Toxicity and chemical descriptor data for 500 aliphatic chemicals modeled by Schultz et al. in Chemical Research in Toxicology.

ID	CAS	Name	Group	Log $(IGC_{50})^{-1}$	Log K_{ow}	E_{lumo}	E_{lumo}^{**}	$^3\chi_c$	A_{max}	EllipsVol
Saturated alcohols***										
1	67-56-1	methyl alcohol	1	-2.6656	-0.77	3.778	1.700			
2	64-17-5	ethyl alcohol	1	-1.9912	-0.31	3.565	1.700			
3	71-23-8	1-propanol	1	-1.7464	0.25	3.489	1.700			
4	67-63-0	2-propanol)	1	-1.8819	0.05	3.575	1.700			
5	71-36-3	1-butanol	1	-1.4306	0.88	3.425	1.700			
6	15892-23-6	(+/-)-2-butanol	1	-1.5420	0.61	3.477	1.700			
7	78-83-1	2-methyl-1-propanol	1	-1.3724	0.76	3.547	1.700			
8	71-41-0	1-pentanol	1	-1.0304	1.56	3.391	1.700			
9	6023-29-7	2-pentanol	1	-1.1596	1.19	3.516	1.700			
10	584-02-1	3-pentanol	1	-1.2437	1.21	3.481	1.700			
11	598-75-4	3-methyl-2-butanol	1	-0.9959	1.28	3.436	1.700			
12	75-85-4	tert-amylalcohol	1	-1.1729	0.89	3.435	1.700			
13	137-32-6	2-methyl-1-butanol	1	-0.9528	1.22	3.544	1.700			
14	123-51-3	3-methyl-1-butanol	1	-1.0359	1.16	3.384	1.700			

15	75-84-3	2,2-dimethyl-1-propanol	1	-0.8702	1.31	3.439	1.700
16	75-65-0	2-methyl-2-propanol	1	-1.7911	0.35	3.438	1.700
17	111-76-2	2-butoxyethanol	1	-1.3743	0.83	2.657	1.700
18	111-27-3	1-hexanol	1	-0.3789	2.03	3.368	1.700
19	624-95-3	3,3-dimethyl-1-butanol	1	-0.7368	1.62	3.376	1.700
20	626-89-1	4-methyl-1-pentanol	1	-0.6372	1.75	3.367	1.700
21	111-70-6	1-heptanol	1	0.1050	2.72	3.353	1.700
22	600-36-2	2,4-dimethyl-3-pentanol	1	-0.7052	1.93	3.386	1.700
23	111-87-5	1-octanol	1	0.5827	3.00	3.343	1.700
24	4128-31-8	2-octanol	1	0.0011	2.90	3.440	1.700
25	20296-29-1	3-octanol	1	0.0309	2.72	3.398	1.700
26	104-76-7	2-ethyl-1-hexanol	1	0.1673	2.81	3.472	1.700
27	58175-57-8	2-propyl-1-pentanol	1	0.1344	2.81	3.465	1.700
28	143-08-8	1-nonanol	1	0.8551	3.77	3.337	1.700
29	628-99-9	2-nonanol	1	0.6183	3.25	3.455	1.700
30	66793-96-2	3-ethyl-2,2-dimethyl-	1	-0.1691	2.86	3.386	1.700

		3-pentanol					
31	112-30-1	1-decanol	1	1.3354	4.57	3.332	1.700
32	2051-31-2	(+/-)-4-decanol	1	0.8499	3.78	3.360	1.700
33	78-69-3	3,7-dimethyl-	1	0.3404	3.52	3.356	1.700
		3-octanol					
34	112-42-5	1-undecanol	1	1.9547	4.53	3.329	1.700
35*	112-53-8	1-dodecanol	1	2.1612	5.13	3.326	1.700
36*	112-70-9	1-tridecanol	1	2.4497	5.58	3.324	1.700
37	108-93-0	Cyclohexanol	1	-0.7659	1.23	3.369	1.700
Diols***							
38	26171-83-5	(+/-)-1,2-butanediol	1	-2.0482	-0.53	3.258	1.700
39*	107-88-0	(+/-)-1,3-butanediol	1	-2.3013	-1.38	3.214	1.700
40	110-63-4	1,4-butanediol	1	-2.2365	-0.83	3.140	1.700
41	5343-92-0	1,2-pentanediol	1	-1.6269	0.00	3.173	1.700
42	111-29-5	1,5-pentanediol	1	-1.9344	-0.64	3.169	1.700
43	107-41-5	2-methyl-2,	1	-1.9531	-0.68	3.274	1.700
		4-pentanediol					
44	6920-22-5	(+/-)-1,2-hexanediol	1	-1.2669	0.53	3.169	1.700
45	629-11-8	1,6-hexanediol	1	-1.4946	-0.11	3.195	1.700

