

## Supplementary Material

Table The experimental and predicted *K<sub>oc</sub>* of 592 chemicals

Chemical Names	Exp. logK <sub>oc</sub>	Cal. LogK <sub>oc</sub>	Res.
2-propenal	-0.31	-0.246	-0.064
acetic acid	0.00	-0.160	0.160
ethanol	0.20	0.449	-0.249
3,4,5-trichloro veratrole	0.20	2.468	-2.268
3,6-dichloropicolinic acid	0.30	1.475	-1.175
ethylene oxide	0.34	0.213	0.127
propyleneglycol	0.36	0.441	-0.081
methanol	0.44	0.219	0.221
1,2,3,4-tetrachloro-5,6-dimethoxy-benzene	0.45	2.853	-2.403
maleic hydrazide	0.45	1.088	-0.638
acetylphosphoramidothioic acid O,S-dimethyl ester	0.48	-0.290	0.770
2,2-dichloropropionic acid	0.48	0.737	-0.257
1-propanol	0.48	0.680	-0.200
1-butanol	0.50	0.910	-0.410
2,6-dichlorobenzamide	0.53	2.231	-1.701
formaldehyde	0.56	0.378	0.182
aldicarb sulfoxide	0.56	0.938	-0.378
methamidophos	0.70	0.699	0.001
1-pentanol	0.70	1.141	-0.441
benzylalcohol	0.70	1.610	-0.910
phosphamidon	0.81	1.436	-0.626
6-chloropicolinic acid	0.95	1.090	-0.140
O,O-dimethyl S-(N-methylcarbamoyl-methyl)phosphorodithioate	0.96	0.918	0.042
trichloroacetamide	0.99	1.010	-0.020
aldoxycarb	1.00	0.678	0.322
1-hexanol	1.01	1.371	-0.361
chlorsulfuron	1.02	1.610	-0.590
m-dihydroxybenzene	1.03	1.370	-0.340
phthalic acid	1.07	0.871	0.199
oxydemeton-methyl	1.10	0.923	0.177
1-heptanol	1.14	1.371	-0.231
bis(2-chloroethyl) ether	1.15	1.473	-0.323
urea	1.15	1.269	-0.119
4-amino-3,5,6-trichloropicolinic acid	1.23	1.915	-0.685
propoxur	1.23	1.756	-0.526
fenthion	1.24	2.631	-1.391
trichlorfon	1.29	1.099	0.191

3-phenyl-1-methylurea	1.29	1.224	0.066
fenac	1.30	2.388	-1.087
1,3,5-trinitrobenzene	1.30	2.173	-0.873
2,4-dichlorophenoxyacetic acid	1.30	1.836	-0.536
2,4-DB	1.30	1.924	-0.623
2-fluro-phenylurea	1.32	1.590	-0.270
3-amino-2,5-dichlorobenzoic acid	1.32	2.175	-0.855
o-cresol	1.34	1.969	-0.629
3,4,5-trichlorocatechol	1.35	2.526	-1.176
phenylurea	1.35	1.556	-0.206
4-methoxyphenylcarbamate	1.40	1.126	0.274
4-methoxyacetanilide	1.40	1.337	0.063
4-methoxy-3-phenyl-1,1-dimethylurea	1.40	2.133	-0.733
trans-1,3-dichloropropene	1.41	1.853	-0.443
aniline	1.41	1.883	-0.473
oxycarboxin	1.41	1.406	0.009
N-methylbenzamide	1.42	1.848	-0.428
phenol	1.43	1.599	-0.169
3-phenyl-1,1-dimethylurea	1.43	1.278	0.152
3-(4-fluro)-phenyl-1,1-dimethylurea	1.43	1.369	0.061
4-hydroxybenzoic acid	1.43	1.121	0.310
3,5,6-trichloro-2-pyridyloxy acetic acid	1.43	1.576	-0.146
acetanilide	1.43	1.507	-0.077
3-methoxyphenylcarbamate	1.44	1.126	0.314
dichloromethane	1.44	1.366	0.074
2-nitrobenzamide	1.45	1.575	-0.125
phenylacetic acid	1.45	1.232	0.218
3-methylacetanilide	1.45	1.876	-0.426
hexanoic acid	1.46	0.762	0.698
benzamide	1.46	1.460	0.000
pentafluorophenyl methyl sulfone	1.46	1.397	0.063
2,3-dihydro-2,2-dimethyl-7-benzofuranyl methylcarbamate	1.46	1.857	-0.397
1,1-dichloroethane	1.48	1.619	-0.139
3-methylphenylcarbamate	1.48	1.665	-0.185
iprodione	1.48	2.292	-0.812
4-fluroacetanilide	1.48	1.452	0.028
sec-phenylethyl alcohol	1.50	1.841	-0.341
2-methoxy-3,6-dichlorobenzoic acid	1.50	1.951	-0.451
sec-phenethyl alcohol	1.50	1.761	-0.261
benzoic acid	1.50	1.350	0.150
phenyl N,N'-dimethyl phosphorodiamidate	1.51	2.077	-0.567
2-chlorobenzamide	1.51	1.846	-0.336
naptalam	1.51	1.756	-0.246
