

Table 1. Toxicity to *T. pyriformis* ($\log(\text{IGC}_{50}^{-1})$), Octanol/water Partitioning ($\log K_{ow}$) and Maximum Acceptor superdelocalisability (A_{max}) Values for Selected Benzenes. (Schultz, T.W. 1999. Structure-toxicity relationships for benzenes evaluated with *Tetrahymena pyriformis*. Chemical Research in Toxicology 12:1262-1267.)

No	CAS	Name	$\log(\text{IGC}_{50}^{-1})$	$\log K_{ow}$	A_{max}
	171-43-2	Benzene	-0.12	2.13	0.280
	2106-42-3	p-xylene	0.25	3.15	0.283
	3120055-09-6	1-phenyl-2-butanol	-0.16	2.02	0.284
	4108-88-3	Toluene	0.25	2.73	0.284
	5104-51-8	n-butylbenzene	1.25	4.26	0.284
	6538-68-1	n-amylbenzene	1.79	4.90	0.284
	7100-46-9	Benzylamine	-0.24	1.09	0.284
	898-82-8	Isopropylbenzene	0.69	3.66	0.285
	92430-16-2	6-phenyl-1-hexanol	0.87	3.30	0.285
	1010521-91-2	5-phenyl-1-pentanol	0.42	2.77	0.285
	11103-05-9	α,α -dimethylbenzenepropanol	-0.07	2.42	0.285
	123360-41-6	4-phenyl-1-butanol	0.12	2.35	0.285
	13122-97-4	3-phenyl-1-propanol	-0.21	1.88	0.285
	14100-51-6	benzyl alcohol	-0.83	1.05	0.285
	1598-85-1	(sec)phenethyl alcohol	-0.66	1.42	0.285
	16768-59-2	4-ethylbenzyl alcohol	0.07	2.13	0.285
	172722-36-3	3-phenyl-1-butanol	0.01	2.11	0.286
	1822144-60-1	(R+-)-1-phenyl-1-butanol	-0.01	2.47	0.286
	193597-91-9	4-biphenylmethanol	0.92	2.99	0.287
	205707-44-8	4-ethylbiphenyl	1.97	5.06	0.288
	2192-52-4	Biphenyl	1.05	3.98	0.288
	221565-75-9	(\pm)-2-phenyl-2-butanol	0.06	2.34	0.288
	235342-87-0	(\pm)-1,2-diphenyl-2-propanol	0.80	3.23	0.290
	2429338-49-6	1,1-diphenyl-2-propanol	0.75	2.93	0.290
	2595-64-7	3,4-dimethylaniline	-0.16	1.86	0.293
	261877-77-6	3-aminobenzyl alcohol	-1.13	-0.55	0.293
	274344-55-2	4-butoxyaniline	0.61	2.59	0.293
	2839905-50-5	4-pentyloxyaniline	0.97	3.12	0.293
	2939905-57-2	4-hexyloxyaniline	1.38	3.65	0.293
	30106-49-0	4-methylaniline	-0.05	1.39	0.293
	3199-88-7	4-isopropylaniline	0.22	2.47	0.293
	32587-02-0	3-ethylaniline	-0.03	1.94	0.294
	33589-16-2	4-ethylaniline	0.03	1.96	0.294
	34108-44-1	3-methylaniline	-0.28	1.40	0.294
	35104-13-2	4-butylaniline	1.07	3.18	0.294
	36103-63-9	(2-bromoethyl)benzene	0.42	3.09	0.294
	3795-53-4	2-methylaniline	-0.16	1.43	0.294
	3824544-04-5	2,6-diisopropylaniline	0.76	3.18	0.294
	3962-53-3	Aniline	-0.23	0.90	0.295
	40578-54-1	2-ethylaniline	-0.22	1.74	0.295
	41579-66-8	2,6-diethylaniline	0.31	2.87	0.295
	42100-68-5	Thioanisole	0.18	2.74	0.296

43150-76-5	4-methoxyphenol	-0.14	1.34	0.298
44527-54-8	3,4,5-trimethylphenol	0.93	2.87	0.298
45100-44-7	benzyl chloride	0.06	2.30	0.298
46104-93-8	4-methylanisole	0.25	2.81	0.299
47697-82-5	2,3,5-trimethylphenol	0.36	2.92	0.299