46	2935-44-6	2,5-hexanediol	1	-1.9598	-0.55	3.310	1.700
47	1119-86-4	1,2-decanediol	1	0.7640	2.64	3.163	1.700
48	112-47-0	1,10-decanediol	1	0.2240	2.01	3.255	1.700
Unsaturated alcohols***							
49	627-27-0	3-buten-1-ol	1	-1.6952	0.34	1.241	1.241
50	763-36-6	3-methyl-3-buten-1-ol	1	-1.1848	0.74	1.152	1.152
51	115-18-4	2-methyl-3-buten-2-ol	1	-1.3889	0.52	1.195	1.195
52	821-09-0	4-penten-1-ol	1	-1.2151	0.87	1.299	1.299
53	625-31-0	4-penten-2-ol	1	-1.5172	0.65	1.424	1.424
54	5390-04-5	4-pentyn-1-ol	1	-1.4204	-0.01	1.867	1.700
55	115-19-5	2-methyl-3-butyn-2-ol	1	-1.3114	0.28	1.677	1.677
56	928-97-2	trans-3-hexen-1ol	1	-0.7772	1.40	1.187	1.187
57	928-96-1	cis-3-hexen-1-ol	1	-0.8091	1.40	1.185	1.185
58	928-90-5	5-hexyn-1-ol	1	-1.2948	0.52	1.885	1.700
59	77-75-8	3-methyl-1-pentyn-3-ol	1	-1.3226	1.07	1.696	1.696
60	Not found	4-methyl-2-heptyn-4-ol	1	-0.4815	2.13	1.604	1.604
61	142-30-3	2,5-dimethyl-3-hexyne-2,5-diol	1	-1.5849	0.69	1.584	1.584

62	107-54-0	3,5-dimethyl-1-hexyne-3-ol	1	-0.5530	2.00	1.713	1.700
63	928-92-7	4-hexen-1-ol	1	-0.7540	1.40	1.227	1.227
64	821-41-0	5-hexen-1-ol	1	-0.8411	1.40	1.316	1.316
65	927-74-2	3-butyn-1-ol	1	-1.8390	-0.18	1.782	1.700
66	10229-10-4	3-pentyn-1-ol	1	-1.1750	0.34	1.690	1.690
67	2117-11-5	(+/-)-4-pentyn-2-ol	1	-1.6324	0.12	1.795	1.700
68	1002-28-4	3-hexyn-1-ol	1	-1.0243	0.87	1.710	1.700
69	19780-84-8	5-hexyn-3-ol	1	-1.4043	0.65	1.875	1.700
70	14916-79-1	3-heptyn-1-ol	1	-0.3231	1.40	1.697	1.697
71	19781-81-8	4-heptyn-2-ol	1	-0.6160	1.18	1.791	1.700
72	14916-80-4	3-octyn-1-ol	1	0.0170	1.93	1.696	1.696
73	53723-18-5	5-octyn-3-ol	1	-0.3759	1.71	1.798	1.700
74	53723-19-6	5-nonyl-3-ol (TECH.)	1	-0.0425	2.24	1.784	1.700
75	31333-13-8	3-nonyn-1-ol	1	0.3401	2.46	1.694	1.694
76	51721-39-2	3-decyn-1-ol	1	1.1273	2.99	1.693	1.693
77*	55182-74-6	3-tetradecyn-1-ol	1	2.3768	5.11	1.692	1.692
78	107-18-6	2-propen-1-ol	1	-1.9178	0.17	1.364	1.364
79	6117-91-5	2-buten-1-ol	1	-1.4719	0.34	1.295	1.295

80	513-42-8	2-methyl-2-propen-1-ol	1	-1.6628	0.21	1.298	1.298
81	598-32-3	(+/-)-3-buten-2-ol	1	-1.0529	0.12	1.247	1.247
82	6117-80-2	cis-2-buten-1,4-diol	1	-2.1495	-0.81	1.295	1.295
83	556-82-1	3-methyl-2-buten-1-ol	1	-1.2392	0.74	1.092	1.092
84	1576-95-0	cis-2-penten-1-ol	1	-1.1052	0.87	1.307	1.307
85	1569-50-2	3-penten-2-ol	1	-1.4010	0.65	1.178	1.178
86	616-25-1	1-penten-3-ol	1	-1.3475	0.65	1.133	1.133
87	928-95-0	trans-2-hexen-1-ol	1	-0.4718	1.40	1.301	1.301
88	4798-44-1	1-hexen-3-ol	1	-0.8113	1.18	1.134	1.134
89	928-94-9	cis-2-hexen-1-ol	1	-0.7767	1.40	1.301	1.301
90	33467-76-4	trans-2-hepten-1-ol	1	0.0452	1.93	1.299	1.299
91	18409-17-1	trans-2-octen-1-ol	1	0.3654	2.45	1.298	1.298
92	22104-79-6	cis-2-nonen-1-ol	1	0.7701	2.98	1.297	1.297
93	31502-14-4	trans-2-nonen-1-ol	1	0.7520	2.98	1.297	1.297
94	22104-80-9	2-decen-1-ol	1	1.1284	3.51	1.296	1.296
95	75039-84-8	trans-2-undecen-1-ol	1	1.6108	4.04	1.295	1.295
96	22104-81-0	2-dodecen-1-ol	1	2.0915	4.57	1.295	1.295
Monoesters***							
97	79-20-9	methyl acetate	1	-1.5954	0.18	1.098	1.098

