P	2	D
1832	bromoxynil octanoate	1689-99-2	-3.94	2	T	1	D
1833	fluazolate	174514-07-9	-4.12	2	T	2	D
1834	ethychlozate	27512-72-7	-7.6	2	T	1	D
1835	fenchlorazole-ethyl	103112-35-2	-6.44	2	T	2	D
1836	3,6-dichloropicolinic acid	1702-17-6	-7.93	2	T	1	M
1837	halacrinat	34462-96-9	-5.55	2	T	2	M
1838	picloram	1918-02-1	-9.95	2	T	1	M

1839	aminocyclopyrachlor	858956-08-8	-10.5	2	T	2	D
1840	eglinazine-ethyl	6616-80-4	-8.01	2	T	1	D
1841	proglinazine-ethyl	68228-18-2	-7.41	2	P	2	D
1842	flupyradifurone	951659-40-8	-10.209	2	T	1	D
1843	flurtamone	96525-23-4	-11.59	2	T	2	D
1844	cyhalofop	122008-78-0	-8.626	2	T	1	D
1845	tralomethrin	66841-25-6	-7.8	2	T	2	D
1846	alpha-cypermethrin	67375-30-8	-4.32	2	T	1	D
1847	beta-cypermethrin	1224510-29-5	-5.14	2	T	2	D
1848	zeta-cypermethrin	1315501-18-8	-6.03	1	T	1	D
1849	theta-cypermethrin	71697-59-1	-6.18	2	P	2	D
1850	gamma-cyhalothrin	76703-62-3	-4.25	2	T	1	D
1851	lambda-cyhalothrin	91465-08-6	-4.75	2	T	2	D
1852	cyfluthrin I	86560-92-1	-3.74	2	T	1	D
1853	cyfluthrin II	86560-94-3	-5.42	1	P	2	D
1854	beta-cyfluthrin (cis)	86560-93-2	-5.55	1	P	1	D
1855	beta-cyfluthrin (trans)	86560-95-4	-4.95	1	P	2	D
1856	esfenvalerate	66230-04-4	-6.62	2	T	1	D
1857	fenvalerate	51630-58-1	-4.77	2	T	2	M
1858	cyhalofop-butyl	122008-85-9	-6.08	2	T	1	D
1859	flucythrinate	70124-77-5	-5.72	2	T	2	D
1860	brofluthrinate	160791-64-0	-4.601	2	T	1	M
1861	acrinathrin	101007-06-1	-4.9	2	T	2	D
1862	triadimenol A	89482-17-7	-8.5	2	T	1	D
1863	triadimenol B	82200-72-4	-8.45	1	P	2	D
1864	pyrazoxyfen	71561-11-0	-5.14	2	T	1	D
1865	triadimefon	43121-43-3	-8.48	2	T	2	D
1866	flurprimidol	56425-91-3	-7.27	2	T	1	M
1867	triclopyr	55335-06-3	-7.4	2	T	2	M
1868	fluazifop	69335-91-7	-10.93	2	P	1	M
1869	fluazifop-P	83066-88-0	-9.4	2	T	2	M
1870	cloquintocet-mexyl	99607-70-2	-5.91	2	T	1	D
1871	fluazifop-butyl	69806-50-4	-5.59	2	T	2	D
1872	fluazifop-P-butyl	79241-46-6	-5.35	1	T	1	D
1873	R-haloxyfop-methyl	72619-32-0	-5.91	2	P	2	D
1874	picoxystrobin	117428-22-5	-6.53	2	T	1	M
1875	clodinafop-propargyl	105512-06-9	-6.95	2	T	2	D
1876	haloxyfop-etotyl	87237-48-7	-7.97	2	T	1	D
1877	quizalofop-ethyl	76578-14-8	-6.12	1	P	2	D
1878	quizalofop-P-ethyl	100646-51-3	-7.08	2	T	1	D
1879	fluacrypyrim	229977-93-9	-5.7	2	T	2	D
1880	fenoxaprop-P-ethyl	71283-80-2	-6.53	2	T	1	D
1881	fenoxaprop-ethyl	66441-23-4	-6.19	2	T	2	M
1882	drazoxolon[2]	5707-69-7	-5.54	2	T	1	D
1883	fluroxypyr	69377-81-7	-10.51	2	T	2	M
1884	florpyrauxifen	943832-81-3	-10.893	2	T	1	D
1885	fluroxypyr-meptyl	81406-37-3	-5.28	2	P	2	D
1886	halauxifen-methyl	943831-98-9	-8.942	2	T	1	D
1887	fluroxypyr-2-butoxy-1-methylethyl	154486-27-8	-6.77	2	P	2	D
1888	tau-fluvalinate	102851-06-9	-7.315	2	P	1	D
1889	pyriminostrobin	1257598-43-8	-7.312	2	T	2	D
1890	methazole	20354-26-1	-5.03	2	T	1	D
1891	N,N-dichloromethylamine	7651-91-4	-0.947	1	T	2	D
1892	N-methylformamide	123-39-7	-6.57	1	T	1	D
1893	acetamide	60-35-5	-7.13	1	T	2	D
1894	propionamide	79-05-0	-6.91	1	T	1	D

1895	N,N'-dimethylformamide	68-12-2	-5.73	1	T	2	D
1896	N-methylacetamide	79-16-3	-6.9	1	T	1	D
1897	butylamide	541-35-5	-6.95	2	T	2	M
1898	N,N'-dimethylacetamide	127-19-5	-6.04	1	T	1	D
1899	hexanamide	628-02-4	-6.66	2	P	2	M
1900	N-butylacetamide	1119-49-9	-6.83	1	T	1	D
1901	N-methylpyrrolidone	872-50-4	-6.883	1	T	2	D
1902	epsilon-caprolactam	105-60-2	-7.65	2	T	1	M
1903	N-acetylpyrrolidine	4030-18-6	-7.19	1	T	2	D
1904	methacrylamide	79-39-0	-7.34	2	T	1	M
1905	*N*-(2-ethylhexyl)bicyclo-(2,2,1)-5-hep-tene-2,3-dicarboximide	113-48-4	-4.75	2	T	2	D
1906	benzamide	55-21-0	-8	1	T	1	D
1907	pyroquilon	57369-32-1	-7.1	2	T	2	D
1908	diphenamid	957-51-7	-8.81	2	P	1	M
1909	naphthaleneacetamide	86-86-2	-9.107	2	T	2	D
1910	dymron	42609-52-9	-7.54	2	T	1	M
1911	fenuron	101-42-8	-7.085	2	T	2	D
1912	isoproturon	34123-59-6	-7.94	2	P	1	M
1913	siduron	1982-49-6	-8.557	2	T	2	D
1914	emylcamate	78-28-4	-2.86	2	T	1	D
1915	m-tolyl methylcarbamate	1129-41-5	-5.19	2	P	2	M
1916	3,4-xylyl methylcarbamate	2425-10-7	-5.37	2	T	1	M
1917	3,5-xylyl methyl carbamate	2655-14-3	-6.02	2	T	2	M
1918	isopropyl phenyl carbamate	122-42-9	-4.87	2	T	1	M
1919	isoprocarb	2631-40-5	-5.89	2	T	2	D
1920	promecarb	2631-37-0	-5.44	2	T	1	M
1921	fenobucarb	3766-81-2	-5.57	1	P	2	M
1922	butacarb	2655-19-8	-5.55	2	T	1	D
1923	carbaryl	63-25-2	-7.43	2	T	2	D
1924	desmedipham	13684-56-5	-9.76	1	T	1	D
1925	phenmedipham	13684-63-4	-10.11	2	P	2	M
1926	maleic hydrazide	10071-13-3	-10.48	2	T	1	D
1927	1-methylthymine	4160-72-9	-7.63	1	T	2	D
1928	lenacil	2164-08-1	-10.25	2	T	1	D
1929	amicarbazone	129909-90-6	-10.25	2	T	2	D
1930	propamocarb	24579-73-5	-7.22	1	T	1	M
1931	hexazinon	51235-04-2	-10.08	2	T	2	M
1932	metamitron	41394-05-2	-10.46	2	T	1	D
1933	aminocarb	2032-59-9	-6.85	2	T	2	M
1934	pirimicarb	23103-98-2	-7.46	2	P	1	M
1935	carbendazim	10605-21-7	-8.62	2	T	2	M
1936	dimetilane	644-64-4	-7.93	2	T	1	M
1937	benomyl	17804-35-2	-9.7	1	T	2	D
1938	carbetamide	16118-49-3	-10.735	2	P	1	D
1939	(SR)-iprovalicarb	140923-25-7	-8.78	2	T	2	D
1940	(SS)-iprovalicarb		-8.77	2	T	1	D
1941	karbutilate	4849-32-5	-11.64	2	T	2	D
1942	isocyanic acid	75-13-8	-2.72	1	T	1	D
1943	oxamide	471-46-5	-9.27	2	T	2	D
1944	phenacetin	62-44-2	-8.13	2	P	1	M
1945	napropamide	15299-99-7	-7.47	2	T	2	D
1946	napropamide-M	41643-35-0	-7.972	2	T	1	D
1947	naproanilide	52570-16-8	-9.2	2	T	2	D
1948	mandestrobin	173662-97-0	-9.136	2	T	1	D
1949	fenfuram	24691-80-3	-7.79	1	T	2	M

1950	difenoxuron	14214-32-5	-10.78	2	T	1	M
1951	propoxur	114-26-1	-6.99	1	T	2	D
1952	diethofencarb	87130-20-9	-7.42	2	T	1	M
1953	fenoxycarb	72490-01-8	-7.79	2	P	2	D
1954	carbofuran	1563-66-2	-7.69	2	T	1	M
1955	dioxacarb	6988-21-2	-9.22	2	T	2	M
1956	bendiocarb	22781-23-3	-5.63	2	P	1	M
1957	isouron	55861-78-4	-7.8	2	T	2	D
1958	isoxaben	82558-50-7	-6.85	2	T	1	D
1959	acetoacetanilide	102-01-2	-8.94	2	T	2	M
1960	(1R)-tetramethrin		-7.52	2	T	1	D
1961	daminozide	1596-84-5	-12.04	2	T	2	M
1962	imiprothrin	72963-72-5	-8.61	2	T	1	D
1963	imazamethabenz-methyl	81405-85-8	-9.59	2	T	2	D
1964	imazaquin	81335-37-7	-14.55	2	T	1	M
1965	metalaxyl	57837-19-1	-7.91	2	T	2	M
1966	metalaxyl-M	70630-17-0	-7.84	2	T	1	D
1967	furalaxyl	57646-30-7	-7.28	2	T	2	M
1968	pinoxaden	243973-20-8	-9.43	2	T	1	D
1969	pefurazoate	101903-30-4	-6.65	2	P	2	D
1970	imazamox	114311-32-9	-14.206	2	P	1	D
1971	oxadixyl	77732-09-3	-9.7	2	P	2	D
1972	furmecyclox	60568-05-0	-3.18	2	T	1	D
1973	pyrametostrobin	915410-70-7	-7.734	2	T	2	D
1974	bifenazate	149877-41-8	-7.7	2	T	1	D
1975	chloroacetamide	79-07-2	-6.46	2	T	2	D
1976	randox	93-71-0	-5.15	2	T	1	D
1977	*N*,*N*-diallyldichloroacetamide	37764-25-3	-4.88	2	T	2	M
1978	propanil	709-98-8	-7.53	2	T	1	M
1979	propachlor	1918-16-7	-5.35	2	P	2	M
1980	monalide	7287-36-7	-6.01	2	T	1	M
1981	bromobutide	74712-19-9	-5.68	2	T	2	D
1982	flurochloridon	61213-25-0	-5.8	2	T	1	D
1983	carpropamid	104030-54-8	-6.32	2	T	2	D
1984	pronamide	23950-58-5	-6.4	2	P	1	M
1985	benodanil	15310-01-7	-6.93	2	T	2	M
1986	procymidone	32809-16-8	-6.066	2	T	1	D
1987	fluoroimide	41205-21-4	-3.28	2	T	2	D
1988	chlorphthalim	39985-63-2	-6.1	2	T	1	D
1989	fluometuron	2164-17-2	-6.97	2	T	2	D
1990	monuron	150-68-5	-7.32	1	T	1	D
1991	chlortoluron	15545-48-9	-7.67	2	T	2	D
1992	diuron	330-54-1	-7.52	2	P	1	M
1993	buturon	3766-60-7	-7.5	2	T	2	D
1994	cumyluron	99485-76-4	-9.8	2	T	1	D
1995	pencycuron	66063-05-6	-9.25	1	P	2	D
1996	chlorpropham	101-21-3	-4.52	1	T	1	D
1997	barban	101-27-9	-6.45	2	T	2	M
1998	chlorbufam	1967-16-4	-6.27	2	T	1	M
1999	bromacil	314-40-9	-8.43	1	T	2	D
2000	terbacil	5902-51-2	-8.15	2	T	1	M
2001	chloridazon	1698-60-8	-12.17	2	T	2	M
2002	norflurazon	27314-13-2	-8.69	2	P	1	M
2003	flonicamid	158062-67-0	-10.4	2	T	2	D
2004	metazachlor	67129-08-2	-7.25	1	T	1	D
2005	penflufen	494793-67-8	-7.9	2	T	2	D