48527-60-6	2,4,6-trimethylphenol	0.42	2.73	0.299
4998-54-4	4-(tert.)butylphenol	0.91	3.31	0.300
5080-46-6	4-tert-pentylphenol	1.23	3.83	0.300
512416-94-6	2,3,6-trimethylphenol	0.28	2.67	0.300
52103-73-1	Phenetole	-0.14	2.51	0.300
53100-66-3	Anisole	-0.10	2.11	0.300
54105-67-9	2,4-dimethylphenol	0.14	2.35	0.300
55127-66-2	2-phenyl-3-butyn-2-ol	-0.18	1.88	0.300
56106-44-5	p-cresol (4-methylphenol)	-0.16	1.97	0.300
57123-07-9	4-ethylphenol	0.21	2.50	0.300
58645-56-7	4-propylphenol	0.64	3.20	0.300
59620-17-7	3-ethylphenol	0.29	2.50	0.300
60104-40-5	Nonylphenol	2.47	5.76	0.300
61108-39-4	m-cresol (3-methylphenol)	-0.08	1.98	0.300
6295-48-7	o-cresol (2-methylphenol)	-0.29	1.98	0.301
6390-00-6	2-ethylphenol	0.16	2.47	0.301
64108-95-2	Phenol	-0.35	1.50	0.301
651745-81-9	2-allylphenol	0.33	2.55	0.301
66591-50-4	Iodobenzene	0.36	3.25	0.301
67106-47-8	4-chloroaniline	0.05	1.83	0.302
68529-19-1	2-tolunitrile	-0.24	2.21	0.302
69501-94-0	4-hydroxyphenethyl alcohol	-0.83	0.52	0.303
70615-65-6	2-chloro-4-methylaniline	0.18	2.41	0.303
7195-51-2	2-chloroaniline	-0.17	1.88	0.304
72500-66-3	5-pentylresorcinol	1.31	3.42	0.305
73150-19-6	3-methoxyphenol	-0.33	1.58	0.305
74136-77-6	4-hexylresorcinol	1.80	3.45	0.306
7588-04-0	4-chloro-3,5-dimethylphenol	1.20	3.48	0.306
76106-38-7	4-bromotoluene	0.47	3.50	0.306
771585-07-5	1-bromo-4-ethylbenzene	0.67	4.03	0.306
78623-12-1	4-chloroanisole	0.60	2.79	0.307
7959-50-7	4-chloro-3-methylphenol	0.80	3.10	0.307
80108-46-3	1,3-dihydroxybenzene	-0.65	0.80	0.307
81108-86-1	Bromobenzene	0.08	2.99	0.308
82106-48-9	4-chlorophenol	0.54	2.39	0.308
83540-38-5	4-iodophenol	0.85	2.90	0.311
84156-41-2	2(4-chlorophenyl)ethylamine	0.14	2.00	0.311
85104-86-9	4-chlorobenzylamine	0.16	1.81	0.311
86554-00-7	2,4-dichloroaniline	0.56	2.78	0.311
87108-90-7	Chlorobenzene	-0.13	2.84	0.311
88108-42-9	3-chloroaniline	0.22	1.88	0.312
8999-51-4	1,2-dimethyl-4-nitrobenzene	0.59	2.91	0.314
905736-91-4	4-(pentyloxy)benzaldehyde	1.18	3.89	0.315
9199-99-0	4-nitrotoluene	0.65	2.37	0.315
92122-03-2	4-isopropylbenzaldehyde	0.67	2.92	0.316

9383-41-0	1,2-dimethyl-3-nitrobenzene	0.56	2.83	0.316
94108-43-0	3-chlorophenol	0.87	2.50	0.317
9599-08-1	3-nitrotoluene	0.42	2.45	0.317
9688-72-2	2-nitrotoluene	0.26	2.30	0.317
97106-37-6	1,4-dibromobenzene	0.68	3.79	0.317
98100-52-7	Benzaldehyde	-0.20	1.48	0.317
99121-32-4	3-ethoxy-4-hydroxybenzaldehyde	0.02	1.58	0.317
100121-33-5	3-methoxy-4-hydroxybenzaldehyde	-0.03	1.21	0.318
10170-70-2	4'-hydroxypropiophenone	0.12	2.03	0.318
102120-83-2	2,4-dichlorophenol	1.04	3.17	0.318
1031009-14-9	Valerophenone	0.56	3.17	0.318