98	141-78-6	ethyl acetate	1	-1.2968	0.73	1.149	1.149
99	109-60-4	propyl acetate	1	-1.2382	1.24	1.154	1.154
100	108-21-4	isopropyl acetate	1	-1.5900	1.02	1.194	1.194
101	123-86-4	butyl acetate	1	-0.4864	1.78	1.154	1.154
102	105-46-4	(+/-)-sec-butyl acetate	1	-0.6794	1.72	1.200	1.200
103	628-63-7	amyl acetate	1	0.1625	2.30	1.154	1.154
104	142-92-7	hexyl acetate	1	-0.0087	2.83	1.154	1.154
105	1003-87-5	2-ethylbutyl acetate	1	-0.1202	2.70	1.162	1.162
106	112-14-1	octyl acetate	1	1.0570	3.88	1.152	1.152
107	121-17-4	decyl acetate	1	1.8794	4.94	1.152	1.152
108	105-37-3	ethyl propionate	1	-0.9450	1.21	1.197	1.197
109	590-01-2	butyl propionate	1	0.1704	2.30	1.202	1.202
110	540-42-1	isobutyl propionate	1	-0.6935	2.17	1.202	1.202
111	106-36-5	propyl propionate	1	-0.8148	1.77	1.198	1.198
112	20487-40-5	tert butyl propionate	1	-0.4095	1.95	1.303	1.303
113	105-54-4	ethyl butyrate	1	-0.4903	1.77	1.201	1.201
114	97-62-1	ethyl isobutyrate	1	-1.2709	1.55	1.250	1.250
115	7452-79-1	(+/-)-ethyl-2-methylbutyrate	1	-0.8893	1.59	0.778	0.778

116	539-82-2	ethyl valerate	1	-0.3580	2.30	1.202	1.202
117	108-64-5	ethyl isovalerate	1	-0.7231	2.17	1.218	1.218
118	105-66-8	propyl butyrate	1	-0.4138	2.30	1.202	1.202
119	109-21-7	butyl butyrate	1	0.5157	2.83	1.201	1.201
120	141-06-0	propyl valerate	1	0.0094	2.83	1.203	1.203
121	624-54-4	amyl propionate	1	-0.0431	2.83	1.197	1.197
122	97-85-8	isobutyl isobutyrate	1	-0.5908	2.48	1.254	1.254
123	123-66-0	ethyl hexanoate	1	0.0637	2.83	1.201	1.201
124	554-12-1	methyl propionate	1	-1.6092	0.82	1.148	1.148
125	623-42-7	methyl butyrate	1	-1.2463	1.29	1.152	1.152
126	624-24-8	methyl valerate	1	-0.8448	1.96	1.153	1.153
127	53955-81-0	(+/-)-methyl-2-methylbutyrate	1	-1.1650	1.55	1.206	1.206
128	106-70-7	methyl hexanoate	1	-0.5611	2.30	1.153	1.153
129	106-73-0	methyl heptanoate	1	0.1039	2.83	1.153	1.153
130	111-11-5	methyl octanoate	1	0.5358	3.36	1.152	1.152
131	1731-84-6	methyl nonanoate	1	1.0419	3.88	1.152	1.152
132	110-42-9	methyl decanoate	1	1.3778	4.41	1.151	1.151
133	1731-86-8	methyl undecanoate	1	1.4248	4.79	1.151	1.151

134	107-31-3	methyl formate	1	-1.4982	0.03	1.076	1.076
135	110-74-7	propyl formate	1	-1.0221	0.83	1.136	1.136
136	592-84-7	butyl formate	1	-0.9336	1.32	1.137	1.137
137	542-55-2	isobutyl formate	1	-1.3081	1.19	1.140	1.140
138	762-75-4	tert butyl formate	1	-1.3719	0.97	1.276	1.276
139	629-33-4	n-hexyl formate	1	-0.3824	2.38	1.137	1.137
140	638-49-3	n-amyl formate	1	-0.7826	1.85	1.138	1.138
141	2408-20-0	allyl propionate	1	-0.8791	1.28	1.081	1.081
142	2051-78-7	allyl butyrate	1	-0.6355	1.81	1.083	1.083
143	123-68-2	allyl hexanoate	1	0.2128	2.87	1.084	1.084
144	142-19-8	allyl heptanoate	1	0.7282	3.40	1.084	1.084
145	108-22-5	isopropenyl acetate	1	-0.4892	1.07	0.813	0.813
146	108-05-4	vinyl acetate	1	-0.8595	0.73	0.650	0.650
147	94-04-2	vinyl-2-ethylhexanoate	1	1.0462	3.71	0.749	0.749
148	627-09-8	propargyl acetate	1	-1.1664	0.28	1.010	1.010
149	1932-92-9	propargyl propionate	1	-0.6554	0.81	1.057	1.057
150	105-38-4	vinyl propionate	1	-0.6530	1.29	0.693	0.693
151	123-20-6	vinyl butyrate	1	-0.3825	1.81	0.697	0.697
152	20515-19-9	methyl trans.-	1	-0.2761	1.28	0.866	0.866