4-methyl-3-phenyl-1,1-dimethylurea	1.51	1.780	-0.270
4-fluro-phenylurea	1.52	1.590	-0.070
3,4-dinitrobenzoic acid	1.53	1.579	-0.049
m-cresol	1.54	1.969	-0.429
anisole	1.54	1.659	-0.119
4-nitrobenzoic acid	1.54	1.465	0.075
N,N-dimethylbenzamide	1.54	1.156	0.384
N-(1,1-dimethyl-2-propynyl) benzamide	1.54	1.645	-0.105
m-methoxyphenol	1.55	1.429	0.121
1,2-dichloroethane	1.56	1.516	0.044
3-methyl-phenylurea	1.56	1.926	-0.366
dinitrobenzene	1.56	2.058	-0.498
tetrachlorocatechol	1.56	2.912	-1.352
1-octanol	1.56	1.832	-0.272
fenamiphos sulfoxide	1.57	1.675	-0.105
3-fluroacetanilide	1.57	1.452	0.118
ethofumesate	1.57	1.411	0.157
o-chloroacetanilide	1.58	1.892	-0.312
o-methoxyphenol	1.60	1.429	0.171
2-chloro-phenylurea	1.61	1.942	-0.332
acetophenone	1.63	1.543	0.087

	1.03	1.05	0.005
2-methyl-2(methylthio)propionaldehyde O-(methylcarbamoyl)oxime	1.64	1.655	-0.015
fenamiphos sulfone	1.64	1.586	0.054
1,2-dibromoethane	1.64	1.780	-0.140
1,2-dibromoethylene	1.65	2.253	-0.603
3-methylaniline	1.65	1.929	-0.279
trichloromethane	1.65	1.363	0.287
thiameturon-methyl	1.66	0.851	0.809
dicrotophos	1.67	1.695	-0.025
2,2-dichlorvinyl dimethyl phosphate	1.68	1.678	0.002
4-fluoro-N-(1,1-dimethyl-2-propynyl) benzamide	1.69	2.412	-0.722
metalexyl	1.69	1.644	0.046
benzyltriazole	1.69	1.969	-0.279
p-cresol	1.70	1.336	0.364
methyl N',N'-dimethyl-N{(methyl-carbamoyl)oxy}-1-thioxamidate	1.70	1.796	-0.096
4-chloro-3-phenyl-1,1-dimethylurea	1.71	1.769	-0.059
1,2-dichloropropane	1.71	1.985	-0.275
o-chlorophenol	1.71	2.283	-0.573
3,4-xylyl methyl carbamate	1.71	2.163	-0.453
isopropyl carbanilate	1.71	2.525	-0.815
2-sec-butyl phenyl methyl carbamate	1.71	2.000	-0.290
3-tert-butyl-5-chloro-6-methyluracil	1.71	1.968	-0.258
butyranilide	1.72	1.289	0.431
3-phenyl-1-cyclopropylurea	1.72	1.714	0.006
m-nitrophenol	1.72	2.222	-0.502
2,4,5-trichlorophenoxy acetic acid	1.72	2.133	-0.413
3-methoxy-3-phenyl-1,1-dimethylurea	1.73	0.152	1.578
4-chloro-2-methyl phenoxy acetic acid	1.73	1.369	0.361
3-(3-fluro)-phenyl-1,1-dimethylurea	1.73	2.504	-0.774
1,1,1,2-tetrachloroethane	1.73	1.782	-0.052
methyl N-phenylcarbamate	1.73	1.998	-0.268
3-amino nitrobenzene	1.73	2.150	-0.420
3-(3,5-dimethylphenyl)-1,1-dimethylurea	1.74	1.626	0.114
3-(3-chloro-4-methoxy-phenyl)-1,1-dimethylurea	1.74	1.714	0.026
p-nitrophenol	1.75	1.871	-0.121
1,1,2-trichloroethane	1.75	1.429	0.321
p-methoxyphenol	1.75	1.975	-0.225
3-(a,a,a-trifluoro-methyl)-acetanilide	1.76	3.141	-1.381
fluazyfop butyl	1.76	2.014	-0.254
4-methyl-N-(1,1-dimethyl-2-propynyl) benzamide	1.77	2.013	-0.243
4-methylbenzyltriazole	1.77	1.622	0.148
trans-1,2-dichloroethylene	1.77	1.719	0.051
4-methylbenzoic acid	1.77	1.590	0.180
3-fluro-phenylurea	1.77	2.111	-0.341
4-trifluoromethylbenzyltriazole	1.78	1.830	-0.050
4-methylbenzamide	1.78	0.300	1.480
methylurea	1.78	1.959	-0.179
3-methyl-4-fluro-phenylurea	1.79	1.963	-0.173
bromodichloromethane	1.79	1.775	0.015
bis(2-chloroisopropyl) ether	1.79	1.796	-0.006
3-(3-chloro-phenyl)-1,1-dimethylurea	1.80	2.195	-0.395
O-ethyl S,S-dipropyl phosphorodithioate	1.80	2.364	-0.564
N,N-dimethyl-diphenyl acetamide	1.80	1.474	0.326
4-methoxybenzyltriazole	1.81	1.733	0.077
1,1-dichloroethylene	1.82	1.985	-0.165