10493-55-0	Propiophenone	-0.07	2.19	0.318
105495-40-9	Butyrophenone	0.21	2.77	0.318
10690-02-8	2-hydroxybenzaldehyde	0.42	1.81	0.318
1071671-75-6	Heptanophenone	1.56	4.23	0.318
10898-86-2	Acetophenone	-0.46	1.63	0.318
10998-95-3	Nitrobenzene	0.14	1.85	0.318
1101674-37-9	Octanophenone	1.89	4.75	0.318
11195-82-9	2,5-dichloroaniline	0.58	2.75	0.318
11295-75-0	3,4-dichlorotoluene	1.07	3.95	0.318
11399-09-2	3-nitroaniline	0.03	1.43	0.319
114626-43-7	3,5-dichloroaniline	0.71	2.90	0.319
1157530-27-0	4-bromo-6-chloro-o-cresol	1.28	3.61	0.319
11695-50-1	1,2-dichlorobenzene	0.53	3.38	0.319
117555-03-3	3-nitroanisole	0.72	2.17	0.321
118119-61-9	Benzophenone	0.87	3.18	0.321
11965262-96-6	3-chloro-5-methoxyphenol	0.76	2.50	0.322
120100-14-1	4-nitrobenzyl chloride	1.18	2.45	0.323
121615-58-7	2,4-dibromophenol	1.40	3.25	0.323
1225922-60-1	2-amino-5-chlorobenzonitrile	0.44	1.79	0.323
123552-41-0	2-hydroxy-4-methoxyacetophenone	0.55	1.98	0.324
124591-35-5	3,5-dichlorophenol	1.56	3.61	0.325
125104-88-1	4-chlorobenzaldehyde	0.40	2.13	0.325
126134-85-0	4-chlorobenzophenone	1.50	3.97	0.325
127108-70-3	1,3,5-trichlorobenzene	0.87	4.19	0.325
128636-30-6	2,4,5-trichloroaniline	1.30	3.69	0.325
12990-90-4	4-bromobenzophenone	1.26	4.12	0.326
130120-82-1	1,2,4-trichlorobenzene	1.08	4.02	0.326
13188-06-2	2,4,6-trichlorophenol	1.41	3.69	0.326
132616-86-4	4-ethoxy-2-nitroaniline	0.76	2.39	0.326
1332973-76-4	5-bromovanillin	0.62	1.92	0.326
134100-29-8	4-nitrophenetole	0.83	2.53	0.328
13589-59-8	4-chloro-2-nitrotoluene	0.82	3.05	0.328
136585-79-5	1-bromo-3-nitrobenzene	1.03	2.64	0.328
1373217-15-0	4-bromo-2,6-dichlorophenol	1.78	3.52	0.329
13883-42-1	2-chloro-6-nitrotoluene	0.68	3.09	0.329
1393481-20-7	2,3,5,6-tetrachloroaniline	1.76	4.10	0.330
140619-24-9	3-nitrobenzonitrile	0.45	1.17	0.330
14195-95-4	2,4,5-trichlorophenol	2.10	3.72	0.330
14295-94-3	1,2,4,5-tetrachlorobenzene	2.00	4.63	0.331

14389-62-3	4-methyl-2-nitroaniline	0.37	1.82	0.331
144121-73-3	1-chloro-3-nitrobenzene	0.73	2.47	0.332
14588-74-4	2-nitroaniline	0.08	1.85	0.332
146634-83-3	2,3,4,5-tetrachloroaniline	1.96	4.27	0.333
147118-79-6	2,4,6-bromophenol	1.91	4.08	0.334
1487149-70-4	2-bromo-5-nitrotoluene	1.16	3.25	0.334
1493819-88-3	1-fluoro-3-iodo-5-nitrobenzene	1.09	3.15	0.335
15088-75-5	2-nitrophenol	0.67	1.77	0.335
151121-87-9	2-chloro-4-nitroaniline	0.75	2.05	0.336
15242454-06-8	5-hydroxy-2-nitrobenzaldehyde	0.33	1.75	0.336
153576-55-6	3,4,5,6-tetrabromo-o-cresol	2.57	4.97	0.336
15458-90-2	2,3,4,6-tetrachlorophenol	2.18	3.88	0.337
155350-46-9	1-fluoro-4-nitrobenzene	0.10	1.89	0.338