		3-pentenoate					
153	34485-37-5	2-butynyl acetate	1	-0.8834	0.81	1.064	1.064
Ketones***							
154	67-64-1	acetone	1	-2.2036	-0.24	0.844	0.844
155	78-93-3	2-butanone	1	-1.7457	0.29	0.877	0.877
156	107-87-9	2-pentanone	1	-1.2224	0.91	0.877	0.877
157	96-22-0	3-pentanone	1	-1.4561	0.85	0.909	0.909
158	563-80-4	3-methyl-2-butanone	1	-1.1689	0.84	0.913	0.913
159	591-78-6	2-hexanone	1	-1.3435	1.38	0.877	0.877
160	108-10-1	4-methyl-2-pentanone	1	-1.2085	1.31	0.895	0.895
161	108-94-1	cyclohexanone	1	-1.2333	0.81	0.921	0.921
162	75-97-8	3,3-dimethyl-2-butanone	1	-1.4420	1.20	0.943	0.943
163	110-43-0	2-heptanone	1	-0.4872	1.98	0.879	0.879
164	110-12-3	5-methyl-2-hexanone	1	-0.6459	1.88	0.889	0.889
165	123-19-3	4-heptanone	1	-0.6690	1.91	0.909	0.909
166	111-13-7	2-octanone	1	-0.1455	2.37	0.879	0.879
167	821-55-6	2-nonanone	1	0.6598	3.14	0.878	0.878
168	502-56-7	5-nonanone	1	0.0744	2.97	0.909	0.909

169	693-54-9	2-decanone	1	0.5822	3.73	0.874	0.874
170	928-80-3	3-decanone	1	0.6265	3.49	0.907	0.907
171	112-12-9	2-undecanone	1	1.5346	4.09	0.876	0.876
172	6175-49-1	2-dodecanone	1	1.6696	4.55	0.877	0.877
173*	593-08-8	2-tridecanone	1	2.1192	5.08	0.873	0.873
174*	462-18-0	7-tridecanone	1	1.5214	5.08	0.905	0.905
175	109-49-9	5-hexen-2-one	1	-1.1405	1.02	0.832	0.832
176	3240-09-3	5-methyl-5-hexen-2-one	1	-0.8749	1.29	0.845	0.845
177	110-93-0	6-methyl-5-hepten-2-one	1	-0.4523	1.82	0.861	0.861
Cyanides***							
178	75-05-8	methyl cyanide	1	-2.2769	-0.34	1.664	1.664
179	107-12-0	ethyl cyanide	1	-1.9721	0.16	1.709	1.700
180	109-74-0	propyl cyanide	1	-1.4409	0.53	1.702	1.700
181	78-82-0	isopropyl cyanide	1	-1.6193	0.47	1.757	1.700
182	110-59-8	butyl cyanide	1	-1.0071	1.12	1.703	1.700
183	625-28-5	isobutyl cyanide	1	-0.8764	1.12	1.703	1.700
184	630-18-2	tert-butyl cyanide	1	-1.3255	1.08	1.809	1.700

185	628-73-9	pentyl cyanide	1	-0.3758	1.66	1.702	1.700
186	542-54-1	isopentyl cyanide	1	-0.7860	1.54	1.713	1.700
187	629-08-3	hexyl cyanide	1	-0.2373	2.25	1.702	1.700
188	124-12-9	heptyl cyanide	1	0.2834	2.75	1.701	1.700
189	2243-27-8	octyl cyanide	1	0.6247	3.12	1.701	1.700
190	2244-07-7	decyl cyanide	1	1.6498	4.37	1.701	1.700
191	2437-25-4	undecyl cyanide	1	1.9031	4.90	1.700	1.700
192	109-75-1	allyl cyanide	1	-1.4792	0.40	0.798	0.798
193	16529-66-1	trans-3-pentenitrile	1	-0.9528	0.71	0.753	0.753
Halogenated hydrocarbons***							
194	109-65-9	1-bromobutane	1	-0.1802	2.75	0.829	0.829
195	110-53-2	1-bromopentane	1	0.4839	3.37	0.828	0.828
196	111-25-1	1-bromohexane	1	0.9370	3.80	0.828	0.828
197	629-04-9	1-bromoheptane	1	1.4868	4.36	0.827	0.827
198	111-83-1	1-bromooctane	1	1.8697	4.89	0.826	0.826
199	624-20-4	1,2-dibromohexane	1	1.1457	3.85	0.434	0.434
200	629-03-8	1,6-dibromohexane	1	1.0460	3.57	0.692	0.692
201	16230-28-7	3,4-dibromohexane	1	0.9978	3.85	-0.008	-0.008
Sulfur-containing compounds***							