m-chlorophenol	1.82	2.013	-0.193
ethyl N-phenylcarbamate	1.82	1.879	-0.059
1,1-dimethyl-3-(a,a,a-trifluoro-m-tolyl) urea	1.83	1.475	0.355
4-methoxy-N-(1,1-dimethyl-2-propynyl) benzamide	1.84	2.543	-0.703
diethyl phthalate	1.84	0.958	0.882
diethylacetamide	1.84	1.439	0.401
3-(3-chloro-4-methoxy-phenyl)-1-methylurea	1.85	1.985	-0.135
p-chlorophenol	1.85	1.712	0.138
tetrachloromethane	1.86	1.912	-0.052
5-bromo-3-sec-butyl-6-methyluracil			

m-chloroacetanilide	1.00	1.052	0.052
4-fluorobenzyltriazole	1.87	1.677	0.193
1-butylamine	1.88	1.400	0.480
4-amino nitrobenzene	1.88	1.998	-0.118
flutriafol	1.88	2.749	-0.869
ethylphenylacetate	1.89	2.314	-0.424
3-bromophenylcarbamate	1.89	1.647	0.243
1-nonanol	1.89	2.063	-0.173
3,5-dinitrobenzoic acid	1.90	1.579	0.321
4-methyl aniline	1.90	2.253	-0.353
1,1,2,2-tetrachloroethane	1.90	2.226	-0.326
4-chloro-N-(1,1-dimethyl-2-propynyl) benzamide	1.90	2.030	-0.130
2-chloro-4-isopropylamino-6-methylamino-S-triazine	1.91	2.132	-0.222
dibromochloromethane	1.92	1.998	-0.078
benzene	1.92	1.828	0.092
3-chloro-4-methoxy acetanilide	1.92	1.722	0.198
4-nitrobenzamide	1.93	1.575	0.355
3-chloro-4-methoxy aniline	1.93	2.099	-0.169
3-phenyl-1-cyclopentylurea	1.93	2.085	-0.155
3-(3-chloro-phenyl)-1-methylurea	1.93	1.609	0.321
metsulfuron-methyl	1.93	1.741	0.189
nitrobenzene	1.94	1.943	-0.003
4-isopropylphenylcarbamate	1.94	2.401	-0.461
3-nitroacetanilide	1.94	1.622	0.318
p-bromoacetanilide	1.95	1.857	0.093
3-nitrobenzamide	1.95	1.575	0.375
molinate	1.95	2.582	-0.632
3-(trifluoromethyl) phenylurea	1.96	2.024	-0.064
4-bromoaniline	1.96	2.234	-0.274
ethyl pentanoate	1.97	1.614	0.356
sulfometuron methyl	1.97	1.856	0.114
4-amino-6-(1,1-dimethylethyl)-3-(methylthio)-1,2,4-triazin-5(4H)-one	1.98	1.837	0.143
4-chloroaniline	1.98	2.269	-0.289
4-chlorobenzyltriazole	1.98	2.029	-0.049
toluene	2.00	2.198	-0.198
2-chloro-N-(2-ethyl-6-methylphenyl) N-(2-methoxy-1-methylethyl)acetamide	2.00	2.670	-0.670
3-(3-chloro-4-methoxy-phenyl)-urea	2.00	1.772	0.228
thidiazuron	2.00	2.588	-0.588
isazophos	2.01	2.270	-0.260
4-bromo-N-(1,1-dimethyl-2-propynyl) benzamide	2.01	1.995	0.015
m-bromoacetanilide	2.01	1.857	0.153
3-chloro-phenylurea	2.01	1.942	0.068
3-(3-chloro-4-methyl-phenyl)-1,1-dimethylurea	2.02	2.166	-0.146
3-(p-bromophenyl)-1-methoxy-1-methylurea	2.02	2.313	-0.293
3-amino-1H-1,2,4-triazole	2.02	1.502	0.518
1,2-dimethoxybenzene	2.03	1.489	0.541
trichloroethylene	2.03	1.968	0.062
2,4-D amine	2.04	2.035	0.005
4-aminobenzoic acid	2.05	1.404	0.646
o-nitrophenol	2.06	1.714	0.346
ethyl hexanoate	2.06	1.845	0.215
n-propyl N-phenylcarbamate	2.06	2.243	-0.183
3-bromo-phenylurea	2.06	1.907	0.153
o-dihydroxybenzene	2.07	1.370	0.700
3-phenyl-1-cyclohexylurea	2.07	2.483	-0.413
4-t-butylphenylcarbamate	2.07	2.259	-0.189
5-amino-4-chloro-2-phehy-3(2H)-pyridazinone	2.08	2.198	-0.118
ancymidol	2.08	1.653	0.426
2-sec-butyl-4,6-dinitrophenol	2.09	2.810	-0.720
benzoic acid butyl ester	2.10	2.647	-0.547
methyl benzoate	2.10	1.955	0.145
3-(3-chloro-4-methyl-phenyl)-1-methylurea	2.10	1.978	0.122
1,2-dibromo-3-chloropropane	2.11	2.082	0.028
5-bromo-3-isopropyl-6-methyluracil	2.11	1.586	0.524

acetocnor	2.11	2.300	-0.450