156771-60-8	Pentafluoroaniline	0.26	1.87	0.338
157577-19-5	1-bromo-2-nitrobenzene	0.75	2.51	0.338
15890-59-5	3,5-dibromosalicylaldehyde	1.65	3.42	0.338
159618-62-2	3,5-dichloronitrobenzene	1.13	3.09	0.339
160610-78-6	4-chloro-3-nitrophenol	1.27	2.46	0.339
1614901-51-3	2,3,4,5-tetrachlorophenol	2.72	4.21	0.339
1622227-79-4	Thiobenzamide	0.09	1.50	0.339
163100-00-5	1-chloro-4-nitrobenzene	0.43	2.39	0.340
1642357-47-3	α,α,α -4-tetrafluoro-m-toluidine	0.77	2.51	0.341
16588-73-3	1-chloro-2-nitrobenzene	0.68	2.52	0.343
1667147-89-9	4-chloro-6-nitro-m-cresol	1.63	2.93	0.343
16787-86-5	Pentachlorophenol	2.07	5.18	0.343
16899-65-0	1,3-dinitrobenzene	0.76	1.49	0.345
169121-14-2	2,4-dinitrotoluene	0.87	1.98	0.345
1706641-64-1	4,5-dichloro-2-nitroaniline	1.66	3.21	0.345
171771-61-9	Pentafluorophenol	1.63	3.23	0.345
172608-71-9	Pentabromophenol	2.66	4.85	0.346
173350-30-1	3-chloro-4-fluoronitrobenzene	0.80	2.74	0.347
174100-25-4	1,4-dinitrobenzene	1.30	1.47	0.347
17599-54-7	3,4-dichloronitrobenzene	1.16	3.12	0.348
17689-61-2	2,5-dichloronitrobenzene	1.13	3.03	0.349
1772683-43-4	2,4-dichloro-6-nitroaniline	1.26	3.33	0.349
17879544-31-3	3,4-dinitrobenzyl alcohol	1.09	0.59	0.349
179611-06-3	2,4-dichloronitrobenzene	0.99	3.09	0.350
1803209-22-1	2,3-dichloronitrobenzene	1.07	3.05	0.350
181528-29-0	1,2-dinitrobenzene	1.25	1.69	0.351
182103-72-0	phenyl isothiocyanate	1.41	3.28	0.352
18388-30-2	3-trifluoromethyl-4-nitrophenol	1.65	2.77	0.352
184305-85-1	2,6-iodo-4-nitrophenol	1.81	3.52	0.353
185609-89-2	2,4-chloro-6-nitrophenol	1.75	3.07	0.354
18618708-70-8	1,3,5-trichloro-2-nitrobenzene	1.43	3.69	0.354
18789-69-0	1,2,4-trichloro-5-nitrobenzene	1.53	3.47	0.354
18817700-09-3	1,2,3-trichloro-4-nitrobenzene	1.51	3.61	0.357
1896361-21-3	2-chloro-5-nitrobenzaldehyde	0.53	2.25	0.357
190653-37-2	Pentafluorobenzaldehyde	0.82	2.39	0.357
191709-49-9	2,4-dinitro-1-iodobenzene	2.12	2.50	0.359
192117-18-0	2,3,5,6-tetrachloronitrobenzene	1.82	4.38	0.360

193329-71-5	2,5-dinitrophenol	1.04	1.86	0.361
19497-02-9	2,4-dinitroaniline	0.72	1.72	0.361
195879-39-0	2,3,4,5-tetrachloronitrobenzene	1.78	3.93	0.361
196771-69-7	1,2,3-trifluoro-4-nitrobenzene	1.89	2.01	0.362
1976306-39-4	1,2-dichloro-4,5-dinitrobenzene	2.21	2.93	0.365
198606-22-4	2,6-dinitroaniline	0.84	1.79	0.366
199534-52-1	4,6-dinitro-2-methylphenol	1.73	2.12	0.366
2004097-49-8	4-(tert)butyl-2,6-dinitrophenol	1.80	3.61	0.367
201584-48-5	1-bromo-2,4-dinitrobenzene	2.31	2.29	0.368
20251-28-5	2,4-dinitrophenol (nonneutralized)	1.06	1.54	0.368
20328689-08-9	1,5-dichloro-2,3-dinitrobenzene	2.42	2.85	0.369