202	111-47-7	propyl sulfide	1	-0.0029	2.96	0.876	0.876
203	544-40-1	butyl sulfide	1	1.0400	4.02	0.866	0.866
204	1639-09-4	1-heptanethiol	1	1.0200	3.82	0.839	0.839
205	1191-43-1	1,6-hexanedithiol	1	0.6261	2.71	0.751	0.751
206	1569-69-3	cyclohexyl mercaptan	1	-0.0040	2.68	0.876	0.876
207	1191-62-4	1,8-octanedithiol	1	1.1911	3.77	0.797	0.797
208*	67-68-5	dimethylsulfoxide	1	-2.4518	-1.35	0.808	0.808
209	4253-91-2	n-propylsulfoxide	1	-1.2205	0.74	0.724	0.724
210	2168-93-6	butyl sulfoxide	1	-0.2567	1.80	0.719	0.719
211	623-98-3	di-n-propyl sulfite	1	0.0861	2.47	0.589	0.589
212	598-04-9	butyl sulfones	1	-0.2563	1.76	-0.622	-0.622
213	64-67-5	diethyl sulfate	1	-0.6977	1.14	-0.574	-0.574
214	625-22-9	di-n-butyl sulfate	1	0.6207	3.21	-0.653	-0.653
Oximes***							
215	107-29-9	acetaldoxime	1	-1.6100	-0.13	1.067	1.067
216	127-06-0	acetone oxime	1	-1.2485	0.12	1.051	1.051
217	96-29-7	2-butanone oxime	1	-1.0697	0.65	1.079	1.079
218	100-64-1	cyclohexanone oxime	1	-0.7963	1.19	1.114	1.114
219	5314-31-8	2-heptanone oxime	1	0.1025	2.24	1.068	1.068

Carbamates***							
220	598-55-0	methyl carbamates	1	-1.9749	-0.66	1.558	1.558
221	51-79-6	ethyl carbamates	1	-1.6500	-0.15	1.543	1.543
222	592-35-8	n-butylcarbamate	1	-0.9663	0.85	1.536	1.536
Diesters***							
223	105-53-3	diethyl malonates	2	-0.9975	0.96	0.852	0.852
224	110-40-7	diethyl sebaccate	2	1.3536	3.90	1.173	1.173
225	2050-23-9	diethyl suberate	2	0.7018	2.84	1.153	1.153
226	123-25-1	diethyl succinate	2	-0.8511	1.19	0.969	0.969
227	108-59-8	dimethyl malonates	2	-1.2869	-0.05	0.775	0.775
228	105-99-7	dibutyl adipate	2	0.7918	3.90	1.106	1.106
229	106-65-0	dimethyl succinate	2	-1.0573	0.35	0.856	0.856
230	141-28-6	diethyl adipate	2	-0.1265	1.79	1.104	1.104
231	1472-87-3	dimethyl brassylate	2	1.6536	4.43	1.135	1.135
232	106-79-6	dimethyl sebaccate	2	1.0106	2.84	1.117	1.117
233	1732-09-8	dimethyl suberate	2	0.2962	1.79	1.090	1.090
234	1119-40-0	dimethyl glutarate	2	-1.1679	0.62	0.956	0.956
235	2050-20-6	diethyl pimelate	2	0.4069	2.31	1.142	1.142
236	16090-77-0	dibutyl suberate	2	1.6556	4.96	1.154	1.154

237	6802-75-1	diethyl isopropylidene malonates	2	-0.0728	2.66	-0.247	-0.247
238	133-08-4	diethyl butylmalonate	2	0.5566	3.02	0.850	0.850
239	133-13-1	diethyl ethylmalonate	2	-0.2422	1.96	0.797	0.797
240	40420-22-2	diethyl-3-oxopimelate	2	-0.3778	1.49	0.270	0.270
241	6317-49-3	diethyl-4-oxopimelate	2	-0.6378	1.54	0.448	0.448
242	609-08-5	diethyl methylmalonate	2	-0.5114	1.44	0.820	0.820
243	2163-48-6	diethyl propylmalonate	2	0.1341	2.49	0.801	0.801
244	1068-90-2	diethyl acetamidomalonate	2	-1.2037	0.34	0.540	0.540
245	2049-80-1	diethyl allylmalonate	2	-0.0559	2.01	0.735	0.735
246	141-03-7	dibutyl succinate	2	0.5123	3.60	0.971	0.971
Carboxylic sodium salts***							
247	137-40-6	propionic acid, sodium	3	-1.4503	0.33	1.023	1.023

		salt					
248	156-54-7	butyric acid, sodium salt	3	-1.3722	0.79	1.028	1.028
249	10051-44-2	hexanoic acid sodium salt	3	-0.6802	1.92	1.030	1.030
250	1984-06-1	octanoic acid sodium salt	3	-0.0796	3.05	1.029	1.029
251	26522-85-0	malonic acid disodium salt monohydrate	3	-1.5780	-0.81	0.566	0.566
252	150-90-3	succinic acid disodium salt	3	-1.6510	-0.59	0.713	0.713
Aldehydes***							
253	123-38-6	propionaldehyde	4	-0.4855	0.59	0.864	0.864
254	123-72-8	butyraldehyde	4	-0.3805	0.88	0.869	0.869
255	78-84-2	isobutyraldehyde	4	-0.4328	0.61	0.897	0.897
256	110-62-3	valeraldehyde	4	-0.0223	1.36	0.870	0.870
257	96-17-3	2-methyl-buteraldehyde	4	-0.3107	1.14	0.901	0.901