2006	sedaxane	874967-67-6	-11.791	2	T	1	D
2007	syn-isopyrazam	683777-13-1	-10.11	2	T	2	D
2008	anti-isopyrazam	683777-14-2	-9.81	2	T	1	D
2009	benzovindiflupyr	1072957-71-1	-9.28	2	T	2	D
2010	fluxapyroxad	907204-31-3	-9.441	2	T	1	D
2011	bixafen	581809-46-3	-7.45	2	P	2	D
2012	fluquinconazole	136426-54-5	-8.6	1	T	1	D
2013	fluopicolide	239110-15-7	-7.45	2	P	2	D
2014	forchlorfenuron	68157-60-8	-9.96	2	T	1	D
2015	fentrazamide	158237-07-1	-8.1	2	T	2	D
2016	diflubenzuron	35367-38-5	-7.29	2	T	1	M
2017	teflubenzuron	83121-18-0	-6.67	2	P	2	D
2018	fenhexamid	126833-17-8	-8.5	2	T	1	D
2019	dimethachlor	50563-36-5	-7	1	P	2	D
2020	alachlor	15972-60-8	-5.47	1	T	1	O
2021	acetochlor	34256-82-1	-5.75	2	T	2	D
2022	butachlor	23184-66-9	-5.68	1	T	1	D
2023	pretilachlor	51218-49-6	-5.96	2	T	2	D
2024	metolachlor	51218-45-2	-5.1	1	T	1	O
2025	S-metolachlor	87392-12-9	-6.05	1	T	2	D
2026	propisochlor	86763-47-5	-5.14	2	P	1	D
2027	butenachlor	87310-56-3	-5.4	2	T	2	D
2028	pethoxamid	106700-29-2	-6.12	2	T	1	D
2029	flutolanil	66332-96-5	-7.78	2	P	2	M
2030	beflubutamid	113614-08-7	-7.35	1	T	1	D
2031	benoxacor	98730-04-2	-5.3	2	T	2	D
2032	furilazole	121776-33-8	-6.25	2	T	1	D
2033	metoxuron	19937-59-8	-9.03	2	T	2	M
2034	chloroxuron	1982-47-4	-8	2	T	1	M
2035	cloethocarb	51487-69-5	-8.94	2	P	2	M
2036	oxadiazon	19666-30-9	-4.61	2	T	1	D
2037	oxadiargyl	39807-15-3	-6.03	2	T	2	D
2038	proquinazid	189278-12-4	-4.84	2	T	1	D
2039	fenoxanil	115852-48-7	-10.09	2	T	2	D
2040	prochloraz	67747-09-5	-6.174	2	P	1	D
2041	furametpyr	123572-88-3	-10.17	2	T	2	D
2042	etoxazole	153233-91-1	-5.87	2	T	1	D
2043	triflumuron	64628-44-0	-6.44	2	T	2	D
2044	hexaflumuron	86479-06-3	-7.39	2	T	1	D
2045	flufenoxuron	101463-69-8	-8.52	1	T	2	D
2046	quinonamide	27541-88-4	-6.3	1	T	1	D
2047	diethatyl-ethyl	38727-55-8	-6.29	2	T	2	D
2048	cyprofuram	69581-33-5	-8.89	2	T	1	M
2049	ofurace	58810-48-3	-7.45	2	T	2	D
2050	benzoylprop-ethyl	22212-55-1	-7.46	1	T	1	M
2051	flamprop-methyl	52756-25-9	-6.74	1	T	2	D
2052	flamprop-M-isopropyl	57973-67-8	-6.16	2	P	1	M
2053	carfentrazone-ethyl	128639-02-1	-6.92	2	T	2	D
2054	valifenalate	283159-90-0	-8.86	2	T	1	D
2055	benzoximate	29104-30-1	-5.66	2	T	2	D
2056	indoxacarb	144171-61-9	-9.69	2	P	1	D
2057	vinclozolin	50471-44-8	-5.75	2	T	2	M
2058	clomazone	81777-89-1	-5.77	2	T	1	D
2059	pydiflumetofen	1228284-64-7	-7.216	2	T	2	D
2060	iprodione	36734-19-7	-8	2	T	1	D
2061	pyraclostrobin	175013-18-0	-8.03	2	T	2	D

2062	chlozolinate	84332-86-5	-6.06	2	T	1	D
2063	acetaldoxime	107-29-9	-3.26	2	T	2	D
2064	2-butanone oxime	96-29-7	-3.26	2	T	1	M
2065	N-nitrosodimethylamine	62-75-9	-4.69	1	T	2	D
2066	N-nitrosodiethylamine	55-18-5	-4.21	1	T	1	D
2067	N-nitrosomethylbutylamine	7068-83-9	-4.12	1	T	2	D
2068	N-nitrosodipropylamine	621-64-7	-4.22	1	P	1	D
2069	N-nitrosomethylpentylamine	13256-07-0	-4.34	1	T	2	D
2070	N-nitrosoethylbutylamine	4549-44-4	-4.03	1	T	1	D
2071	N-nitrosodibutylamine	924-16-3	-3.96	1	P	2	D
2072	di-i-propylnitrosoamine	601-77-4	-4.13	1	T	1	D
2073	N-nitrosopyrrolidine	930-55-2	-6.15	1	P	2	D
2074	N-nitrosopiperidine	100-75-4	-5.06	1	T	1	D
2075	nitrosohexamethyleneimine	932-83-2	-5.46	1	T	2	D
2076	N-Methyl-N-nitrosobenzylamine	937-40-6	-3.72	1	T	1	D
2077	nitromethane	75-52-5	-2.93	1	T	2	D
2078	nitroethane	79-24-3	-2.71	1	T	1	D
2079	1-nitropropane	108-03-2	-2.505	1	T	2	O
2080	1-nitrobutane	627-05-4	-2.27	1	T	1	D
2081	1-nitropentane	628-05-7	-2.07	1	T	2	D
2082	2-nitropropane	79-46-9	-2.314	1	P	1	O
2083	nitrobenzene	98-95-3	-3.01	1	T	2	D
2084	2-nitrotoluene	88-72-2	-2.63	1	T	1	D
2085	3-nitrotoluene	99-08-1	-2.84	1	T	2	O
2086	4-nitrotoluene	99-99-0	-2.57	1	T	1	D
2087	1-nitronaphthalene	86-57-7	-4.14	1	P	2	D
2088	1,3-dinitrobenzene	99-65-0	-4.96	1	P	1	D
2089	1,4-dinitrobenzene	100-25-4	-5	1	T	2	D
2090	2,4-dinitrotoluene	121-14-2	-5.15	2	T	1	M
2091	2,5-dinitrotoluene	619-15-8	-5.07	1	P	2	D
2092	2,6-dinitrotoluene	606-20-2	-5.05	1	T	1	D
2093	1,3,5-trinitrobenzene	99-35-4	-6.91	2	T	2	D
2094	2,4,6-trinitrotoluene	118-96-7	-6.15	2	T	1	M
2095	2,4,6-trinitro-5-*tert*-butyl-*m*-xylene	81-15-2	-2.9	1	T	2	D
2096	cyclonite	121-82-4	-8.92	2	T	1	M
2097	1,3,5,7-tetranitro-1,3,5,7-tetrazocane	2691-41-0	-12.93	1	T	2	D
2098	methyl nitrate	598-58-3	-1.69	1	T	1	D
2099	ethyl nitrate	625-58-1	-1.6	1	T	2	O
2100	1-propyl nitrate	627-13-4	-1.284	1	T	1	O
2101	1-butyl nitrate	928-45-0	-1.201	1	T	2	O
2102	1-pentyl nitrate	1002-16-0	-1.167	1	P	1	O
2103	1-hexyl nitrate	20633-11-8	-1.215	1	T	2	D
2104	2-propyl nitrate	1712-64-7	-1.18	1	P	1	O
2105	2-butyl nitrate	924-52-7	-1.036	1	T	2	O
2106	2-methyl-propyl-1-nitrate	543-29-3	-1.36	1	T	1	O
2107	2-pentyl nitrate	21981-48-6	-0.914	1	T	2	O
2108	3-pentyl nitrate	82944-59-0	-0.951	1	T	1	D
2109	3-methyl-1-butyl nitrate	543-87-3	-1.046	1	T	2	D
2110	1,2-ethane dinitrate	628-96-6	-3.29	1	T	1	O
2111	1,3-propyl dinitrate	3457-90-7	-3.51	1	T	2	O
2112	1,4-butyl dinitrate	3457-91-8	-3.59	1	T	1	O
2113	1,5-pentyl dinitrate	3457-92-9	-3.46	1	T	2	O
2114	1,6-hexyl dinitrate		-3.57	1	T	1	O
2115	1,7-heptyl dinitrate		-3.45	1	P	2	O
2116	1,8-octyl dinitrate		-3.29	1	T	1	O

2117	1,10-decyl dinitrate	3457-97-4	-3.02	1	P	2	O
2118	1,2-propyleneglycol dinitrate	6423-43-4	-2.9	1	T	1	O
2119	1,2-butyl dinitrate	20820-41-1	-2.71	1	T	2	O
2120	1,3-butyl dinitrate	6423-44-5	-3.15	1	T	1	O
2121	2,3-butyl dinitrate	6423-45-6	-2.48	1	T	2	O
2122	1,2-pentyl dinitrate		-2.52	1	P	1	O
2123	1,4-pentyl dinitrate		-2.98	1	P	2	O
2124	cis-2,4-pentyl dinitrate		-2.73	1	T	1	O
2125	trans-2,4-pentyl dinitrate		-2.55	1	T	2	O
2126	1,2-hexyl dinitrate	110539-07-6	-2.38	1	T	1	O
2127	1,5-hexyl dinitrate		-2.83	1	P	2	O
2128	2,5-hexyl dinitrate		-2.89	1	T	1	O
2129	1,2-octyl dinitrate		-2.11	1	T	2	O
2130	1,2-decyl dinitrate		-1.69	1	P	1	O
2131	cis-1,2-cyclohexyl dinitrate		-3.5	1	T	2	O
2132	cis-1,3-cyclohexyl dinitrate		-3.93	1	T	1	O
2133	trans-1,2-cyclohexyl dinitrate		-3.11	1	T	2	O
2134	trans-1,3-cyclohexyl dinitrate		-3.23	1	T	1	O
2135	trans-1,2-cycloheptyl dinitrate		-3.34	1	T	2	O
2136	nitroglycerol	55-63-0	-4.81	2	T	1	D
2137	pentaerythrittetranitrate	78-11-5	-8.52	2	T	2	D
2138	o-nitroaniline	88-74-4	-4.77	2	T	1	D
2139	m-nitroaniline	99-09-2	-6.49	1	T	2	D
2140	p-nitroaniline	100-01-6	-7.288	1	T	1	D
2141	4-amino-2,6-dinitrotoluene	19406-51-0	-7.26	1	T	2	D
2142	4-((4-nitrophenyl)azo)benzenamine	730-40-5	-8.14	2	P	1	M
2143	pendimethalin	40487-42-1	-3.38	2	T	2	M
2144	butralin	33629-47-9	-3.17	2	T	1	M
2145	isopropalin	33820-53-0	-2.83	2	P	2	D
2146	4-nitroazobenzene	2491-52-3	-4.65	2	T	1	M
2147	N-methyl-N,2,4,6-tetranitroaniline	479-45-8	-8.4	2	T	2	M
2148	ethylnitrosocyanamide	38434-77-4	-3.05	1	T	1	D
2149	methylnitrosoacetamide	7417-67-6	-2.6	1	T	1	D
2150	orysastrobin	248593-16-0	-8.86	2	T	2	D
2151	cymoxanil	57966-95-7	-7.47	2	T	2	D
2152	2-nitrophenol	88-75-5	-3.36	1	T	1	D
2153	3-nitrophenol	554-84-7	-7.05	1	T	2	D
2154	4-nitrophenol	100-02-7	-7.58	2	T	1	D
2155	4-methyl-2-nitrophenol	119-33-5	-3.05	1	T	2	O
2156	5-methyl-2-nitrophenol	700-38-9	-3.12	1	P	1	O
2157	3-methyl-4-nitrophenol	2581-34-2	-6	1	T	2	D
2158	3-methyl-2-nitrophenol	4920-77-8	-3.8	1	T	1	O
2159	2-methyl-6-nitrophenol	13073-29-5	-2.72	1	P	2	O
2160	4-sec-butyl-2-nitrophenol	3555-18-8	-2.3	1	T	1	O
2161	2,4-dinitrophenol	51-28-5	-5.37	1	T	2	O
2162	2,5-dinitrophenol	329-71-5	-5.5	2	P	1	D
2163	4,6-dinitro-o-cresol	534-52-1	-4.9	1	T	2	O
2164	2,6-dinitro-p-cresol	609-93-8	-5.57	1	T	1	O
2165	dinoseb	88-85-7	-4.58	2	T	2	M
2166	dinoterb	1420-07-1	-4.77	2	T	1	M
2167	2,4,6-trinitrophenol	88-89-1	-8.87	2	P	2	M
2168	2-nitrooxy-ethanol	16051-48-2	-5.98	1	T	1	O
2169	4-nitrooxy-1-butanol	22911-39-3	-5.75	1	T	2	O
2170	5-nitrooxy-1-pentanol		-5.7	1	T	1	O
2171	2-nitrooxy-1-propanol	20266-74-4	-5.24	1	P	2	O
2172	2-nitrooxy-1-butanol	147794-12-5	-5.166	1	T	1	D