2043531-19-9	6-chloro-2,4-dinitroaniline	1.12	2.46	0.370
2051817-73-8	2-bromo-4,6-dinitroaniline	1.24	2.61	0.372
206314-41-0	2,3,4,6-tetrafluoronitrobenzene	1.87	1.86	0.372
207573-56-8	2,6-dinitrophenol	0.83	1.33	0.372
20897-00-7	1-chloro-2,4-dinitrobenzene	2.16	2.14	0.374
20970-34-8	2,4-dinitro-1-fluorobenzene	1.71	1.47	0.375
210880-78-4	Pentafluoronitrobenzene	2.43	2.00	0.378
21120098-38-8	1,4-dinitrotetrachlorobenzene	2.82	3.44	0.380
212327-92-4	1,5-difluoro-2,4-dinitrobenzene	2.08	1.31	0.384
2132678-21-9	1,3-dinitro-2,4,5-trichlorobenzene	2.60	3.05	0.385
2146284-83-9	1,3,5-trichloro-2,4-dinitrobenzene hemihydrate	2.19	2.97	0.385
2151930-72-9	4-chloro-3,5-dinitrobenzotrile	2.66	1.37	0.393
21682-68-8	Pentachloronitrobenzene	NTAS	4.64	0.364
217608-93-5	Pentachlorobenzene	NTAS	5.17	0.339
2181825-21-4	Pentachloroanisole	NTAS	5.45	0.339

NTAS, not toxic at saturation.

Table 2. Toxicity to *T. pyriformis* ($\log(\text{IGC}_{50}^{-1})$), Octanol/water Partitioning ($\log K_{ow}$) and Maximum Acceptor superdelocalisability (A_{max}) Values for Additional Benzenes. (Schultz T.W., Netzeva, T.I., and Cronin, M.T.D. 2003. The use of diversity versus representivity in the training and validation of quantitative structure-activity relationships. SAR QSAR in Environmental Research 14: 59-81.)

No	CAS	NAME	$\log(\text{IGC}_{50}^{-1})$	$\log K_{ow}$	A_{max}
	114898-87-4	1-phenyl-2-propanol	-0.62	1.97	0.283
	2589-18-4	4-methylbenzyl alcohol	-0.49	1.58	0.284
	3705-73-7	(±)-1-phenyl-2-pentanol	0.16	2.55	0.284
	4536-60-7	4-isopropylbenzyl alcohol	0.18	2.53	0.284
	53261-62-9	2-(p-tolyl)ethylamine	-0.04	1.78	0.284
	6104-84-7	4-methyl benzylamine	-0.01	2.81	0.284
	7587-03-1	3-methylbenzyl alcohol	-0.24	1.60	0.285
	8104-54-1	3-phenyl-2-propen-1-ol	-0.08	1.95	0.285
	9877-65-6	4-(tert)butylbenzyl alcohol	0.48	2.93	0.285
	10699-02-5	4-methylphenethyl alcohol	-0.26	1.68	0.285
	11618-36-0	1-phenylethylamine	-0.18	1.40	0.285
	1289-95-2	2-methylbenzyl alcohol	-0.43	1.55	0.285
	13100-86-7	2-methyl-1-phenyl-2-propanol	-0.41	1.86	0.285
	14589-08-2	n-methylphenethylamine	-0.41	1.43	0.285
	15582-22-9	β-methylphenethylamine	-0.28	1.68	0.285
	1622135-49-5	(S±)-1-phenyl-1-butanol	-0.09	2.47	0.286
	1793-54-9	(±)1-phenyl-1-propanol	-0.43	1.94	0.286
	1860-12-8	phenethyl alcohol	-0.59	1.36	0.286
	191123-85-9	2-phenyl-1-propanol	-0.40	1.58	0.286
	20617-94-7	2-phenyl-2-propanol	-0.57	1.81	0.288
	2189104-46-1	2-phenyl-1-butanol	-0.11	2.11	0.288
	2291-01-0	Benzhydrol	0.50	2.67	0.289
	23622-32-2	benzaloxime	-0.11	1.75	0.291
	24108-69-0	3,5-dimethylaniline	-0.36	1.91	0.293