isoproturon	2.11	2.263	-0.153
3,5,6-trichloro-2-pyridinol	2.11	2.110	0.000
4-bromo-phenylurea	2.12	1.907	0.213
2-chloro-4,6-bis(ethylamino)-S-triazine	2.13	2.132	-0.002
2-chloro-N-(pyrazol-1-ylmethyl) acet-2',6'-xylidide	2.14	2.115	0.025
methyl N-(3-chlorophenyl) carbamate	2.15	2.167	-0.017
4-n-butylbenzyltriazole	2.16	2.095	0.065
4-methylsulfonyl-2,6-dinitro-W,N-dimethylaniline	2.16	1.993	0.167
2-chloro-4-ethylamino-6-isopropylamino-1,3,5-triazine	2.17	2.283	-0.113
fensulfothion sulfone	2.17	2.394	-0.224
4-amino-4,5-dihydro-3-methyl-6-phenyl-1,2,4-triazin-5-one	2.17	2.569	-0.399
4-iso-propyl-N-(1,1-dimethyl-2-propynyl) benzamide	2.17	2.395	-0.225
bromobenzene	2.18	2.179	0.001
terbufos sulfoxide	2.18	2.772	-0.592
terbufos sulfone	2.18	2.511	-0.331
naled	2.19	2.424	-0.237
propanil	2.19	2.508	-0.318
methomyl	2.20	1.746	0.454
trichlorofluoromethane	2.20	2.338	-0.138
2-chloro-4,6-bis(isopropylamino)-S-triazine	2.20	2.914	-0.714
chlorbufam	2.21	1.751	0.459
ethyl 4-hydroxybenzoate	2.21	1.956	0.254
pendimethalin	2.21	3.996	-1.786
dimethyl-1-methyl-2-(1-phenylethoxycarbonyl) vinyl phosphate	2.23	3.018	-0.788
1,1,1-trichloroethane	2.26	2.243	0.017
n-butyl N-phenylcarbamate	2.26	2.474	-0.214
N,N-dimethylaniline	2.26	2.362	-0.102
3-methyl-4-bromo-aniline	2.26	2.603	-0.343
2-chloro-2',6'-diethyl-N-(methoxymethyl)acetanilide	2.28	2.655	-0.375
3,5-dibromo-4-hydroxyphenylcyanide	2.28	2.322	-0.042
N-methylaniline	2.28	2.186	0.094
3,4-dichloroaniline	2.29	2.654	-0.364
ethyl benzoate	2.30	2.186	0.114
1-naphthyl acetic acid	2.30	2.344	-0.043
3-(p-chlorophenyl)-1-methoxy-1-methylurea	2.30	2.246	0.054
2-methoxy carbonyl-1-methyl vinyl dimethyl phosphate	2.30	1.578	0.722
cis-N-[(trichloromethyl)thio]-4-cyclohexene-1,2-dicarboximide	2.30	2.342	-0.042
3,6-dichlorosalicylic acid	2.30	1.891	0.409
N-(1,1-dimethyl-2-propynyl)3,5-dichlorobenzamide	2.30	2.416	-0.116
5-butyl-2-dimethylamino-6-methyl pyrimidin-4-ol	2.30	2.728	-0.428
2-(4-chloro-6-ethylamino-S-triazin-2-ylamino)-2-methylpropionitrile	2.30	2.621	-0.321
carbaryl	2.31	2.657	-0.347
3,5-dinitrobenzamide	2.31	1.690	0.620
terbutylazine	2.32	2.496	-0.176
3,5-dimethyl-4-(methylthio) phenol methylcarbamate	2.32	2.517	-0.197
1-naphthalenemethanol	2.33	2.722	-0.392
3,4-dichlorobenzyltriazole	2.33	2.414	-0.084
tribromomethane	2.34	2.033	0.307
3,4-dichloroacetanilide	2.34	2.278	0.062
1,2-dimethylbenzene	2.35	2.567	-0.217
methyl benzimidazol-2-yl carbamate	2.35	2.400	-0.050
4-propylsulfonyl-2,6-dinitro-W,N-dimethylaniline	2.35	2.454	-0.104
pirimicarb	2.35	1.595	0.755
1-naphthyl N-methylcarbamate	2.36	2.657	-0.297
O,O-diethyl O-(2-isopropyl-4-methyl-6-pyrimidinyl) phosphorothioate	2.36	3.027	-0.667
3-trifluoromethyl aniline	2.36	2.351	0.009
4-methylsulfonyl-2,6-dinitro-W,N-diethylaniline	2.36	2.454	-0.094
2,6-dichlorobenzonitrile	2.37	2.621	-0.251
3-methyl-4-bromo-phenylurea	2.37	2.276	0.094
N,N-diethylaniline	2.37	2.823	-0.453
3-phenyl-1-cycloheptylurea	2.37	2.882	-0.512
3,5-dichloroaniline	2.38	2.654	-0.274
S-ethyl dipropylthiocarbamate	2.38	2.418	-0.038

dimethyl phthalate	2.39	2.082	0.308
S-benzyl O,O-di-isopropyl phosphorothioate	2.40	2.577	-0.177
isoxaben	2.40	2.154	0.246
chlorobenzene	2.41	2.214	0.196