2173	3-nitrooxy-1-butanol		-5.25	1	T	2	O
2174	4-nitrooxy-1-pentanol		-5.45	1	T	1	O
2175	1-nitrooxy-2-propanol	20266-65-3	-5.426	1	T	2	D
2176	1-nitrooxy-2-butanol	147794-11-4	-5.15	1	T	1	O
2177	4-nitrooxy-2-butanol		-5.26	1	P	2	O
2178	2-nitrooxy-3-butanol	147794-10-3	-5.393	1	P	1	O
2179	2-[ethyl[4-[(4-nitrophenyl)azo]phenyl]-amino]ethanol	2872-52-8	-10.63	2	T	2	D
2180	4-(4-nitrophenylazo)phenol	1435-60-5	-9	2	T	1	D
2181	N-nitrosomorpholine	59-89-2	-6.35	1	T	2	D
2182	2,6-dimethyl-N-nitrosomorpholine	1456-28-6	-4.96	1	T	1	D
2183	o-nitroanisole	91-23-6	-3.79	1	T	2	D
2184	p-nitroanisole	100-17-4	-4.09	1	T	1	D
2185	diethylene diglycol dinitrate	693-21-0	-4.797	2	T	2	D
2186	oxabetrinil	74782-23-3	-5.33	2	T	1	D
2187	metominostrobin	133408-50-1	-7.79	2	T	2	D
2188	dimoxystrobin	149961-52-4	-9.324	2	T	1	D
2189	musk ketone	81-14-1	-4.38	2	T	2	M
2190	nitrooxyacetone	6745-71-7	-4.39	1	T	1	O
2191	nitrothal-isopropyl	10552-74-6	-6.15	2	T	2	M
2192	dinoseb acetate	2813-95-8	-6.58	2	T	1	M
2193	binapacryl	485-31-4	-5.73	2	T	2	M
2194	dinocap[3]	39300-45-3	-5.49	2	P	1	D
2195	methyldinocap	131-72-6	-5.37	2	T	2	D
2196	4-methoxy-2-nitrophenol	1568-70-3	-3.95	1	T	1	O
2197	4-formyl-2-nitrophenol	3011-34-5	-4.19	2	T	2	D
2198	tralkoxydim	87820-88-0	-7.57	2	T	1	D
2199	kresoxim-methyl	143390-89-0	-6.61	1	P	2	D
2200	fenpyroximate	111812-58-9	-4.26	2	T	1	D
2201	(Z)-pyriminobac-methyl	147411-70-9	-7.68	2	T	2	D
2202	(E)-pyriminobac-methyl	147411-69-6	-6.26	2	T	1	D
2203	peroxyacetyl nitrate	2278-22-0	-1.835	1	T	2	D
2204	peroxypropionyl nitrate	5796-89-4	-1.71	1	T	1	D
2205	peroxybutyryl nitrate	138779-12-1	-1.61	1	T	2	D
2206	peroxyisobutyryl nitrate	65424-60-4	-1.27	1	T	1	D
2207	peroxymethacryloyl nitrate	88181-75-3	-1.5	1	P	2	D
2208	1-nitroguanidin	556-88-7	-13.5	2	T	1	M
2209	N-nitroso-N-methylurethane	615-53-2	-3.3	1	T	2	D
2210	1-chloro-1-nitroethane	598-92-5	-1.7	2	T	1	M
2211	1-chloro-1-nitropropane	600-25-9	-2.06	2	P	2	M
2212	1,1-dichloro-1-nitroethane	594-72-9	-1.28	2	T	1	D
2213	trichloronitromethane	76-06-2	-1.066	1	T	2	O
2214	2-chloro-1-nitrobenzene	88-73-3	-2.74	1	T	1	D
2215	m-chloronitrobenzene	121-73-3	-3.26	1	T	2	D
2216	p-chloronitrobenzene	100-00-5	-2.92	2	T	1	M
2217	2,3-dichloronitrobenzene	3209-22-1	-3.57	2	P	2	M
2218	2,5-dichloronitrobenzene	89-61-2	-3.31	1	T	1	D
2219	3,4-dichloronitrobenzene	99-54-7	-3.48	1	T	2	D
2220	2,4-dichloronitrobenzene	611-06-3	-3.14	2	T	1	D
2221	quintozene	82-68-8	-3.82	1	T	2	O
2222	3-bromo-1-nitrobenzene	585-79-5	-4.12	2	P	1	D
2223	1-chloro-2,4-dinitrobenzene	97-00-7	-5.01	2	T	2	M
2224	2-chloro-4-nitroaniline	121-87-9	-6.41	1	T	1	D
2225	2,6-dichloro-4-nitroaniline	99-30-9	-5.46	2	P	2	M
2226	fluazinam	79622-59-6	-2.91	2	T	1	M
2227	trifluralin	1582-09-8	-2.25	1	T	2	O

2228	benefin	1861-40-1	-2.04	2	T	1	D
2229	fluchloralin	33245-39-5	-2.94	2	P	2	M
2230	profluralin	26399-36-0	-1.92	2	T	1	D
2231	ethalfluralin	55283-68-6	-2.28	2	T	2	D
2232	flumetralin	62924-70-3	-2.75	2	T	1	D
2233	dinitramine	29091-05-2	-4.246	2	T	2	D
2234	prodiamine	29091-21-2	-3.5	2	P	1	M
2235	formaldehyde O-((perfluorophenyl)methyl) oxime	86356-73-2	-1.607	1	T	2	O
2236	acetaldehyde-O-pentafluorobenzyloxime	114611-59-5	-1.67	1	T	1	O
2237	n-hexanal, O-[(pentafluorophenyl)-methyl]oxime		-1.156	1	T	2	O
2238	n-octanal, O-[(pentafluorophenyl)-methyl]oxime		-1.294	1	T	1	O
2239	n-decanal, O-[(pentafluorophenyl)-methyl]oxime		-1.781	1	P	2	O
2240	N-[(pentafluorophenyl)methoxy]-propan-2-imine	899828-53-6	-1.438	1	T	1	O
2241	N-[(pentafluorophenyl)methoxy]-butan-2-imine		-1.062	1	P	2	O
2242	(E)-N-[(pentafluorophenyl)methoxy]-pentan-2-imine		-0.966	1	T	1	O
2243	(E,E)-N-[(pentafluorophenyl)methoxy]prop2-en-1-imine	932710-55-9	-1.372	1	T	2	O
2244	N-[(pentafluorophenyl)methoxy]but-2-en-1-imine	932710-52-6	-1.227	1	T	1	O
2245	N-[(pentafluorophenyl)methoxy]-1-phenyl-methanimine		-1.095	1	T	2	O
2246	1-(4-methylphenyl)-N-[(pentafluorophenyl)-methoxy]methanimine		-1.215	1	P	1	O
2247	1-(9H-fluoren-9-yl)-N-[(pentafluorophenyl)-methoxy]methanimine		-1.435	1	T	2	O
2248	N1,N2-bis[(pentafluorophenyl)-methoxy]-ethane-1,2-diimine	618858-54-1	-1.602	1	T	1	O
2249	pyrifenox	88283-41-4	-5.76	2	T	2	D
2250	monolinuron	1746-81-2	-6.53	1	T	1	D
2251	linuron	330-55-2	-6.92	1	T	2	M
2252	metobromuron	3060-89-7	-7.16	2	P	1	D
2253	chlorbromuron	13360-45-7	-6.74	2	T	2	D
2254	bronopol	52-51-7	-8.49	2	T	1	D
2255	5-fluoro-2-nitrophenol	446-36-6	-2.94	1	T	2	O
2256	4-chloro-2-nitrophenol	89-64-5	-3.29	2	T	1	D
2257	4-chloro-5-methyl-2-nitrophenol	7147-89-9	-2.7	2	T	2	D
2258	2-{[(pentafluorophenyl)methoxy]-imino}-propan-1-ol		-1.826	1	T	1	O
2259	2-methyl-3-{[(pentafluorophenyl)-methoxy]-imino}-butan-2-ol		-1.486	1	T	2	O
2260	bromofenoxim	13181-17-4	-10.28	2	T	1	M
2261	nitrofen	1836-75-5	-3.91	2	T	2	M
2262	chlomethoxyfen	32861-85-1	-3.1	2	T	1	D
2263	oxyfluorfen	42874-03-3	-4.47	2	T	2	M
2264	fluorodifen	15457-05-3	-6.13	2	P	1	M
2265	aclonifen	74070-46-5	-5.66	2	T	2	M
2266	fluxofenim	88485-37-4	-3.53	2	T	1	D
2267	trifloxystrobin	141517-21-7	-6.03	2	T	2	D
2268	bifenox	42576-02-3	-7.34	2	T	1	D
2269	lactofen	77501-63-4	-5.8	2	T	2	M
2270	tepraloxydim	149979-41-9	-8.11	2	P	1	D

2271	propaquizafop	111479-05-1	-9.9	2	T	2	D
2272	imidacloprid	138261-41-3	-12.87	2	T	1	D
2273	fluoxastrobin	361377-29-9	-10.39	1	T	2	D
2274	methanethiol	74-93-1	-0.995	1	T	1	O
2275	ethanethiol	75-08-1	-0.838	1	T	2	O
2276	n-propanethiol	107-03-9	-0.777	1	T	1	O
2277	n-butanethiol	109-79-5	-0.57	1	P	2	O
2278	pentyl mercaptan	110-66-7	-0.3	2	P	1	D
2279	n-heptyl mercaptan	1639-09-4	0	2	T	2	D
2280	isopropyl mercaptan	75-33-2	-0.52	2	T	1	O
2281	isobutyl mercaptan	513-53-1	-0.53	2	T	2	D
2282	sec-butyl mercaptan	513-44-0	-0.53	2	T	1	D
2283	dimethyl sulfide	75-18-3	-1.6	1	T	2	D
2284	methyl ethyl sulfide	624-89-5	-1.1	1	P	1	D
2285	diethyl sulfide	352-93-2	-1.07	1	T	2	D
2286	dipropyl sulfide	111-47-7	-0.903	1	T	1	O
2287	diisopropyl sulfide	625-80-9	-0.869	1	T	2	O
2288	allyl methyl sulfide	10152-76-8	-1.02	1	T	1	O
2289	diallyl sulfide	592-88-1	-1.01	1	T	2	D
2290	thiophenol	108-98-5	-1.87	1	T	1	D
2291	phenyl methyl sulfide	100-68-5	-2	1	T	2	D
2292	dimethyl disulfide	624-92-0	-1.26	1	T	1	D
2293	diethyl disulfide	110-81-6	-1	1	T	2	D
2294	dipropyl disulfide	629-19-6	-0.77	1	P	1	O
2295	diallyl disulfide	2179-57-9	0.23	2	T	2	D
2296	thiophene	110-02-1	-1.033	1	T	1	O
2297	2-methylthiophene	554-14-3	-1.01	1	P	2	D
2298	3-methylthiophene	616-44-4	-0.534	2	T	1	D
2299	dibenzothiophene	132-65-0	-2.86	2	T	2	M
2300	2,3,4-trithiapentane	3658-80-8	-1.72	1	T	1	D
2301	2,2'-dichlorodiethylsulfide	505-60-2	-3	1	T	2	D
2302	1,2-bis(2-chloroethylthio)ethane	3563-36-8	-5.34	2	T	1	D
2303	tetrasul	2227-13-6	-3.16	2	T	2	D
2304	isoprothiolane	50512-35-1	-5.97	2	T	1	D
2305	2,2'-thiobis-4,6-dichlorophenol	97-18-7	-8.45	2	T	2	D
2306	*S*-ethyl-2-methyl-4-chlorophenoxythio-acetate	25319-90-8	-2.76	2	T	1	M
2307	4-(pentafluorothio)phenol	774-94-7	-5	2	T	2	O
2308	methyl isothiocyanate	556-61-6	-1.95	1	T	1	M
2309	allyl isothiocyanate	57-06-7	-1.97	2	T	2	M
2310	phenyl isothiocyanate	103-72-0	-0.92	2	T	1	M
2311	thiram	137-26-8	-6.98	2	T	2	M
2312	dazomet	533-74-4	-7.69	1	P	1	D
2313	tricyclazole	41814-78-2	-8.896	2	T	2	M
2314	acibenzolar-S-methyl	135158-54-2	-5.31	2	T	1	D
2315	simetryn	1014-70-6	-7.56	2	T	2	D
2316	desmetryn	1014-69-3	-7.38	2	P	1	M
2317	ametryn	834-12-8	-6.74	2	T	2	D
2318	prometryn	7287-19-6	-6.49	1	T	1	M
2319	dipropretryn	4147-51-7	-6.2	2	T	2	M
2320	dimethatryn	22936-75-0	-6.41	1	T	1	M
2321	terbutryn	886-50-0	-6.3	1	T	2	D
2322	thiabendazole	148-79-8	-10.96	1	T	1	D
2323	cymiazole	61676-87-7	-5.57	2	P	2	D
2324	buthiobate	51308-54-4	-4.92	2	T	1	D
2325	methoprotryne	841-06-5	-8.06	2	T	2	M