	25769-92-6	4-(tert)butylaniline	0.36	2.70	0.293
	2695-68-1	2,4-dimethylaniline	-0.29	1.68	0.293
	272046-18-6	4-phenylbutyronitrile	0.15	2.21	0.293
	2888-05-1	2,4,6-trimethylaniline	-0.05	2.31	0.293
	29645-59-0	3-phenylpropionitrile	-0.16	1.72	0.294
	3030273-11-1	4-sec-butylaniline	0.61	2.87	0.294
	3187-59-2	2,3-dimethylaniline	-0.43	1.81	0.294
	32140-29-4	benzyl cyanide	-0.36	1.56	0.294
	3395-78-3	2,5-dimethylaniline	-0.33	1.83	0.294
	341823-91-2	α-methylbenzyl cyanide	0.01	1.87	0.294
	35643-28-7	2-isopropylaniline	0.12	2.12	0.294
	3687-62-7	2,6-dimethylaniline	-0.43	1.84	0.294
	37103-69-5	n-ethylaniline	0.07	2.16	0.295
	381821-39-2	2-propylaniline	0.08	2.42	0.295
	39100-61-8	n-methylaniline	0.06	1.66	0.295
	401199-46-8	2-amino-4-(tert)butylphenol	0.37	2.44	0.295
	4190-04-0	2-methoxyaniline	-0.69	1.18	0.295
	421008-88-4	3-phenylpyridine	0.47	2.53	0.296
	435344-90-1	2-aminobenzyl alcohol	-1.07	-0.17	0.296

44101-82-6	2-benzylpyridine	0.38	2.71	0.296
451138-52-9	3,5-di-tert-butylphenol	1.64	5.13	0.298
465651-88-7	phenyl propargyl sulfide	0.54	3.30	0.298
47622-62-8	4-ethoxyphenol	0.01	1.81	0.298
48122-94-1	4-butoxyphenol	0.70	2.90	0.298
492116-65-6	4-benzylpyridine	0.63	2.62	0.298
501008-89-5	2-phenylpyridine	0.27	2.63	0.299
5195-65-8	3,4-dimethylphenol	0.12	2.23	0.299
52585-34-2	3-tert-butylphenol	0.74	3.30	0.300
53108-68-9	3,5-dimethylphenol	0.11	2.35	0.300
541879-09-0	6-tert-butyl-2,4-dimethylphenol	1.16	4.30	0.300
5599-89-8	4-isopropylphenol	0.47	2.90	0.300
56618-45-1	3-isopropylphenol	0.61	2.90	0.300
57526-75-0	2,3-dimethylphenol	0.12	2.42	0.300
5895-87-4	2,5-dimethylphenol	0.14	2.34	0.300
59498-00-0	4-hydroxy-3-methoxybenzyl alcohol	-0.70	0.29	0.300
6088-69-7	2-isopropylphenol	0.61	2.88	0.301
6153222-92-7	3-amino-2-cresol	-0.55	0.70	0.301
6295-69-2	4-chloro-2-methylaniline	0.35	2.36	0.301
6397-54-1	2-methoxy-4-propenylphenol	0.75	3.31	0.302
6490-72-2	2,4,6-tris(dimethylaminomethyl)phenol	-0.52	0.92	0.302
65348-54-9	2-fluoroaniline	-0.37	1.26	0.302
663544-25-0	4-aminobenzyl cyanide	-0.76	0.34	0.302
67626-01-7	3-iodoaniline	0.65	2.90	0.302
684360-47-8	cinnamonitrile	0.16	1.95	0.303
69456-47-3	3-fluorobenzyl alcohol	-0.39	1.25	0.305
702237-30-1	3-cyanoaniline	-0.47	1.07	0.306
71371-41-5	4-fluorophenol	0.02	1.77	0.307
72615-43-0	2-iodoaniline	0.35	2.32	0.307
73372-19-0	3-fluoroaniline	-0.10	1.30	0.307
741570-64-5	4-chloro-2-methylphenol	0.70	2.78	0.307
7514143-32-9	4-chloro-3-ethylphenol	1.08	3.51	0.308
761124-04-5	2-chloro-4,5-dimethylphenol	0.69	3.10	0.309
77500-99-2	3,5-dimethoxyphenol	-0.09	1.64	0.309
7814191-95-8	4-hydroxybenzyl cyanide	-0.38	0.90	0.309