ethylbenzene	2.41	2.428	-0.018
4-bromophenol	2.41	1.950	0.460
carboxin	2.41	2.302	0.108
vernolate	2.42	2.750	-0.334
1,4-dimethylbenzene	2.42	2.567	-0.147
4-bromonitrobenzene	2.42	2.294	0.126
2-chloro-N-isopropylacetanilide	2.42	1.670	0.750
1,4-dichlorobenzene	2.44	2.599	-0.159
thiodicarb	2.44	2.817	-0.377
3,4-chloro-pheny-1-methylurea	2.46	1.994	0.466
1,3-dichlorobenzene	2.47	2.599	-0.129
chlorfenvinphos	2.47	2.325	0.145
isouron	2.47	2.422	0.048
methyl (4-aminophenyl) sulfonyl carbamate	2.48	1.095	1.385
ethyl 4-nitrobenzoate	2.48	2.301	0.179
3-(3,4-dichloro-phenyl)urea	2.49	2.327	0.163
1,2-dichlorobenzene	2.51	2.599	-0.089
4-ethylsulfonyl-2,6-dinitro-W,N-diethylaniline	2.51	2.684	-0.174
triadimefon	2.51	1.910	0.600
fensulfothion	2.52	2.415	0.105
fenamiphos	2.52	2.400	0.120
3,4-dichloronitrobenzene	2.53	2.714	-0.184
methidathion	2.53	2.492	0.038
3-(3,5-dimethyl-4-bromo-phenyl)-1,1-dimethylurea	2.53	2.500	0.030
S-ethylcyclohexylethylthiocarbamate	2.54	2.986	-0.446
2,4-bis(isopropylamino)-6-methoxy-S-triazine	2.54	2.439	0.101
o-chlorotoluene	2.55	2.583	-0.033
flurochloridone	2.55	1.686	0.864
3,5-dinitroaniline	2.55	2.113	0.437
tetrachloroethylene	2.56	2.315	0.245
2,6-dinitro-α, α, α -trifluoro-p-toluidine	2.56	2.581	-0.021
2,4,5-trichlorophenol	2.56	2.755	-0.195
4-phenoxy phenyl urea	2.56	3.535	-0.975
2-(ethylamino)-4-(isopropylamino)-6-(methylthio)-S-triazine	2.59	2.705	-0.115
ethyl 4-methylbenzoate	2.59	2.555	0.035
1-decanol	2.59	2.293	0.297
3-chloro-4-bromonitrobenzene	2.60	2.679	-0.079
diuron	2.60	2.182	0.418
ethyl heptanoate	2.61	2.075	0.535
n-pentyl N-phenylcarbamate	2.61	2.704	-0.094
malathion	2.61	2.919	-0.309
siduron	2.62	2.758	-0.138
2-chloro-6-(trichloromethyl) pyridine	2.62	3.069	-0.449
fenitrothion	2.63	3.017	-0.387
anthracene-9-carboxylic acid	2.63	3.574	-0.944
dimethylamine	2.63	1.011	1.619
4-biphenylmethanol	2.64	3.332	-0.692
2,3,4-trichloroaniline	2.65	3.039	-0.389
2,3-dichlorophenol	2.65	2.370	0.280
fluridone	2.65	3.916	-1.263
sulfotepp	2.66	2.521	0.139
3-(4-bromo-3-chlorophenyl)-1-methoxy-1-methylurea	2.66	2.699	-0.039
2,5-dichloro-N-methylphenyl carbamate	2.71	2.781	-0.071
methyl 1-(butyl carbamoyl) benzimidazol-2-yl carbamate	2.71	2.322	0.388
benzophenone	2.71	2.800	-0.090
2,4,6-trinitrotoluene	2.72	2.542	0.178
2,4-dichloro aniline	2.72	2.654	0.066
isofenphos	2.73	3.473	-0.743
methyl N(3,4-dichlorophenyl) carbamate	2.74	2.553	0.187
ethyl 3,5-dinitrobenzoate	2.74	2.415	0.325

	2.75	2.370	0.300
2,4-dichlorophenol	2.76	3.306	-0.546
S-{{(1,1-dimethylethyl)thio}methyl}O,O-diethyl phosphorodithioate	2.76	1.812	0.948
2,2-dimethyl-1,3-benzodioxol-4- <sup>a</sup> methylcarbamate	2.76	3.147	-0.387
oryzalin	2.76	2.496	0.264
clopidol	2.76	3.735	-0.975
quizalofop-ethyl	2.77	2.548	0.222
isopropyl-N-(3-chlorophenyl) carbamate	2.78	3.507	-0.727
diphenylamine	2.78	2.438	0.342
2-chloro-4-(diethylamino)-6-(ethylamino)-S-triazine	2.78	2.322	0.458
secbumeton	2.79	2.032	0.758
phosmet	2.79	2.852	-0.062
N-{5-(1,1-dimethylethyl)-1,3,4-thiodiazol-2-yl}-N,N'-dimethylurea	2.80	2.990	-0.190
1,2,3-trimethylbenzene	2.80	2.790	0.010
S-propyl butylethylthiocarbamate	2.80	2.738	0.062
1-(1,3-benzothiazol-2-yl)-1,3-dimethyl urea	2.82	2.937	-0.117