2326	dithianon	3347-22-6	-9.07	2	T	1	D
2327	pyriftalid	135186-78-6	-8.8	2	P	2	D
2328	octhilinone	26530-20-1	-6.07	2	T	1	D
2329	quinomethionate	2439-01-2	-5.22	2	T	2	M
2330	thiodicarb	59669-26-0	-7.69	2	T	1	M
2331	carbosulfan	55285-14-8	-4.68	2	P	2	D
2332	furathiocarb	65907-30-4	-7.26	2	T	1	D
2333	pyributicarb	88678-67-5	-5.03	2	T	2	D
2334	benfuracarb	82560-54-1	-6.082	2	T	1	D
2335	chloromethiuron	28217-97-2	-8.5	2	T	2	D
2336	2-chloroallyl diethyldithiocarbamate	95-06-7	-3.53	1	T	1	D
2337	chlorpromazine	50-53-3	-8.21	2	P	2	M
2338	dithiopyr	97886-45-8	-4.21	1	T	1	M
2339	2,6-dichlorothiobenzamide	1918-13-4	-7.65	2	T	2	M
2340	flubenzimine	37893-02-0	-3.72	2	T	1	D
2341	imibenconazole	86598-92-7	-8.08	2	T	2	D
2342	thiacloprid	111988-49-9	-12.35	2	T	1	D
2343	etridiazole	2593-15-9	-4.944	2	P	2	M
2344	flutianil	958647-10-4	-5.25	2	T	1	D
2345	flurazole	72850-64-7	-5	2	T	2	D
2346	thiazopyr	117718-60-2	-4.81	2	T	1	M
2347	pyridate	55512-33-9	-6.37	2	T	2	D
2348	captan	133-06-2	-6.75	2	T	1	M
2349	captafol	2425-06-1	-7.69	2	T	2	M
2350	folpet	133-07-3	-5.5	2	T	1	D
2351	benazolin	3813-05-6	-10.02	2	T	2	M
2352	benazolin-ethyl	25059-80-7	-6.11	2	T	1	M
2353	3-aminophenylsulfur pentafluoride	2993-22-8	-4.2	2	T	2	O
2354	4-aminophenylsulfur pentafluoride	2993-24-0	-4	2	T	1	O
2355	metsulfovax	21452-18-6	-9.36	2	T	2	D
2356	methiocarb	2032-65-7	-7	1	T	1	D
2357	ethiofencarb	29973-13-5	-7.33	2	T	2	M
2358	benzthiazuron	1929-88-0	-9.68	1	T	1	D
2359	methabenzthiazuron	18691-97-9	-7.64	2	T	2	M
2360	tebuthiuron	34014-18-1	-7.96	2	P	1	M
2361	thidiazuron	51707-55-2	-10.75	2	T	2	M
2362	metribuzin	21087-64-9	-7.72	2	T	1	M
2363	ethiozin	64529-56-2	-6.45	2	T	2	D
2364	isomethiozin	57052-04-7	-5.94	2	P	1	D
2365	fenamidone	161326-34-7	-8.33	1	T	2	D
2366	S-ethyl dipropylthiocarbamate	759-94-4	-3.14	1	P	1	D
2367	pebulate	1114-71-2	-3.01	2	T	2	D
2368	vernolate	1929-77-7	-2.97	2	T	1	M
2369	butylate	2008-41-5	-2.46	2	T	2	M
2370	molinate	2212-67-1	-4.31	2	T	1	O
2371	cycloate	1134-23-2	-3.51	2	T	2	M
2372	prosulfocarb	52888-80-9	-4.27	2	T	1	D
2373	esprocarb	85785-20-2	-3.66	2	P	2	D
2374	dimepiperate	61432-55-1	-5.84	2	T	1	D
2375	buprofezin	69327-76-0	-4.62	2	T	2	D
2376	carboxine	5234-68-4	-7.94	2	T	1	D
2377	mefenacet	73250-68-7	-7.27	2	T	2	M
2378	fenothiocarb	62850-32-2	-6.12	2	P	1	M
2379	triazamate	112143-82-5	-8.33	2	T	2	M
2380	isofetamid	875915-78-9	-7.942	2	T	1	D
2381	aldicarb	116-06-3	-7	1	T	2	M

2382	methomyl	16752-77-5	-9.07	1	P	1	M
2383	oxamyl	23135-22-0	-10.8	1	T	2	M
2384	penthiopyrad	183675-82-3	-6.95	2	T	2	D
2385	tiadinil	223580-51-6	-8.12	2	T	1	D
2386	thiazafluron	25366-23-8	-7.63	2	T	1	M
2387	diallate	2303-16-4	-4.36	2	T	2	M
2388	triallate	2303-17-5	-3.31	2	T	1	D
2389	thiobencarb	28249-77-6	-4.74	2	P	2	D
2390	orbencarb	34622-58-7	-4.7	2	P	1	D
2391	hexythiazox	78587-05-0	-6.05	2	T	2	M
2392	dimethenamid	87674-68-8	-5.475	1	P	1	D
2393	dimethenamid-P	163515-14-8	-6.71	1	T	2	D
2394	thenylchlor	96491-05-3	-6.48	2	T	1	D
2395	thifluzamide	130000-40-7	-9.47	2	T	2	D
2396	flufenacet	142459-58-3	-6.24	2	T	1	D
2397	butocarboxim	34681-10-2	-7.41	2	P	2	D
2398	thiofanox	39196-18-4	-6.42	2	T	1	M
2399	cycloxiydim	101205-02-1	-7.26	2	T	2	D
2400	sethoxydim	74051-80-2	-6.95	2	T	1	D
2401	clethodim	99129-21-2	-7.87	2	T	2	D
2402	clothianidin	210880-92-5	-13.42	2	T	1	D
2403	thiamethoxam	153719-23-4	-12.72	2	T	2	D
2404	4-nitrophenylsulfur pentafluoride	2613-27-6	-2.6	2	T	1	O
2405	dimethipin	55290-64-7	-9.03	2	T	2	D
2406	ethyl methanesulfonate	62-50-0	-5.36	2	T	1	D
2407	1,3-propane sultone	1120-71-4	-6.59	2	T	2	M
2408	dimethyl sulfate	77-78-1	-3.79	2	T	1	M
2409	diethyl sulfate	64-67-5	-3.6	2	T	2	M
2410	dimethyl sulfoxide	67-68-5	-6.31	4	T	1	M
2411	benfuresate	68505-69-1	-5.96	2	T	2	D
2412	ethofumesate	26225-79-6	-7.4	1	T	1	D
2413	propargite	2312-35-8	-5.4	2	T	2	D
2414	endosulfan sulfate	1031-07-8	-4.88	2	T	1	D
2415	tetradifon	116-29-0	-3.915	2	T	2	D
2416	alpha-endosulfan	959-98-8	-3.56	1	T	1	D
2417	endosulfan II	33213-65-9	-4.574	1	P	2	O
2418	fluoromethyl sulfone	558-25-8	-2.6	2	T	1	D
2419	sulcotrione	99105-77-8	-8.4	2	T	2	D
2420	tembotrione	335104-84-2	-10.68	2	T	1	D
2421	tralopyril	122454-29-9	-7.05	2	T	2	M
2422	bentazon	25057-89-0	-8.87	2	P	1	D
2423	bupirimate	41483-43-6	-6.12	2	T	2	M
2424	sulfometuron-methyl	74222-97-2	-14.77	2	T	1	M
2425	ethametsulfuron-methyl	97780-06-8	-12.72	2	T	2	D
2426	bensulfuron-methyl	83055-99-6	-12.65	2	T	1	D
2427	metsulfuron-methyl	74223-64-6	-12.04	2	T	2	D
2428	tribenuron-methyl	101200-48-0	-9.886	2	P	1	D
2429	thifensulfuron-methyl	79277-27-3	-12.75	1	P	2	M
2430	fluensulfone	318290-98-1	-5.178	2	T	1	D
2431	ethiprole	181587-01-9	-8.8	2	T	2	D
2432	fipronil	120068-37-3	-6.78	2	T	1	D
2433	flumetsulam	98967-40-9	-14.56	2	T	2	M
2434	N-methylperfluorooctane-sulfonamido-ethanol	24448-09-7	-3.95	2	T	1	O
2435	N-ethyl-N-(2-hydroxyethyl)-perflu-orooctyl-sulfonamide	1691-99-2	-3.35	2	P	2	O

2436	2-(N-ethylperfluorooctane-sulfona-mido)ethyl acrylate	423-82-5	-3.44	2	T	1	O
2437	triafamone	874195-61-6	-7.31	2	T	2	D
2438	isoxaflutole	141112-29-0	-7.7	1	T	1	D
2439	dichlofluanid	1085-98-9	-4.55	2	T	2	M
2440	tolylfluanid	731-27-1	-4.2	2	T	1	D
2441	chlorsulfuron	64902-72-3	-11.24	2	T	2	D
2442	triasulfuron	82097-50-5	-12.3	2	T	1	M
2443	chlorimuron-ethyl	90982-32-4	-11	2	T	2	M
2444	cafenstrole	125306-83-4	-9.3	2	P	1	D
2445	ethidimuron	30043-49-3	-10.25	2	T	2	M
2446	aldicarb sulfone	1646-88-4	-6.97	2	T	1	M
2447	aldicarb sulfoxide	1646-87-3	-7.4	2	T	2	D
2448	thiencarbazone-methyl	317815-83-1	-10.26	2	T	1	D
2449	sulfentrazone	122836-35-5	-9.73	2	T	2	D
2450	diclosulam	145701-21-9	-13.8	2	T	1	D
2451	metosulam	139528-85-1	-15.5	1	P	2	D
2452	penoxsulam	219714-96-2	-14.48	2	T	1	D
2453	pyrasulfotole	365400-11-9	-10.65	2	T	2	D
2454	cloransulam-methyl	147150-35-4	-14.6	2	P	1	D
2455	nitralin	4726-14-1	-6.18	2	T	2	M
2456	oryzalin	19044-88-3	-10.49	2	T	1	D
2457	butoxycarboxim	34681-23-7	-9.67	2	T	2	D
2458	flusulfamide	106917-52-6	-7	2	T	1	D
2459	trimethyl phosphate	512-56-1	-6.33	1	T	2	D
2460	triethyl phosphate	78-40-0	-5.53	1	T	1	D
2461	tripropyl phosphate	513-08-6	-4.47	1	T	2	D
2462	tributyl phosphate	126-73-8	-4.585	1	P	1	D
2463	2-ethylhexanol phosphate	78-42-2	-1.99	2	T	2	M
2464	diisopropyl methyl phosphonate	1445-75-6	-4.72	2	T	1	M
2465	2-ethylhexyl diphenyl phosphate	1241-94-7	-3.59	2	T	2	M
2466	triphenylphosphate	115-86-6	-4.61	2	T	1	M
2467	tert-butylphenyl diphenyl phosphate[4]	56803-37-3	-4.44	1	T	2	D
2468	tri-2-butoxyethyl phosphate	78-51-3	-7.92	2	T	1	M
2469	crotoxyphos	7700-17-6	-6.42	2	T	2	M
2470	trichloroethyl phosphate	115-96-8	-7.38	2	P	1	M
2471	naled	300-76-5	-5.33	2	T	2	M
2472	1-chloro-2-propanol phosphate 2473	13674-84-5	-6.77	2	T	1	M
tris(1,3-dichloroisopropyl) phosphate 2474		13674-87-8	-8.01	2	T	2	M
dichlorvos		62-73-7	-4.98	1	T	1	D
2475	heptenophos	23560-59-0	-5.34	1	T	2	D
2476	etephon	16672-87-0	-11.147	2	T	1	D
2477	isofluorphate	55-91-4	-3.28	2	T	2	M
2478	dimethylvinphos	2274-67-1	-5.874	2	T	1	D
2479	chlorfenvinphos	470-90-6	-6.06	2	T	2	M
2480	tetrachlorvinphos	961-11-5	-6.77	2	T	1	M
2481	soman	96-64-0	-3.41	2	T	2	M
2482	trichlorfon	52-68-6	-9.37	2	T	1	M
2483	tabun	77-81-6	-5.11	2	T	2	M
2484	isopestox	371-86-8	-6.46	2	T	1	M
2485	monocrotophos	6923-22-4	-10.04	2	T	2	D
2486	dicrotophos	141-66-2	-8.687	1	T	1	D
2487	paraoxon	311-45-5	-7.05	2	T	2	M
2488	ethoprophos	13194-48-4	-5.02	2	T	1	M
2489	cadusafos	95465-99-9	-4.278	2	T	2	D
2490	tribufos	78-48-8	-4.4	2	T	1	M