792374-05-2	4-bromo-2,6-dimethylphenol	1.16	3.63	0.309
8018982-54-2	2-bromobenzyl alcohol	0.10	1.97	0.309
81615-74-7	2-chloro-5-methylphenol	0.54	2.65	0.309
82367-12-4	2-fluorophenol	0.19	1.67	0.309
83100-10-7	4-(dimethylamino)benzaldehyde	0.23	1.81	0.310
84106-41-2	4-bromophenol	0.68	2.59	0.311
8595-79-4	5-chloro-2-methylaniline	0.50	2.36	0.311
8695-74-9	3-chloro-4-methylaniline	0.39	2.41	0.311
8787-60-5	3-chloro-2-methylaniline	0.38	2.36	0.312
881875-88-3	4-chlorophenethyl alcohol	0.32	1.90	0.312
89873-76-7	4-chlorobenzyl alcohol	0.25	1.96	0.312
906627-55-0	2-bromo-4-methylphenol	0.60	2.85	0.312
91603-71-4	1,3,5-trimethyl-2-nitrobenzene	0.86	3.22	0.313
92873-63-2	3-chlorobenzyl alcohol	0.15	1.94	0.314
9395-56-7	2-bromophenol	0.33	2.33	0.314

944421-08-3	4-hydroxy-3-methoxybenzonitrile	-0.03	1.42	0.315
95619-25-0	3-nitrobenzyl alcohol	-0.22	1.21	0.315
9616532-79-9	4-bromophenyl acetonitrile	0.60	2.43	0.315
97874-90-8	4-methoxybenzonitrile	0.10	1.70	0.315
9836436-65-4	2-hydroxy-4,5-dimethylacetophenone	0.71	2.86	0.316
99135-02-4	2-anisaldehyde	0.15	1.72	0.316
10095-88-5	4-chlororesorcinol	0.13	1.80	0.316
10118358-63-9	methyl-4-methylaminobenzoate	0.31	2.16	0.316
10267-36-7	4-phenoxybenzaldehyde	1.26	3.96	0.317
103621-59-0	3-hydroxy-4-methoxybenzaldehyde	-0.14	0.97	0.317
1043218-36-8	4-biphenylcarboxaldehyde	1.12	3.38	0.317
1054460-86-0	2,4,5-trimethoxybenzaldehyde	-0.10	1.19	0.317
1061137-41-3	4-benzoylaniline	0.68	2.46	0.317
1075991-31-1	3-anisaldehyde	0.23	1.71	0.317
1087778-83-8	n-propyl cinnamate	1.23	3.52	0.318
109103-36-6	(trans)ethyl cinnamate	0.99	2.99	0.318
110942-92-7	hexanophenone	1.19	3.70	0.318
111538-65-8	n-butyl cinnamate	1.53	4.05	0.318
112140-53-4	4-chlorobenzyl cyanide	0.66	2.47	0.319
113103-26-4	(trans)methyl cinnamate	0.58	2.62	0.319
11494-30-4	ethyl-4-methoxybenzoate	0.77	2.81	0.319
115937-39-3	phenylacetic acid hydrazide	-0.48	0.14	0.319
116100-83-4	3-hydroxybenzaldehyde	0.08	1.38	0.320
11787-65-0	2,6-dichlorophenol	0.73	2.64	0.320
1182495-37-6	benzyl methacrylate	0.65	2.53	0.320
1196521-30-8	isoamyl-4-hydroxybenzoate	1.48	3.97	0.320
1202491-32-9	benzyl-4-hydroxyphenyl ketone	1.07	3.22	0.321
121120-51-4	benzyl benzoate	1.45	3.97	0.321
1221137-42-4	4-benzoylphenol	1.02	3.07	0.321
1235428-54-6	2-methyl-5-nitrophenol	0.66	2.35	0.321
124621-42-1	3-acetamidophenol	-0.16	0.73	0.322
1253034-34-2	4-cyanobenzamide	-0.38	0.48	0.322
12686-00-0	2-nitrobiphenyl	1.30	3.77	0.322
1277120-43-6	5-chloro-2-hydroxybenzamide	0.59	2.13	0.323
128554-84-7	3-nitrophenol	0.51	2.00	0.324
129626-19-7	phenyl-1,3-dialdehyde	0.18	1.36	0.324