1,3,5-trimethylbenzene	2.83	2.338	0.492
3,5-dimethylphenol	2.83	1.188	1.642
trimethylamine	2.83	3.331	-0.501
disulfoton	2.83	2.812	0.018
2-( <sup>a</sup> -naphthoxy)-N,N-diethylpropionamide	2.85	2.985	-0.140
1,3,5-trichlorobenzene	2.85	2.971	-0.121
tetrachloroguaiacol	2.85	3.422	-0.572
2-(tert-butylamino)-4-(ethylamino)-6-(methylthio)-S-triazine	2.87	2.659	0.211
n-propylbenzene	2.88	3.145	-0.265
4-ethylsulfonyl-2,6-dinitro-W,N-dipropylaniline	2.89	2.328	0.562
quinoline	2.91	2.632	0.278
3-(3,4-dichlorophenyl)-1-methoxy-1-methylurea	2.91	2.855	0.055
2,4-bis(isopropylamino)-6-(methylthio)-S-triazine	2.93	2.656	0.275
2-acetonaphthone	2.93	3.350	-0.420
O-ethyl-S-phenylethylphosphonodithioate	2.94	2.985	-0.045
1,2,4-trichlorobenzene	2.95	3.526	-0.576
pentachlorophenol	2.95	2.124	0.826
hydroxy atrazine	2.96	3.189	-0.229
lindane	2.96	2.169	0.791
2-methoxy-3,5,6-trichloropyridine	2.96	2.543	0.417
styrene	2.98	2.915	0.065
4-methylsulfonyl-2,6-dinitro-W,N-dipropylaniline	2.99	2.586	0.404
4,5,6-trichloroguaiacol	3.00	2.874	0.126
azinphos-methyl	3.00	3.062	-0.062
pirimiphos-methyl	3.00	1.987	1.013
dichlorprop	3.00	3.000	0.000
amitraz	3.01	2.827	0.183
profenofos	3.02	2.306	0.714
ethyl octanoate	3.03	2.755	0.275
2,4,6-trichlorophenol	3.03	3.213	-0.183
profenophos	3.04	3.425	-0.385
2,3,4,5-tetrachloroaniline	3.07	3.376	-0.306
4-propylsulfonyl-2,6-dinitro-W,N-dipropylaniline	3.07	3.086	-0.016
2-ethylthio-4,6-bis(isopropylamino)-S-triazine	3.08	2.259	0.821
1,4-dichloro-2,5-dimethoxybenzene	3.09	2.370	0.720
3,4-dichlorophenol	3.09	3.097	-0.007
tricyclazole	3.09	3.247	-0.157
lineai alkylate sulfonate	3.11	2.941	0.170
naphthalene	3.11	2.947	0.163
diethyltethyl-ethyl	3.11	3.886	-0.773
fenarimol	3.12	3.306	-0.186
1,2,4,5-tetramethylbenzene	3.12	3.657	-0.537
EPN	3.13	3.638	-0.508
diphenyl diimide	3.14	2.452	0.688
toxaphene	3.14	3.413	-0.273
chlorothalonil	3.14	3.465	-0.325
di-n-butyl phthalate	3.16	3.212	-0.052
phenyl benzoate	3.17	3.084	0.086

penturon	3.18	3.241	-0.061
permethrin	3.19	4.286	-1.096
1,3-dimethylbenzene	3.20	2.144	1.056
1,2,4,5-tetrachlorobenzene	3.20	3.370	-0.170
O,O-dimethyl O-(2,4,5-trichlorophenyl)-phosphorothioate	3.20	3.689	-0.489
4-acetyl biphenyl	3.22	3.265	-0.045
2-chloro-4-(diethylamino)-6-(isopropylamino)-S-triazine	3.22	2.588	0.632
biphenyl	3.23	3.550	-0.320
thiabendazole	3.24	3.182	0.058
O,O-diethyl S-{2-(ethylthio)ethyl}phosphorodithioate	3.25	2.695	0.555
2,6-dichloro aniline	3.25	2.654	0.596
N-(trichloromethylthio)phthalimide	3.27	3.289	-0.019
thiobencarb	3.27	3.605	-0.335
S-ethyl diisobutylthiocarbamate	3.28	2.786	0.494
norfluorazon	3.28	3.076	0.204
2-(2,4,5-trichlorophenoxy) propionic acid	3.28	2.372	0.908
4-chloro-5-(methylamino)-2-( $\alpha$ , $\alpha$ , $\alpha$ -trifluoro-m-tolyl)-3(2H)-pyridazinone	3.28	3.348	-0.068
diphenylether	3.29	2.919	0.371
butachlor	3.29	3.257	0.037
desmedipharm	3.30	3.301	-0.001
triforine	3.30	3.360	-0.059
methyl 5-(2,4-dichlorophenoxy)-2-nitrobenzoate	3.32	3.931	-0.611
cis-N-[(1,1,2,2-tetrachloroethyl)thio]-4-cyclohexene-1,2-dicarboximide	3.32	2.671	0.649
phosalone	3.32	4.309	-0.989
1-naphthol	3.33	2.711	0.619
hexachloroethane	3.34	3.492	-0.152
2,3,4,6-tetrachlorophenol	3.35	3.141	0.209