2491	ethion	563-12-2	-4.91	2	T	2	M
2492	iprobenfos	26087-47-8	-5.93	2	T	1	M
2493	salithion	3811-49-2	-2.94	2	T	2	M
2494	ediphenphos	17109-49-8	-6.99	2	T	1	M
2495	fonofos	944-22-9	-3.68	1	P	2	M
2496	propaphos	7292-16-2	-5.93	2	T	1	M
2497	demeton-S-methyl	919-86-8	-6.55	2	T	2	M
2498	demeton-O-methyl	867-27-6	-3.9	2	T	1	M
2499	demeton-S	126-75-0	-5.51	2	P	2	M
2500	demeton-O	298-03-3	-4.01	2	T	1	D
2501	thiometon	640-15-3	-4.48	2	T	2	M
2502	phorate	298-02-2	-3.748	2	T	1	D
2503	disulfoton	298-04-4	-3.91	2	P	2	M
2504	terbufos	13071-79-9	-3.47	2	T	1	M
2505	fenthion	55-38-9	-4.15	2	T	2	D
2506	sulprofos	35400-43-2	-3.81	2	P	1	M
2507	temephos	3383-96-8	-5.46	2	T	2	M
2508	(E)-methacrifos	62610-77-9	-4.21	2	T	1	M
2509	malaoxon	1634-78-2	-7.37	2	T	2	D
2510	malathion	121-75-5	-5.62	1	P	1	D
2511	phenthoate	2597-03-7	-4.95	2	T	2	M
2512	sulfotep	3689-24-5	-3.76	2	T	1	M
2513	tetrapropyl dithiopyrophosphate	3244-90-4	-4.18	2	P	2	D
2514	chlorethoxyfos	54593-83-8	-1.85	1	T	1	D
2515	chlormephos	24934-91-6	-3.05	2	T	2	M
2516	tolclofos-methyl	57018-04-9	-3.23	2	P	1	M
2517	dichlofenthion	97-17-6	-2.77	2	T	2	D
2518	ronnel	299-84-3	-2.63	2	T	1	D
2519	profenophos	41198-08-7	-5.724	2	P	2	M
2520	bromophos	2104-96-3	-1.8	2	T	1	M
2521	bromophos-ethyl	4824-78-6	-2.79	2	T	2	M
2522	iodophenphos	18181-70-9	-3.43	2	T	1	M
2523	prothiofos	34643-46-4	-2.92	2	T	2	D
2524	trichloronate	327-98-0	-3.07	2	T	1	M
2525	leptophos	21609-90-5	-4.77	2	P	2	M
2526	chlorthiophos	21923-23-9	-3.57	2	T	1	D
2527	carbophenothion	786-19-6	-4.75	2	T	2	M
2528	coumaphos	56-72-4	-5.45	2	T	1	M
2529	fenamiphos	22224-92-6	-7.62	2	T	2	D
2530	fosthietam	21548-32-3	-9.08	1	T	1	D
2531	cyolane	947-02-4	-8.1	2	T	2	M
2532	O-ethyl S-diisopropylaminoethyl methylphosphonothioate	50782-69-9	-6.475	2	T	1	D
2533	cyanophos	2636-26-2	-4.43	2	T	2	M
2534	phoxim	14816-18-3	-5.09	2	P	1	M
2535	triazophos	24017-47-8	-6.19	2	T	2	M
2536	thionazin	297-97-2	-4.9	1	T	1	D
2537	diazinon	333-41-5	-4.22	1	T	2	D
2538	tebupirimfos	96182-53-5	-3.73	2	T	1	D
2539	quinalphos	13593-03-8	-5.42	2	P	2	M
2540	imicyafos	140163-89-9	-12.57	2	T	1	D
2541	pirimiphos-methyl	29232-93-7	-4.91	2	P	2	M
2542	pirimiphos-ethyl	23505-41-1	-4.52	2	T	1	M
2543	etrimfos	38260-54-7	-4.48	2	T	2	D
2544	isoxathion	18854-01-8	-4.67	2	P	1	M
2545	propetamphos	31218-83-4	-5.43	2	T	2	M

2546	isofenphos	25311-71-1	-5.6	1	T	1	D
2547	acephate	30560-19-1	-10.58	2	P	2	D
2548	ditalimfos	5131-24-8	-6.75	2	T	1	M
2549	fosthiazate	98886-44-3	-8.148	1	T	2	D
2550	methidathion	950-37-8	-6.53	2	T	1	D
2551	pyraclofos	77458-01-6	-7.75	2	T	2	D
2552	isazophos	42509-80-8	-4.35	2	T	1	M
2553	methylchlorpyrifos	5598-13-0	-3.66	2	T	2	D
2554	chlorpyrifos	2921-88-2	-3.77	1	P	1	O
2555	dimethoate	60-51-5	-8.11	2	P	2	M
2556	prothoate	2275-18-5	-7.36	1	P	1	D
2557	piperophos	24151-93-7	-6.34	2	T	2	D
2558	formothion	2540-82-1	-6.62	2	T	1	M
2559	phosmet	732-11-6	-5.87	2	T	2	M
2560	pyridaphenthion	119-12-0	-8.1	2	T	1	D
2561	azinphos-methyl	86-50-0	-8.35	2	T	2	M
2562	azinphos-ethyl	2642-71-9	-6.36	2	T	1	M
2563	dialifor	10311-84-9	-5.14	2	T	2	D
2564	phosalone	2310-17-0	-5.6	2	T	1	M
2565	azamethiphos	35575-96-3	-8.87	2	T	2	D
2566	parathion-methyl	298-00-0	-4.6	1	T	1	D
2567	fenitrothion	122-14-5	-4.42	1	T	2	D
2568	parathion	56-38-2	-4.47	2	T	1	D
2569	isoparathion	597-88-6	-5.18	2	T	2	D
2570	O-ethyl O-p-nitrophenyl benzenethio-phosphonate	2104-64-5	-5.68	2	T	1	M
2571	butamifos	36335-67-8	-4.92	2	P	2	M
2572	dicapthon	2463-84-5	-5.01	2	T	1	M
2573	chlorthion	500-28-7	-5.22	2	T	2	M
2574	fensulfothion	115-90-2	-6.27	2	T	1	M
2575	bensulide	741-58-2	-7.31	2	T	2	M
2576	methylarsine	593-52-2	1.65	2	T	1	D
2577	ethylarsine	593-59-9	1.42	2	T	2	M
2578	dimethyl selenide	593-79-3	-1.153	1	T	1	D
2579	dimethyl diselenide	7101-31-7	-0.54	2	T	2	D
2580	tetramethylsilane	75-76-3	2.23	2	T	1	D
2581	tetraethylsilane	631-36-7	2.03	1	T	1	D
2582	dimethylmercury	593-74-8	-0.51	1	T	2	D
2583	tetramethyltin	594-27-4	0.86	2	T	2	D
2584	tetramethyllead	75-74-1	0.18	2	T	1	D
2585	tetraethyllead	78-00-2	1.38	1	T	2	D
2586	dichloro(methyl)arsane	593-89-5	-1.1	2	T	1	D
2587	trans-dichloro(2-chlorovinyl)arsine	541-25-3	-2.05	2	P	1	D
2588	chloromethylmercury	115-09-3	-4.57	1	T	2	D
2589	trimethyllead chloride	1520-78-1	-3.79	2	T	2	M
2590	diphenylarsinchlorid	712-48-1	-5.18	2	T	1	D
2591	trimethylsilanol	1066-40-6	-2.74	1	T	2	O
2592	dimethylsilanediol	1066-42-8	-6.7	1	T	1	D
2593	tetraethyl silicate	78-10-4	-1.97	2	T	2	M
2594	hexamethyldisiloxane	107-46-0	2.49	1	T	1	O
2595	octamethyltrisiloxane	107-51-7	3.07	1	P	2	O
2596	decamethyltetrasiloxane	141-62-8	3.45	1	T	1	O
2597	octamethylcyclotetrasiloxane	556-67-2	2.69	1	P	2	O
2598	decamethylcyclopentasiloxane	541-02-6	2.43	1	T	1	O
2599	dodecamethylcyclohexasiloxane	540-97-6	3	1	T	2	D
2600	hydroxymethyl mercury	1184-57-2	-6.38	1	T	1	D

2601	tributyltin oxide	56-35-9	-4.39	2	T	2	M
2602	phenylmercuric acetate	62-38-4	-7.63	2	T	1	M
2603	triphenyltin hydroxide	76-87-9	-8.43	2	T	2	M
2604	fentin acetate	900-95-8	-6.7	1	T	1	D
2605	silafluofen	105024-66-6	-3	2	T	2	D
2606	etacelasil	37894-46-5	-8.86	2	T	1	M
2607	azocyclotin	41083-11-8	-9.57	2	T	1	M
2608	methylmercury dicyandiamide	502-39-6	-7.95	2	T	2	M
2609	diphenylarsanylformonitrile	23525-22-6	-6.44	2	T	2	D
2610	flusilazole	85509-19-9	-7	2	T	1	D
2611	simeconazole	149508-90-7	-7	2	T	2	D
2612	bromine chloride	13863-41-7	-1.36	1	T	1	D
2613	hydrogen peroxide	7722-84-1	-6.31	1	T	2	D
2614	monochlorine monoxide	14989-30-1	-1.24	1	T	1	D
2615	dichlorine monoxide	7791-21-1	-2.62	1	T	2	D
2616	chlorine dioxide	10049-04-4	-1.39	1	T	1	D
2617	hypochlorous acid	7790-92-3	-4.07	1	P	2	D
2618	ammonia	7664-41-7	-3.19	1	T	1	D
2619	hydrazoic acid	7782-79-8	-2.47	1	T	2	D
2620	nitrogen trifluoride	7783-54-2	1.69	1	P	1	D
2621	chloramine	10599-90-3	-3.33	1	T	2	D
2622	dichloramine	3400-09-7	-2.84	1	T	1	D
2623	nitrogen trichloride	10025-85-1	-0.39	1	T	2	D
2624	tetrafluorohydrazine	10036-47-2	1.68	1	T	1	D
2625	pernitric acid	26404-66-0	-4.98	1	T	2	D
2626	hydrogen sulfide	7783-06-4	-0.44	1	T	1	D
2627	dodecamethylpentasiloxane	141-63-9	4.23	2	P	2	D
2628	hexamethylcyclotrisiloxane	541-05-9	1.796	2	T	1	D
2629	tetrakis(trimethylsiloxy)silane	3555-47-3	4.19	2	P	2	D
2630	methyltris(trimethylsiloxy)silane	17928-28-8	4.14	2	T	1	M
2631	gamma-aminopropyltriethoxysilane	919-30-2	-5.48	2	P	2	D
2632	trimethoxyethoxyvinylsilane	1067-53-4	-6.163	2	T	1	D
2633	trisiloxane, 1,1,1,3,5,5,5-heptamethyl-	1873-88-7	3.58	2	T	2	D
2634	γ-glycidoxypropyltrimethoxysilane	2530-83-8	-5.542	2	T	1	D
2635	2-(3,4-epoxycyclohexyl)ethyltriethoxy-silane	10217-34-2	-4.392	2	P	2	D
2636	isobutyltriethoxysilane	17980-47-1	-1.135	2	T	1	M

Data type: 1 = directly measured; 2 = from measured P_v and S_w; 3 = from measured P_v and γ_w^{∞}; 4 = from measured K_{ow} and K_{aw}.

Experimental data from literature, curated and stored in ChemProp.

Set: training set (T) vs prediction set (P).

Group1 vs *group 2* for mutual leave-50%-out cross-validation.

Ref type: O = value from single original paper; D = value from single database or data collection; M = multiple sources used

[1]UVCB, used: p-n-nonylphenol
[2]used tautomer: 4-[(2-chlorophenyl)diazenyl]-3-methyl-1,2-oxazol-5-ol
[3]UVCB, used: 4-(6-methylheptyl)-2,6-dinitrophenyl-(2E)-but-2-enoate
[4]UVCB, used: 3-tert-butylphenyl) diphenyl phosphate

Table S5. Outliers.