258	66-25-1	hexylaldehyde	4	-0.1731	1.78	0.869	0.869
259	123-15-9	2-methylvaleraldehyde	4	-0.4745	1.67	0.902	0.902
260	97-96-1	2-ethylbutyraldehyde	4	-0.0544	1.67	0.939	0.939
261	2987-16-8	3,3-dimethyl butyraldehyde	4	-0.3744	1.63	0.920	0.920
262	111-71-7	heptaldehyde	4	-0.0019	2.42	0.869	0.869
263	124-13-0	octyl aldehyde	4	0.4829	2.95	0.869	0.869
264	123-05-7	2-ethylhexanal	4	0.1608	2.73	0.939	0.939
265	124-19-6	nonyl aldehyde	4	0.8080	3.48	0.868	0.868
266	112-31-2	decyl aldehyde	4	1.2815	4.01	0.868	0.868
267	112-44-7	undecylic aldehyde	4	1.6904	4.54	0.868	0.868
268*	112-54-9	dodecyl aldehyde	4	1.7595	5.07	0.868	0.868
269	65405-70-1	trans-4-decen-1-al	4	1.2076	4.05	0.846	0.846
270	21661-97-2	cis-7-decen-1-al	4	0.9485	3.52	0.863	0.863
Lactones***							
271*	57-57-8	β-propiolactone (TECH)	5	-0.1255	-1.36	0.913	0.913
272	96-48-0	γ-butyrolactone	5	-1.7171	-0.64	1.105	1.105
273	36536-46-6	(+/-)-β-butyrolactone	5	-0.7588	-0.84	0.989	0.989

274	108-29-2	γ-valerolactone	5	-1.5691	-0.28	1.160	1.160	
275	695-06-7	γ-caprolactone	5	-1.2403	0.24	1.163	1.163	
276	502-44-3	ε-caprolactone	5	-1.2609	0.31	0.759	0.759	
277	1679-47-6	α-methyl-δ-butyrolactone	5	-1.1897	-0.28	1.158	1.158	
278	104-50-7	γ-octanoic lactone	5	-0.3798	1.30	1.163	1.163	
279	104-61-0	γ -nonanoic lactone	5	0.0142	1.83	1.162	1.162	
280	706-14-9	γ -decanolactone	5	0.4928	2.72	1.162	1.162	
281	705-86-2	(+/-)-δ-decanolactone	5	-0.0773	2.39	1.218	1.218	
α- acetylenic alcohols***								
282	107-19-7	2-propyn-1-ol	6	-1.0738	-0.38	1.696	-0.048	0.000
283	764-01-2	2-butyn-1-ol	6	-0.8678	0.37	1.617	0.007	0.000
284	65337-13-5	3-butyn-2-ol	6	-0.4024	0.14	1.636	0.049	0.408
285	110-65-6	2-butyn-1,4-diol	6	-1.8836	-0.72	1.420	-0.086	0.000
286	4187-86-4	1-pentyn-3-ol	6	-1.1776	0.67	1.651	0.084	0.289
287	6261-22-9	2-pentyn-1-ol	6	-0.5724	0.89	1.641	0.029	0.000
288	5557-88-0	2-penten-4-yn-1-ol	6	-0.5549	-0.01	0.482	-0.661	0.000
289	105-31-7	1-hexyn-3-ol	6	0.6574	1.2	1.651	0.084	0.289

290	764-60-3	2-hexyn-1-ol	6	-0.384	1.42	1.628	0.034	0.000
291	109-50-2	3-hexyn-2-ol	6	0.5112	1.2	1.576	0.116	0.408
292	20739-59-7	4-hexyn-3-ol	6	-0.1949	1.2	1.562	0.128	0.289
293	3031-66-1	3-hexyne-2,5-diol	6	-0.4604	-0.1	1.351	-0.080	0.816
294	7383-19-9	1-heptyn-3-ol	6	-0.265	1.73	1.651	0.086	0.289
295	1002-36-4	2-heptyn-1-ol	6	-0.1895	1.95	1.628	0.035	0.000
296	32398-69-9	4-heptyn-3-ol	6	-0.0336	1.73	1.587	0.148	0.289
297	20739-58-6	2-octyn-1-ol	6	0.1944	2.48	1.626	0.035	0.000
298	5921-73-3	2-nonyn-1-ol	6	0.6486	3.01	1.626	0.035	0.000
299	4117-14-0	2-decyn-1-ol	6	0.9855	3.54	1.625	0.034	0.000
300*	51887-25-3	2-tridecyn-1-ol	6	2.3665	5.13	1.624	0.034	0.000
301	565-68-4	4-methyl-1-pentyn-3-ol	6	-0.0267	1.07	1.666	0.092	0.569
302	61996-79-0	5-methyl-1-hexyn-3-ol	6	0.6173	1.6	1.660	0.095	0.697
303	87777-46-6	4-methyl-1-heptyn-3-ol	6	0.7426	2.13	1.668	0.105	0.471
304	60657-70-7	2-methyl-5-octyn-4-ol	6	0.4011	2.66	1.596	0.157	0.697
Halogenated alcohols***								
305	540-51-2	2-bromoethanol	7	-0.8457	0.18	0.635	0.635	
306	627-18-9	3-bromo-1-propanol	7	-0.9328	0.15	0.706	0.706	