S-(2,2,3-trichloroallyl) diisopropylthiocarbamate	3.35	3.442	-0.092
1-methylnaphthalene	3.36	3.310	0.050
1-n-butyl-3-(3,4-dichlorophenyl)-1-methylurea	3.36	2.873	0.487
phenazine	3.37	2.827	0.543
propiconazole	3.39	3.527	-0.137
n-butylbenzene	3.40	2.624	0.776
2-methylnaphthalene	3.40	3.310	0.090
2-(3,4-dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dione	3.42	3.031	0.389
piperophos	3.44	3.632	-0.192
dyfonate	3.44	2.697	0.743
phenmediphem	3.44	3.439	0.001
benzidine	3.46	3.659	-0.199
chlorobenzilate	3.46	4.050	-0.590
pyroxychlor	3.48	2.974	0.506
4,6-dichloro-N(2-chloro-phenyl)-1,3,5-triazin-2-amine	3.48	3.364	0.116
1,2,3,5-tetrachlorobenzene	3.49	3.370	0.120
benzo[b]thiophene	3.49	3.079	0.411
O,O-diethyl S-[(ethylthio)methyl] phosphorodithioate	3.51	2.942	0.568
1-naphthylamine	3.51	2.995	0.515
2-tert-butyl-4-(2,4-dichloro-5-isopropoxyphenyl)-1,2,3,4-oxadiazolin-5-one	3.51	3.204	0.306
2,3,5,6-tetrachloroterephthalic acid	3.51	2.412	1.093
3-[p-(p-chlorophenoxy)phenyl]-1,1-dimethylurea	3.51	2.887	0.623
O,O-dimethyl-O-(3,5,6-trichloro-2-pyridyl) phosphorothioate	3.52	3.044	0.476
1-dodecanol	3.52	2.754	0.766
3,4,5-trichlorophenol	3.56	2.755	0.805
N-(2-chloroethyl)- $\alpha$ , $\alpha$ , $\alpha$ -trifluoro-2,6-dinitro-N-propyl-p-toluidine	3.56	3.987	-0.427
2-chlorobiphenyl	3.57	3.935	-0.365
9-acetylanthracene	3.58	3.768	-0.188
1,2,3,4,5,6-hexachlorobenzene	3.59	4.141	-0.551
N <sub>4</sub> ,N <sub>4</sub> -diethyl- $\alpha$ , $\alpha$ , $\alpha$ -trifluoro-3,5-dinitrotoluene 2,4-diamine	3.60	3.474	0.126
1,2,4-trimethylbenzene	3.60	2.937	0.663
9-anthracene methanol	3.61	2.935	0.675
2,3,5-trimethylphenol	3.61	2.708	0.903
2,6-dinitro-N-n-propyl- $\alpha$ , $\alpha$ -trifluoro-p-toluidine	3.61	2.541	1.069
p-ethyl toluene	3.62	2.798	0.822
indane	3.63	2.725	0.905
chlorthal methyl	3.64	3.623	0.017

	3.05	3.805	-0.150
O,O-diethyl-O-p-nitrophenyl phosphorothioate	3.68	3.007	0.673
fluorene	3.70	3.748	-0.048
2,6-dichloro-4-nitroaniline	3.70	2.769	0.930
piperalin	3.70	4.407	-0.708
imazalil	3.73	3.079	0.651
2-ethylnaphthalene	3.76	3.540	0.220
1,2,3,4-tetrachlorobenzene	3.76	3.370	0.390
1-ethylnaphthalene	3.77	3.540	0.230
N-{{(4-chlorophenyl)amino}-carbonyl}-2,6-difluorobenzamide	3.83	3.331	0.499
tetrapropyl dithiopyrophosphate	3.84	3.443	0.397
5-indanol	3.86	2.495	1.365
chlornitrofen	3.90	4.190	-0.290
N-sec-butyl-4-tert-butyl-2,6-dinitroaniline	3.91	3.990	-0.080
2,2'-dichlorobiphenyl	3.92	4.321	-0.401
N-(cyclopropylmethyl)- $\alpha$ , $\alpha$ , $\alpha$ -trifluoro-2,6-dinitro-N-propyl-p-toluidine	3.93	3.817	0.113
2,3,5,6-tetrachloroaniline	3.94	3.425	0.515
9H-carbazole	3.95	3.568	0.382
O-(4-bromo-2,5-dichlorophenyl) O-methylphenylphosphonothioate	3.97	4.911	-0.941
O,O-dimethyl-O-p-nitrophenyl phosphorothioate	3.99	2.546	1.444
ethafluralin	4.00	3.848	0.152
bensulide	4.00	4.113	-0.113
2,2'-biquinoline	4.02	4.548	-0.528
N-butyl-N-ethyl- $\alpha$ , $\alpha$ , $\alpha$ -trifluoro-2,6-dinitro-p-toluidine	4.03	3.982	0.048
2,3,5,6-tetrachloro-nitrobenzene	4.05	3.485	0.565
dibenzothiophene	4.05	4.191	-0.141
2,3-dimethylnaphthalene	4.08	3.256	0.824
S-ethyl diisobutylthiocarbamate	4.09	2.719	1.371
aldrin	4.10	4.747	-0.647
acenaphthene	4.11	3.438	0.672