No.	Compound name	CAS-RN	exp. log K_{aw}	pred. log K_{aw}	Predict. error
992	1,4-benzoquinone	106-51-4	-4.71	-6.83	-2.12
1076	pentadecalactone	106-02-5	-1.56	-3.53	-1.97
1139	spiromesifen	283594-90-1	-4.94	-6.55	-1.61
1186	2-hydroxy-1-methylethyl laurate	107328-11-0	-4.81	-3.31	1.50
1197	milbemectin A4	51596-11-3	-10.28	-12.18	-1.89
1315	pentabromoanisole	1825-26-9	-3.44	-1.92	1.52
1384	decachlorodiphenyl ether	31710-30-2	0.75	-1.38	-2.13
1521	2-chlorosyringaldehyde	76341-69-0	-5.35	-7.53	-2.18
1522	2,6-dichlorosyringaldehyde	76330-06-8	-5.83	-7.34	-1.51
1528	indanofan	133220-30-1	-7.67	-9.50	-1.83
1624	1-pyrroline	5724-81-2	-3.60	-1.85	1.75
1683	diquat	2764-72-9	-8.84	-7.30	1.54
1705	triapenthenol	76608-88-3	-8.00	-6.37	1.63
1753	azoxystrobin	131860-33-8	-11.01	-8.89	2.12
1798	fenbuconazole	114369-43-6	-7.91	-9.83	-1.92
1821	quinoxyfen	124495-18-7	-4.21	-5.78	-1.57
1822	pyridalyl	179101-81-6	-3.90	-6.49	-2.59
1842	flupyradifurone	951659-40-8	-10.21	-11.94	-1.73
1843	flurtamone	96525-23-4	-11.59	-9.46	2.13
1844	cyhalofop	122008-78-0	-8.63	-10.73	-2.11
1845	tralomethrin	66841-25-6	-7.80	-6.29	1.51
1860	brofluthrinate	160791-64-0	-4.60	-7.34	-2.74
1884	florpyrauxifen	943832-81-3	-10.89	-12.70	-1.81
1914	emylcamate	78-28-4	-2.86	-4.89	-2.03
1928	lenacil	2164-08-1	-10.25	-8.36	1.89
1943	oxamide	471-46-5	-9.27	-10.80	-1.53
1963	imazamethabenz-methyl	81405-85-8	-9.59	-7.75	1.84
1972	furmecyclox	60568-05-0	-3.18	-5.02	-1.84
2002	norflurazon	27314-13-2	-8.69	-10.76	-2.07
2006	sedaxane	874967-67-6	-11.79	-9.54	2.25
2011	bixafen	581809-46-3	-7.45	-9.57	-2.12
2019	dimethachlor	50563-36-5	-7.00	-5.22	1.78
2032	furilazole	121776-33-8	-6.25	-4.73	1.52
2055	benzoximate	29104-30-1	-5.66	-7.58	-1.92
2076	N-benzyl-N-methylnitrous amide	937-40-6	-3.72	-5.67	-1.95
2197	4-formyl-2-nitrophenol	3011-34-5	-4.19	-5.76	-1.57
2262	chlomethoxyfen	32861-85-1	-3.10	-5.43	-2.33
2272	imidacloprid	138261-41-3	-12.87	-14.47	-1.60
2327	pyriftalid	135186-78-6	-8.80	-6.81	1.99
2328	octhilinone	26530-20-1	-6.07	-4.29	1.78
2334	benfuracarb	82560-54-1	-6.08	-7.89	-1.81
2346	thiazopyr	117718-60-2	-4.81	-7.14	-2.33
2347	pyridate	55512-33-9	-6.37	-4.63	1.74
2365	fenamidone	161326-34-7	-8.33	-6.43	1.90
2382	methomyl	16752-77-5	-9.07	-7.04	2.03
2385	tiadinil	223580-51-6	-8.12	-10.34	-2.22
2411	dimethyl sulfoxide	67-68-5	-6.31	-4.55	1.76
2424	sulfometuron-methyl	74222-97-2	-14.77	-12.76	2.01
2428	tribenuron-methyl	101200-48-0	-9.89	-11.48	-1.59
2437	triafamone	874195-61-6	-7.31	-8.92	-1.61
2447	aldicarb sulfoxide	1646-87-3	-7.40	-9.86	-2.46
2469	crotoxyphos	7700-17-6	-6.42	-7.94	-1.52

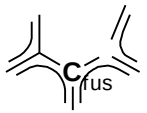
2483	tabun	77-81-6	-5.11	-6.93	-1.82
2531	cyolane	947-02-4	-8.10	-9.65	-1.55
2565	azamethiphos	35575-96-3	-8.87	-10.52	-1.65
2569	isoparathion	597-88-6	-5.18	-7.02	-1.84
2590	chlorodiphenylarsine	712-48-1	-5.18	-3.58	1.60
2624	tetrafluorohydrazine	10036-47-2	1.68	-0.95	-2.63

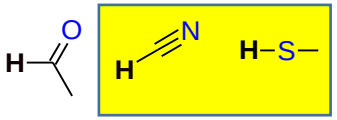
Scheme S2. Fragments and Correction Factors Used in the UFZ Model.

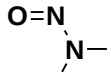
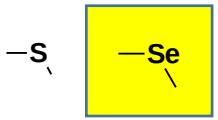
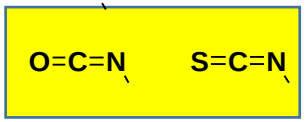
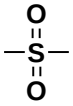
Substructure color code: Bold black: Atoms and bonds to be counted. Blue: chemical environment (has to be present, but is not counted as fragment).
Yellow: Currently tentative (only few occurrences; several substructures combined to one parameter)

#	value	#occurences / #cpds (in sequential calibration)	#occurences / #cpds (in total data set)	substructure
1	0.455	696 / 696	2636 / 2636	regression constant

Basic fragments (each atom has to be counted in exactly one basic fragment)

2	-0.416	3248 / 636	9687 / 2033	C(sp^3)	
3	-0.547	386 / 149	1017 / 469	C(sp^2)	 R=**C**=R R = alkyl C
4	-0.644	46 / 20	72 / 33	C(sp)	
5	-0.575	1577 / 218	11827 / 1451	arom. C	
6	-0.275	58 / 16	126 / 50	fused arom. C with 2 (or 3) fused arom. C as neighbours, as in phenanthrene	
7	-0.496	140 / 59	378 / 178	other fused arom. C (as in naphthalene)	
8	0.275	7203 / 636	20733 / 1970	H at C(sp^3)	
9	0.405	1600 / 363	7258 / 1640	H at C(sp^2) or C(sp)	
10	-1.019	181 / 56	893 / 249	**F**—	

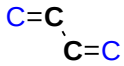
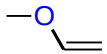
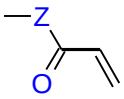
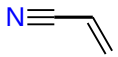
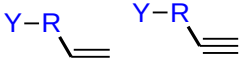
11	-1.39	27 / 27	2629 / 913	**Cl**—	
12	-1.46	26 / 26	299 / 153	**Br**—	
13	-1.53	10 / 10	23/21	**I**—	
14	-4.581	104 / 104	492 / 409	**HO**—	
15	-2.848	48 / 48	1633 / 1010	nonarom. –O-	
16	0.145	40 / 40	52 / 52	arom. O	
17	-3.995	77 / 77	970 / 780	keto group	
18	0.834	43 / 43	87 / 34	H at certain hetero atoms / funct. groups	 **H**-Si-
19	-4.416	46 / 46	402 / 328	prim. or second. amino group	H_2N— 
20	-4.00	11 / 11	264 / 227	tert. amino group	
21	-3.01	25 / 25	535 / 275	arom. N	
22	-0.09	13 / 13	13 / 13	H at arom. N (as in pyrrole)	$H-N_{ar}$
23	-1.09	31 / 24	101 / 80	acyclic –N=	 (R ≠ O)
24	-2.31	42 / 35	42 / 35	cyclic –N=	 (R ≠ O)
25	-3.68	14 / 14	84 / 79	cyano group	

26	-5.99	10 / 10	17 / 17	N-nitroso	
27	-3.60	11 / 11	254 / 172	nitro	
28	-2.60	18 / 18	188 / 153	sulfur or selenium	
29	-0.58	4 / 4	30 / 30	arom. sulfur	
30	-3.33	7 / 6	7 / 6		
31	-2.71	4 / 4	4 / 4		
32	-5.82	8 / 8	8 / 8		
33	-4.23	7 / 6	48 / 47		
34	-6.53	10 / 10	49 / 49		
35	-3.87	45 / 41	72 / 68		
36	-0.58	81 / 13	58 / 25		
37	0.21	4 / 4	6 / 6		
38	-1.73	9 / 8	9 / 8		
39	-1.59	5 / 5	5 / 5		

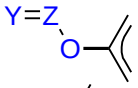
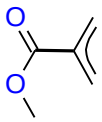
Correction factors

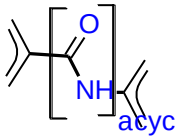
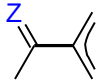
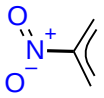
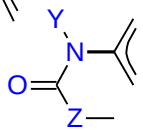
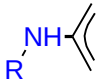
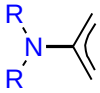
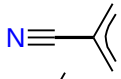
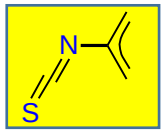
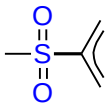
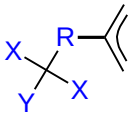
All correction factors occurring in a given structure apply, and atoms may occur in more than one correction factor. Each group of correction factors is independent, so atoms or bonds already counted can be found again in a new group.

Olefinic attachments (the bond adjacent to the olefinic bond is to be counted)

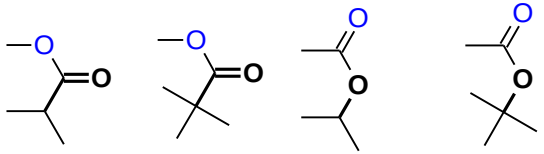
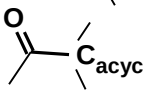
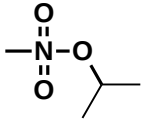
40	-0.34	8 / 8	16 / 16	conj. C=C bonds		
41	0.980	82 / 34	153 / 79			
42	0.96	7 / 6	42 / 41			
43	0.37	19 / 19	70 / 62		Z = O, N	
44	0.92	4 / 4	8 / 7			
45	0.39	18 / 18	118 / 87	allylic / propargylic atoms / groups		Y = halogen, O, >N-, S, C#N

Aromatic attachments (the bond adjacent to the aromatic ring is to be counted)

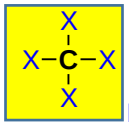
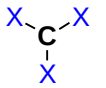
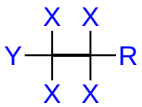
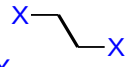
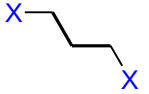
46	0.83	24 / 24	129 / 118			
47	2.30	35 / 29	55 / 49		Y=O, P	Z = P, S
48	1.56	5 / 4	662 / 389			
49	1.13	9 / 7	86 / 67			

50	1.52	16 / 16	16 / 16			
51	1.15	11 / 10	131 / 85		Z = O, S	
52	1.79	5 / 5	140 / 96			
53	1.83	28 / 26	66 / 62		Y = H, C, O	Z = O, N
54	1.59	7 / 7	2191 / 715		X = F, Cl	
55	1.50	8 / 8	230 / 108		X = Br, I	
56	1.45	46 / 46	169 / 130		($R \neq SO_2$)	
57	1.71	4 / 4	66 / 65		($R \neq SO_2$)	
58	2.20	11 / 10	24 / 23	 		
59	0.89	22 / 17	42 / 34			
60	1.66	31 / 29	31 / 29	 		
61	0.91	6 / 2	6 / 2			
62	0.74	12 / 10	246 / 210	benzylic attachment 		Y = halogen, O, >N-, S, C#N
63	0.47	12 / 6	15 / 8	benzylic attachment of CX_2, CX_3 	X = halogen	Y = halogen, H

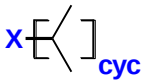
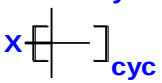
Heteroatoms / functional groups at alkyl branch

64	0.212	36 / 30	107 / 91		to be counted twice for tert. branch
65	0.17	10 / 10	13 / 13		
66	0.375	32 / 23	37 / 28		
67	0.10	11 / 11	190 / 84		X = halogen

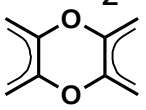
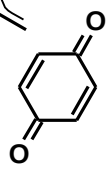
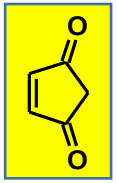
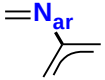
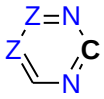
Correction factors for multiple halogenation (X = any halogen)

68	5.93	7 / 7	7 / 7		
69	3.43	32 / 25	144 / 123		
70	3.20	21 / 19	44 / 42		maximum 1 F
71	0.99	9 / 8	10 / 9		Y = Br, I
72	1.07	57 / 45	178 / 118		at least 1 X = Cl or F
73	1.91	27 / 21	81 / 38		Y = C, H, halogen
74	0.480	162 / 39	281 / 60		to be counted twice if CX-CX$_2$
75	0.30	12 / 10	30 / 19		each pair is to be counted (e.g. 3x for CX$_3$-C-CX, 4x for CX$_2$-C-CX$_2$)