307	107-07-3	2-chloroethanol	7	-1.4174	-0.06	1.294	1.294
308	127-00-4	1-chloro-2-propanol	7	-1.4920	0.14	1.399	1.399
309	627-30-5	3-chloro-1-propanol	7	-1.3992	0.50	1.380	1.380
310	928-51-8	4-chloro-1-butanol	7	-0.7594	0.85	1.434	1.434
311	13401-56-4	3-chloro-2,2-dimethyl-1-propanol	7	-0.7822	0.81	1.470	1.470
312	598-38-9	2,2-dichloroethanol	7	-0.9904	0.37	0.368	0.368
313	115-20-8	2,2,2-trichloroethanol	7	-0.4647	1.42	-0.276	-0.276
314	96-23-1	1,3-dichloro-2-propanol	7	-0.7930	0.20	0.917	0.917
315	2009-83-8	6-chloro-1-hexanol	7	-0.2726	1.59	1.474	1.474
316	23144-52-7	8-chloro-1-octanol	7	0.4878	2.65	1.489	1.489
317	4286-55-9	6-bromo-1-hexanol	7	0.0074	1.73	0.794	0.794
318	50816-19-8	8-bromo-1-octanol	7	1.0424	2.79	0.809	0.809
319	75-80-9	2,2,2-tribromoethanol	7	0.1127	2.10	-0.851	-0.851
320	40894-00-6	3-bromo-2,2-dimethyl-1-propanol	7	-0.4603	0.95	0.801	0.801
321	19686-73-8	1-bromo-2-propanol	7	-1.1885	0.28	0.718	0.718

		(TECH.)					
322	96-13-9	2,3-dibromopropanol	7	-0.4861	0.63	0.172	0.172
Halogenated esters***							
323	4753-59-7	4-bromobutylacetate	7	0.3923	1.62	0.696	0.696
324	20395-28-2	5-chloropentylacetate	7	-0.1312	2.01	1.062	1.062
325	5454-83-1	methyl-5-bromovalerate	7	-0.0802	1.62	0.684	0.684
326	15848-22-3	5-bromopentylacetate	7	0.2933	2.15	0.740	0.740
327	14660-52-7	ethyl-5-bromovalerate	7	0.2177	2.15	0.696	0.696
328	25542-62-5	ethyl-6-bromohexanoate	7	0.5936	2.68	0.741	0.741
329	539-74-2	ethyl-3-bromopropionate	7	0.1263	1.44	0.456	0.456
330	623-71-2	ethyl 3-chloropropionate	7	-0.4980	1.30	0.914	0.914
331	3153-36-4	ethyl 4-chlorobutyrate	7	-0.2809	1.48	1.015	1.015
332	2969-81-5	ethyl-4-bromobutyrate	7	-0.0290	1.62	0.609	0.609
Halogenated cyanides***							

333	5332-06-9	4-bromobutyronitrile	7	-0.4655	0.52	0.448	0.448
334	5414-21-1	5-bromovaleronitrile	7	-0.2147	1.05	0.569	0.569
335	20965-27-9	7-bromoheptanonitrile	7	0.5120	2.10	0.689	0.689
336	542-76-7	3-chloropropionitrile	7	-0.9986	0.18	0.857	0.857
337	628-20-6	4-chlorobutyronitrile	7	-0.9303	0.56	1.074	1.074
338	6280-87-1	5-chlorovaleronitrile	7	-0.6345	0.91	1.218	1.218
339	22819-91-6	7-chloroheptanonitrile	7	0.2868	1.96	1.362	1.362
Halogenated acids***							
340	2623-87-2	4-bromobutyric acid (non-neutralized)	7	-0.7711	0.68	0.555	0.555
341	2067-33-7	5-bromovaleric acid (non-neutralized)	7	-0.6929	1.21	0.654	0.654
342	17696-11-6	8-bromooctanoic acid (non-neutralized)	7	1.3233	2.79	0.764	0.764
343	4224-70-8	6-bromohexanoic acid (non-neutralized)	7	0.0305	1.74	0.709	0.709
344	590-92-1	3-bromopropionic acid	7	-0.0444	0.50	0.383	0.383