acridine	4.11	3.440	0.670
1,3,5-triethylbenzene	4.12	3.628	0.492
O,O-diethyl-O-(3,5,6-trichloro-2-pyridyl) phosphorothioate	4.13	3.403	0.727
endosulfan	4.13	3.892	0.238
2,4'-dichlorobiphenyl	4.13	4.321	-0.191
$\alpha$ , $\alpha$ , $\alpha$ -trifluoro-2,6-dinitro-N,N-dipropyl-p-toluidine	4.14	3.880	0.260
phenylcyclohexane	4.18	3.553	0.627
O,O,O,O-tetraethyl S,S-methylene bisphosphorodithioate	4.19	3.753	0.437
1,1'-dimethyl-4,4'-bipyridiniumion	4.19	3.170	1.020
2,5,2'-trichlorobiphenyl	4.23	4.706	-0.476
2,3,4,5-tetrachloro-nitrobenzene	4.23	3.485	0.745
butyl-benzyl phthalate	4.23	4.165	0.065
cypermethrin	4.27	4.393	-0.123
4,4'-dichlorobiphenyl	4.30	4.321	-0.021
dieldrin	4.32	3.840	0.480
chlordan	4.33	4.615	-0.285
3,3'-dichlorobenzidine	4.35	4.430	-0.080
phenanthrene	4.36	4.053	0.307
anthracene	4.41	4.053	0.357
3-chlorobiphenyl	4.42	3.935	0.485
sulprofos	4.42	3.929	0.491
2-aminoanthracene	4.45	4.107	0.343
1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-tetrahydro-4,7-methanoindene	4.48	4.573	-0.093
2,4,4'-trichlorobiphenyl	4.62	4.706	-0.086
pentachloroaniline	4.62	3.810	0.810
2,4,5,2',5'-pentachlorobiphenyl	4.63	5.477	-0.847
S-{{(p-chlorophenyl)thio)methyl} O,O-diethyl phosphorodithioate	4.66	4.120	0.540
p,p'-DDE	4.70	4.991	-0.291
oxyfluorfen	4.72	3.717	1.003
2,3,4,2',5'-pentachlorobiphenyl	4.74	5.477	-0.737
fluoranthrene	4.79	4.555	0.235
9-methylanthracene	4.81	4.422	0.388
2,4,2'-trichlorobiphenyl	4.84	4.706	0.134
2,5,3',4'-tetrachlorobiphenyl	4.86	5.092	-0.232

2,6-dinitro-N,N-dipropyl camidine	4.88	4.265	0.615
dichlofop-methyl	4.89	3.543	1.347
1,1,1-trichloro-2,2- bis(p-methoxyphenyl)ethanol	4.90	5.312	-0.412
2,5,2',5'-tetrachlorobiphenyl	4.91	5.092	-0.182
2,6,2',6'-tetrachlorobiphenyl	4.91	5.092	-0.182
pyrene	4.92	4.555	0.365
di-a(ethylhexyl) phthalate	4.94	3.465	1.475
benzo[f]quinoline	4.97	3.440	1.530
fenvalerate	5.00	3.787	1.213
chlordimeform	5.00	5.064	-0.064
pentachloronitrobenzene	5.00	3.870	1.130
flucythrinate	5.00	4.931	0.069
bis(2-ethylhexyl) phthalate	5.00	5.149	-0.149
temephos	5.00	4.741	0.259
6-aminochrysene	5.16	5.219	-0.059
pentachlorobenzene	5.32	3.755	1.565
7,12-dimethylbenzanthracene	5.35	5.481	-0.131
benzo(b)fluoranthrene	5.36	6.277	-0.917
p,p'-DDT	5.38	5.400	-0.020
p,p'-DDD	5.38	5.120	0.260
1,2-benzofluorene	5.46	4.445	1.015
benz[a]anthracene	5.49	5.165	0.325
perylene	5.49	5.416	0.074
chrysene	5.50	5.165	0.335
benzo(k)fluoranthrene	5.63	5.667	-0.037
tetracene	5.81	5.165	0.645
benzo(a)pyrene	5.83	5.667	0.163
2,3,4,5,6,2',5'-heptachlorobiphenyl	5.95	6.248	-0.298
2,3,4,5,2',5'-hexachlorobiphenyl	5.95	5.862	0.088
7H-dibenzo(c,g)carbazole	6.01	6.080	-0.070
dibenz(a,j)anthracene	6.02	6.277	-0.253
13H dibenzo(a,i)carbazole	6.02	5.792	0.228
benzo(e)pyrene	6.07	5.976	0.094
2,4,5,2',4',5'-hexachlorobiphenyl	6.08	5.862	0.218
2,4,6,2',4',6'-hexachlorobiphenyl	6.08	5.862	0.218
3-methyl cholanthrene	6.10	5.939	0.161
2,3,4,6,2'-pentachlorobiphenyl	6.11	5.477	0.633
benzo(ghi)perylene	6.15	6.170	-0.020
dibenz(a,h)anthracene	6.22	6.277	-0.057
2,3,4,2',3',4'-hexachlorobiphenyl	6.42	5.862	0.558
indeno(1,2,3-cd)pyrene	6.45	6.170	0.280
dicofol	6.90	4.998	1.905
2,3,5,6,2',3',5',6'-octachlorobiphenyl	7.34	6.633	0.707