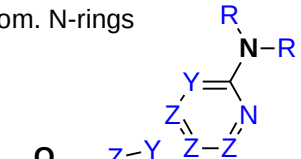
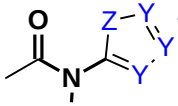
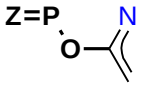
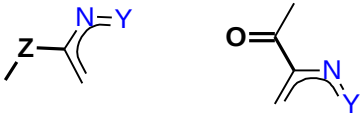
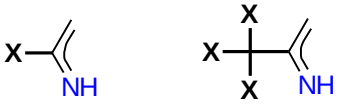
Correction factors for atoms in or at aliphatic ring

76	-0.064	492 / 116	1045 / 305	C_{cyc}	C-atom in aliph. ring (part of only 1 ring, not at ring node)
77	-0.15	25 / 25	413 / 237	Z_{cyc}	Z = O, -N<, S, Si (hetero atom in aliph. ring, not –N=, not –O-P)
78	0.228	87 / 16	133 / 38		X = halogen (halogen at aliph. ring, but not at ring node)
79	0.80	22 / 8	46 / 16		X = halogen (halogen at ring node)

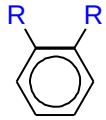
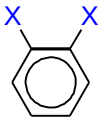
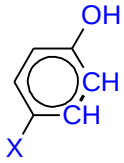
Correction factors for special ring systems / cyclic structures

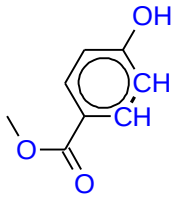
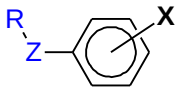
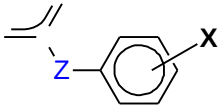
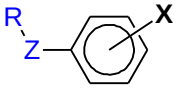
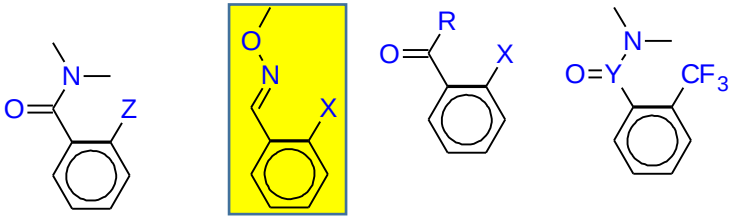
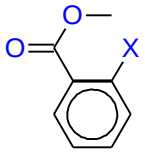
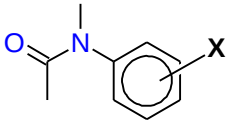
80	2.43	6 / 6	17 / 17		Z = O, S (dioxolane and thio derivatives)
81	0.52	29 / 29	29 / 29		dibenzodioxine
82	1.52	9 / 9	18 / 18	 	quinones and similar 5-rings
83	1.92	6 / 6	12 / 12		Y, Z = N, O, S (dioxane, morpholine, piperidine, …)
84	0.53	11 / 11	11 / 11		arom. ring with S and N in 1,3-position
85	0.46	5 / 4	37 / 29		arom. N in 2-position to fused arom. C (e.g. quinoline)
86	5.48	33 / 33	33 / 33		1,3,5-triazine ring
87	2.36	6 / 6	14 / 14		pyrazines
88	2.74	34 / 34	34 / 34		Z = any arom. atom (arom. ring with1,3-diazine-substructure)

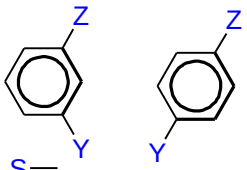
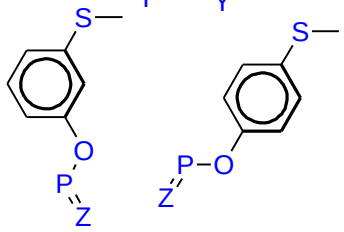
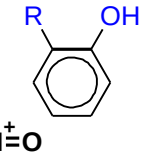
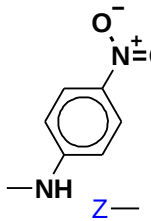
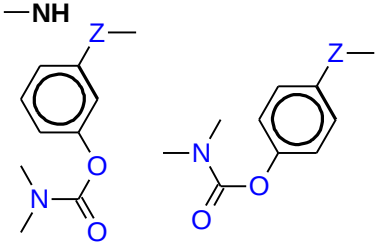
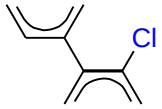
Correction factors for substitutions at arom. N-rings

89	0.527	154 / 54	154 / 54		Y = arom. C, N; Z = any arom. atom R ≠ N; to be counted twice if Y = N
90	2.59	9 / 9	9 / 9		Z = arom. N, O Y = any arom. atom
91	0.72	11 / 11	11 / 11		Z = O, S
92	1.84	78 / 66	78 / 66		Y = arom. C, N Z = O, S
93	1.04	51 / 45	51 / 45		X = halogen
94	1.52	10 / 5	12 / 7		X = halogen, pyrrole-type-N in arom. 5-ring

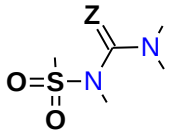
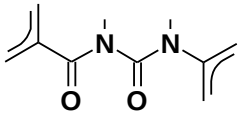
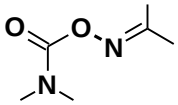
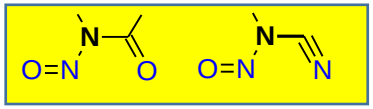
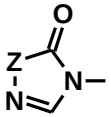
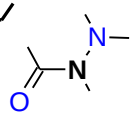
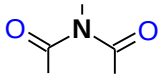
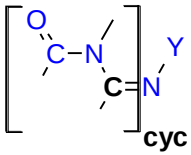
Correction factors for ortho- / meta- / para-positions at arom. rings

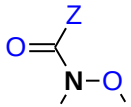
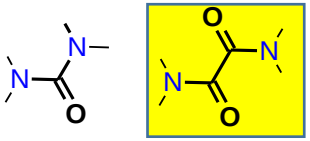
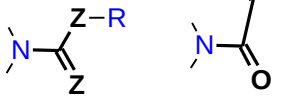
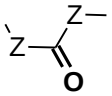
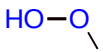
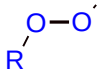
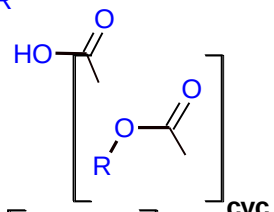
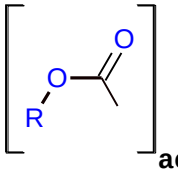
95	-0.171	32 / 21	49 / 36		alkyl groups in ortho-position
96	-0.018	406 / 167	868 / 363		X = halogen
97	-0.20	8 / 7	9 / 8		X = halogen

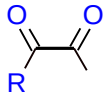
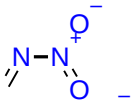
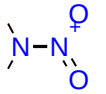
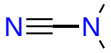
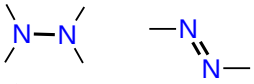
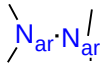
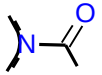
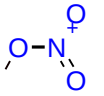
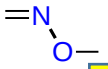
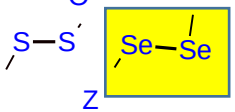
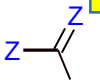
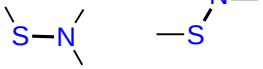
98	0.43	4 / 4	4 / 4		
99	0.397	113 / 49	210 / 106		X = F, Cl, R = alkyl, any position at arom. ring, Z = O,S
100	0.293	178 / 43	217 / 68		X = F, Cl, any position at arom. ring, Z = O,S
101	0.351	58 / 36	61 / 38		X = Br, I, R = alkyl, any position at arom. ring, Z = O,S
102	2.03	12 / 10	12 / 10		X = Cl, Br, I Z = X, -R-O- Y = C, S
103	0.51	6 / 3	6 / 3		X = Cl, Br, I
104	0.26	18 / 14	38 / 29		X = CF_3, Cl, Br, I, any position at arom. ring

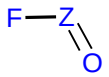
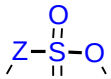
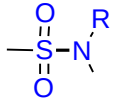
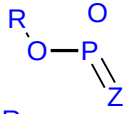
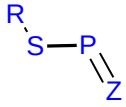
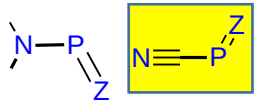
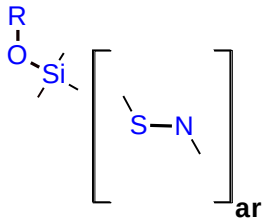
105	-0.31	8 / 8	9 / 9		Y = NO_2, SO_2, C=N-O Z = OH, COOH
106	0.42	7 / 6	7 / 6		Z = O, S
107	0.56	19 / 16	36 / 30		to be used also for non-aromatic rings
108	-0.82	4 / 4	4 / 4		
109	0.77	5 / 5	5 / 5		Z = -N<, -S-, C=O, SO_2
110	0.158	280 / 131	284 / 134		e.g. in PCB‘s

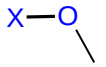
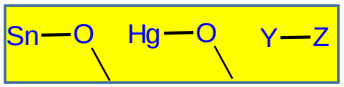
Correction factors for complex functional groups / adjacent hetero atoms

111	4.17	10 / 10	10 / 10		Z = O, S	sulfonyl ureas
112	7.14	5 / 5	5 / 5			
113	3.20	10 / 9	10 / 9			
114	5.90	5 / 5	5 / 5			
115	5.14	2 / 2	2 / 2			
116	6.10	8 / 8	8 / 8		Z = C, N	
117	1.86	23 / 20	23 / 20			
118	4.64	20 / 19	26 / 25			
119	4.27	3 / 3	3 / 3			

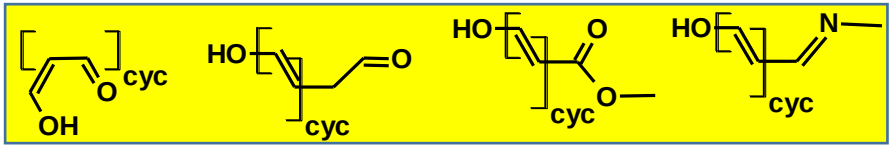
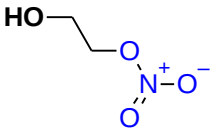
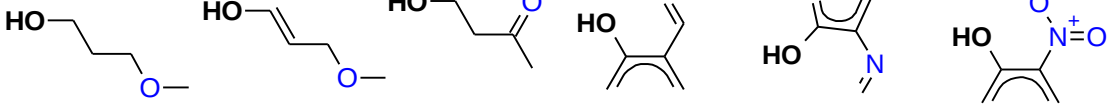
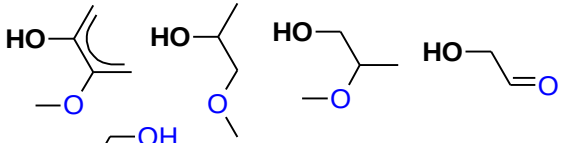
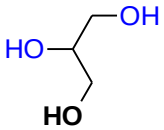
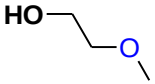
120	4.15	5 / 5	5 / 5		Z = O, R
121	3.17	24 / 21	41 / 38		
122	0.84	17 / 17	63 / 61		Z = O, S
123	-1.04	6 / 6	6 / 6		Z = O, S
124	0.64	18 / 14	193 / 188		nonarom. bond between arom. rings, e.g. in biphenyl
125	2.46	7 / 7	8 / 8		
126	3.56	7 / 7	8 / 8		
127	2.81	26 / 25	92 / 82		
128	2.05	6 / 5	30 / 27		
129	3.191	103 / 99	392 / 339		