1305798-75-4	ethyl-4-bromobenzoate	1.33	3.50	0.325
13189-84-9	2,4-dihydroxyacetophenone	0.25	1.41	0.325
1321016-78-0	3-chlorobenzophenone	1.55	3.97	0.325
13317696-62-7	phenyl-4-hydroxybenzoate	1.37	3.49	0.327
13493-99-2	phenyl benzoate	1.35	3.59	0.327
135131-57-7	2-hydroxy-4-methoxybenzophenone	1.42	3.58	0.327
1362700-22-3	Benzylidene malononitrile	0.64	2.15	0.328
137620-88-2	4-nitrophenyl phenyl ether	1.58	3.83	0.330
138136-36-7	resorcinol monobenzoate	1.11	3.13	0.330
13914548-45-9	4-bromophenyl-3-pyridyl ketone	0.82	2.96	0.331
140121-89-1	3'-nitroacetophenone	0.32	1.42	0.332
14199-61-6	3-nitrobenzaldehyde	0.11	1.47	0.332
1424553-07-5	ethyl phenylcyanoacetate	-0.02	1.63	0.332
14391-23-6	2-nitroanisole	-0.07	1.73	0.332

1444920-77-8	3-methyl-2-nitrophenol	0.61	2.29	0.332
145844-51-9	2,5-diphenyl-1,4-benzoquinone	1.48	3.16	0.332
146610-15-1	2-nitrobenzamide	-0.72	-0.12	0.332
1472905-69-3	methyl-2,5-dichlorobenzoate	0.81	3.16	0.332
148552-89-6	2-nitrobenzaldehyde	0.17	1.74	0.333
149119-33-5	4-methyl-2-nitrophenol	0.57	2.15	0.333
150131-55-5	2,2',4,4'-tetrahydroxybenzophenone	0.96	2.92	0.333
151555-16-8	4-nitrobenzaldehyde	0.20	1.56	0.333
152700-38-9	5-methyl-2-nitrophenol	0.59	2.31	0.333
15390-60-8	3,5-dichlorosalicylaldehyde	1.55	3.07	0.334
15469212-31-3	2-(benzylthio)-3-nitropyridine	1.72	3.42	0.335
15599-77-4	ethyl-4-nitrobenzoate	0.71	2.33	0.335
156874-42-0	2,4-dichlorobenzaldehyde	1.04	3.08	0.335
15713608-87-2	2',3',4'-trichloroacetophenone	1.34	3.21	0.336
158835-11-0	2,2'-dihydroxybenzophenone	1.16	3.47	0.336
159619-50-1	methyl-4-nitrobenzoate	0.39	1.94	0.336
1602973-19-5	2-chloromethyl-4-nitrophenol	0.75	2.42	0.338
161402-45-9	α,α,α -trifluoro-p-cresol	0.62	2.82	0.340
1625292-45-5	Dimethylnitroterephthalate	0.43	1.66	0.340
163637-53-6	Thioacetanilide	-0.01	1.71	0.341
164601-89-8	2-nitroresorcinol	0.66	1.56	0.341
1651689-84-5	3,5-dibromo-4-hydroxybenzotrile	1.16	2.88	0.341
166440-60-8	pentafluorobenzyl alcohol	-0.20	1.82	0.342
16742087-80-9	methyl-4-chloro-2-nitrobenzoate	0.82	2.41	0.342
1681493-27-2	1-fluoro-2-nitrobenzene	0.23	1.69	0.343
169393-39-5	a,a,a-4-tetrafluoro-o-toluidine	-0.02	2.51	0.343
170704-13-2	3-hydroxy-4-nitrobenzaldehyde	0.27	1.47	0.345
1713460-18-2	2,5-dibromonitrobenzene	1.37	3.41	0.346
172613-90-1	benzoyl cyanide	0.31	1.91	0.347
17378056-39-0	4,5-difluoro-2-nitroaniline	0.75	2.19	0.348
174364-74-9	2,5-difluoronitrobenzene	0.33	1.86	0.349
175827-23-6	2,4-dibromo-6-nitroaniline	1.62	3.63	0.352
1763011-34-5	4-hydroxy-3-nitrobenzaldehyde	0.61	1.48	0.352
177532-55-8	benzoyl isothiocyanate	0.10	1.91	0.364