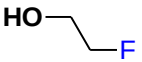
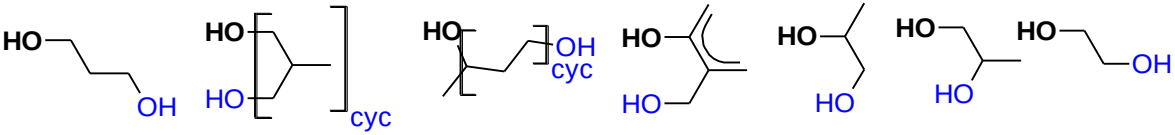
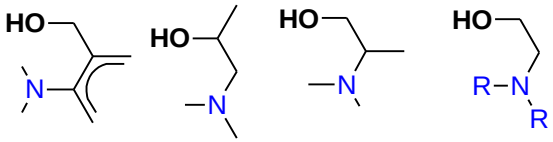
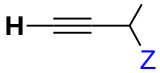
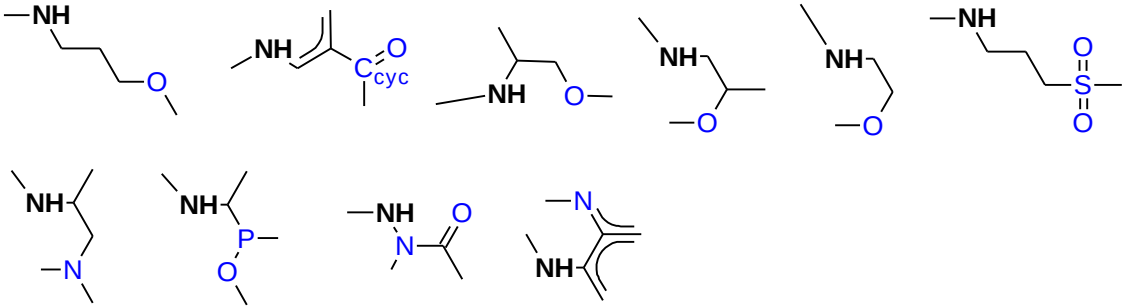
130	0.38	33 / 33	302 / 243		
131	2.39	7 / 7	8 / 8		
132	1.44	4 / 4	4 / 4		
133	4.42	8 / 3	8 / 3		
134	6.11	2 / 2	2 / 2		
135	1.37	10 / 9	47 / 38		
136	2.69	80 / 77	80 / 77		
137	6.30	6 / 6	6 / 6		(C=O with bond to arom. N)
138	3.82	18 / 18	91 / 59		
139	1.44	12 / 12	46 / 40		
140	2.62	6 / 5	8 / 7		
141	4.07	18 / 17	31 / 28		Z = O, S
142	4.46	14 / 10	14 / 10		

143	2.41	4 / 4	4 / 4		Z = S, P
144	1.419	20 / 4	20 / 4		
145	5.34	4 / 4	4 / 4		Z = O, N
146	4.28	6 / 3	6 / 3		
147	2.67	28 / 25	28 / 25		R ≠H
148	2.58	204 / 80	292 / 115		Z = O, S
149	2.43	33 / 27	45 / 39		Z = O, S
150	2.87	10 / 9	14 / 12		Z = O, S
151	0.96	3 / 2	3 / 2		
152	1.681	48 / 15	96 / 18		
153	1.75	4 / 4	4 / 4		
154	2.76	7 / 5	7 / 5		X = halogen

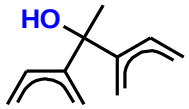
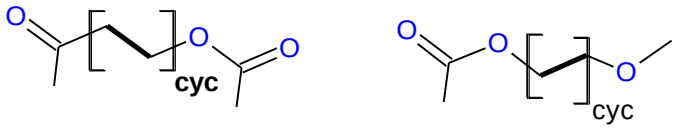
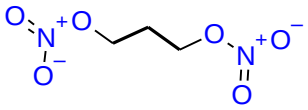
155	2.32	8 / 4	15 / 6		X = halogen
156	1.39	6 / 4	6 / 4		X = Cl, Br, I
157	-1.68	9 / 8	9 / 8		Y = Hg, Sn, Pb Z = Cl, N

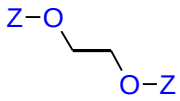
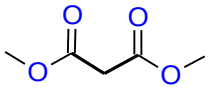
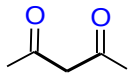
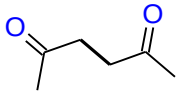
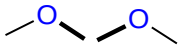
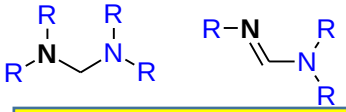
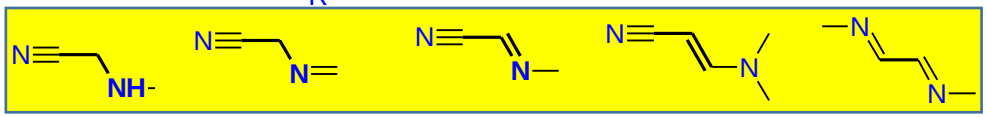
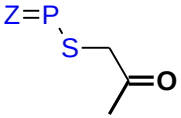
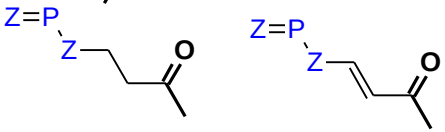
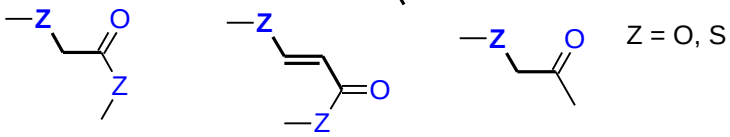
Correction factors for intramoleculare hydrogen bonds

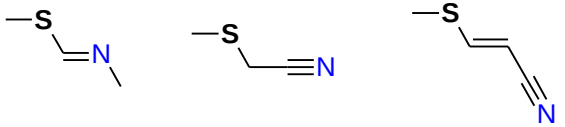
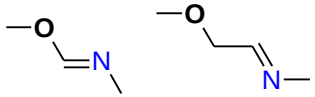
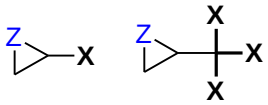
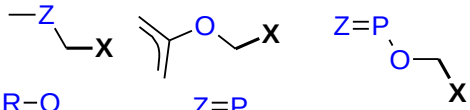
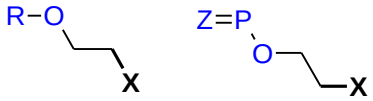
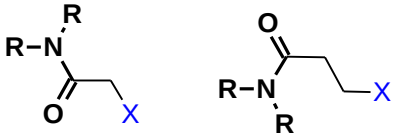
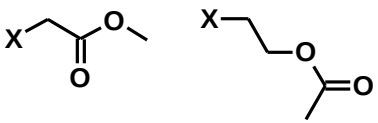
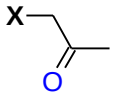
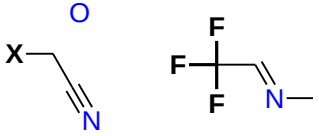
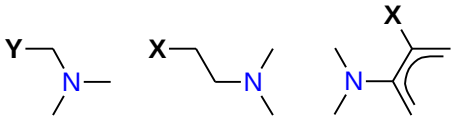
158	5.20	11 / 11	11 / 11		(several cases with large parameter value combined into one parameter)
159	0.72	6 / 6	6 / 6		
160	3.73	21 / 20	34 / 33		
161	2.12	14 / 14	36 / 36		
162	1.915	24 / 8	24 / 8		
163	1.91	20 / 17	30 / 26		X = Cl, Br
164	1.59	11 / 11	12 / 12		

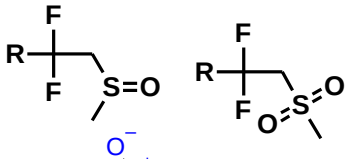
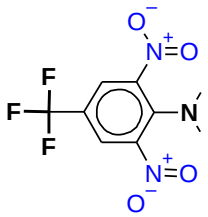
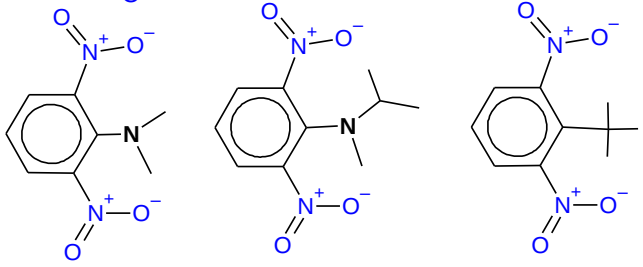
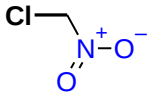
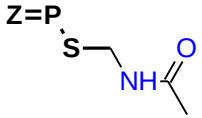
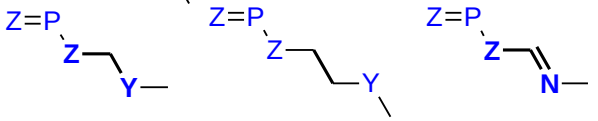
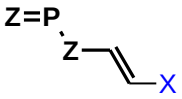
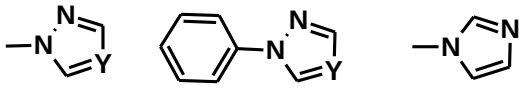
165	1.13	8 / 8	8 / 8	
166	0.700	34 / 17	36 / 18	
167	1.47	13 / 13	13 / 13	 R ≠H
168	0.79	6 / 6	6 / 6	 Z = N,O
169	1.60	13 / 11	33 / 31	

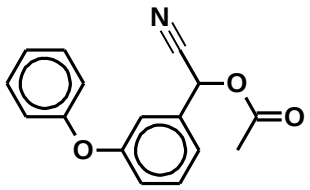
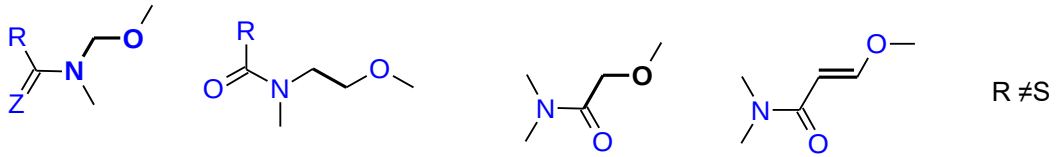
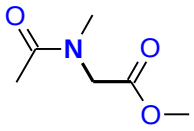
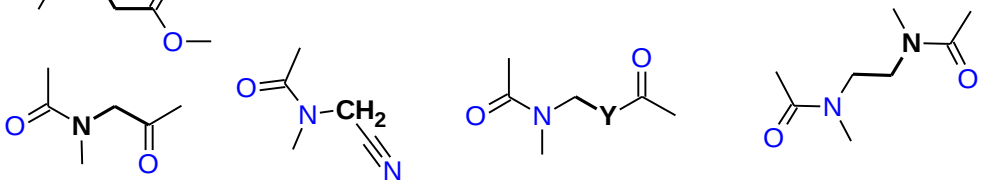
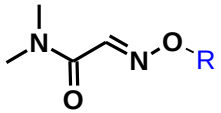
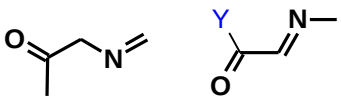
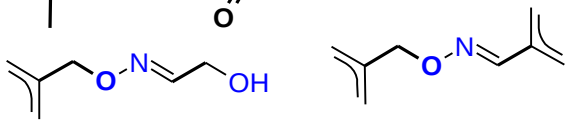
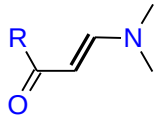
Other correction factors

170	0.86	7 / 7	7 / 7	
171	1.93	3 / 3	3 / 3	
172	0.67	8 / 7	8 / 7	

173	1.10	25 / 23	56 / 43		Z = alkyl, C=O, NO_2
174	1.03	4 / 4	4 / 4		
175	2.22	18 / 16	18 / 16		
176	0.59	10 / 10	15 / 13		
177	1.803	16 / 9	27 / 19		not in dioxolane ring
178	2.01	13 / 8	13 / 8		
179	2.26	13 / 11	13 /11		
180	2.72	7 / 7	7 / 7		Z = O, S
181	1.09	7 / 7	7 / 7		Z = O, S
182	1.36	41 / 40	41 / 40		Z = O, S

183	2.65	14 / 11	14 / 11			
184	2.21	14 / 14	14 / 14			
185	2.36	4 / 2	4 / 2		Z = O, S	X = F, Cl
186	1.67	16 / 12	28 / 23		Z = O, S	
187	0.989	43 / 24	53 / 34		X = halogen, CF_3	Z = O, S
188	2.77	8 / 8	27 / 27		R = C, H	X = halogen
189	1.52	8 / 8	13 / 13		X = halogen	
190	0.82	14 / 8	16 / 10		X = Cl, Br, I	
191	1.75	7 / 3	8 / 4			
192	0.88	8 / 4	59 / 37		X = Cl, Br, I	Y = halogen (incl. F)

193	1.74	5 / 5	5 / 5		R = C, H, F	
194	4.21	9 / 9	9 / 9			
195	2.98	7 / 7	7 / 7			
196	2.87	4 / 4	4 / 4			
197	4.13	7 / 7	7 / 7		Z = O, S	
198	1.20	11 / 11	14 / 14		Z = O, S	Y = O, N, S
199	1.03	5 / 5	5 / 5		Z = O, S	X = Cl, Br, I
200	2.40	57 / 57	57 / 57			Y = arom. C or N

201	4.27	18 / 18	18 / 18		
202	2.27	11 / 11	41 / 38		R ≠S
203	2.58	10 / 10	10 / 10		
204	4.33	8 / 7	8 / 7		
205	4.55	4 / 4	4 / 4		R = alkyl or arom. C
206	2.34	7 / 7	7 / 7		Y = N, O
207	2.69	6 / 6	6 / 6		
208	1.80	6 / 5	6 / 5		R = alkyl or arom. C
209	1.53	4 / 4	4 / 4