		(non-neutralized)					
345	627-00-9	4-chlorobutyric acid (non-neutralized)	7	-0.6773	0.54	0.834	0.834
346	107-94-8	3-chloropropionic acid (non-neutralized)	7	-0.3321	0.41	0.725	0.725
347	1119-46-6	5-chlorovaleric acid (non-neutralized)	7	-0.2857	1.07	0.880	0.880
348	80-58-0	2-bromobutyric acid (non-neutralized)	7	0.1221	1.42	-0.202	-0.202
349	2052-01-9	2-bromoisobutyric acid (non-neutralized)	7	-0.5845	0.86	0.042	0.042
350	565-74-2	2-bromoisovaleric acid (non-neutralized)	7	-0.5492	1.48	-0.149	-0.149
351	584-93-0	2-bromovaleric acid (non-neutralized)	7	-0.0423	1.61	-0.200	-0.200
352	2623-82-7	2-bromooctanoic acid (non-neutralized)	7	0.4907	3.19	-0.200	-0.200
353	616-59-6	2-bromohexanoic	7	0.4547	2.14	-0.199	-0.199

		acid (non-neutralized)					
Miscellaneous***							
355*	1068-57-1	acetic hydrazide	8	-1.3796	-1.58	0.984	0.984
356	3538-65-6	butyric acid hydrazide	8	-0.9720	-0.62	1.024	1.024
357*	1071-93-8	adipic dihydrazide	8	-1.3744	-2.88	0.928	0.928
354*	624-84-0	formylhydrazine	8	-0.8708	-2.05	1.452	1.452
358	110-61-2	succinonitrile	8	-1.8236	-0.99	1.027	1.027
359	544-13-8	glutaronitrile	8	-1.6375	-0.72	1.263	1.263
360	111-69-3	1,4-dicyanobutane	8	-1.5381	-0.32	1.394	1.394
361	123-54-6	2,4-pentanedione	8	-0.2721	0.40	0.327	0.327
362	504-02-9	1,3-cyclohexanedione (neutralized)	8	-0.9290	-0.45	0.399	0.399
363	637-88-7	1,4-cyclohexanedione	8	-1.6677	-0.52	0.364	0.364
364	110-13-4	2,5-hexanedione	8	-1.4034	-0.27	0.730	0.730
365	7424-54-6	3,5-heptanedione	8	-0.3816	0.60	0.360	0.360
366	14090-87-0	2,4-octanedione	8	0.1298	1.13	0.363	0.363
367	6175-23-1	2,4-nonanedione	8	0.5058	1.65	0.357	0.357
Aminoalcohols							

368*	141-43-5	ethanolamine (neutralized)	9	-1.8855	-1.31	3.345	1.700
369*	156-87-6	3-amino-1-propanol (neutralized)	9	-1.6917	-1.12	3.200	1.700
370	109-83-1	2-(methylamino) ethanol (neutralized)	9	-1.8202	-0.94	3.062	1.700
371*	13325-10-5	4-amino-1-butanol (non-neutralized)	9	-0.9752	-1.06	3.228	1.700
372	110-73-6	2-(ethylamino)ethanol (neutralized)	9	-1.6491	-0.46	2.959	1.700
373	124-68-5	2-amino-2-methyl- propanol (neutralized)	9	-1.9315	-0.59	3.208	1.700
374	2508-29-4	5-amino-1-pentanol (neutralized)	9	-1.7649	-0.53	3.242	1.700
375	16369-21-4	2-(propylamino) ethanol (neutralized)	9	-1.6842	0.07	2.938	1.700
376	4146-04-7	DL-2-amino-1-	9	-0.6718	0.07	3.193	1.700

		pentanol (non-neutralized)					
377	26734-09-8	3-amino-2,2-dimethyl- 1-propanol (non-neutralized)	9	-0.9246	-0.79	3.206	1.700
378	4048-33-3	6-amino-1-hexanol (non-neutralized)	9	-0.9580	-0.01	3.257	1.700
379	5665-74-7	DL-2-amino-1-hexanol TECH (non-neutralized)	9	-0.5848	0.60	3.310	1.700
380	16369-05-4	DL-2-amino-3-methyl- 1-butanol (non-neutralized)	9	-0.5852	-0.06	3.312	1.700
381	112245-13-3	2-amino-3,3-dimethyl- butanol (non-neutralized)	9	-0.7178	0.34	3.284	1.700
382	24629-25-2	2-amino-3-methyl-1-	9	-0.6594	0.47	3.264	1.700

		-pentanol (non-neutralized)					
383	7533-40-6	2-amino-4-methyl-pentanol (non-neutralized)	9	-0.6191	0.47	3.321	1.700
384	100-37-8	N,N- diethylethanolamine (neutralized)	9	-1.4955	0.48	2.846	1.700
385	4620-70-6	2-(tert.butylamino) ethanol (neutralized)	9	-1.6730	0.41	3.146	1.700
386*	111-42-2	diethanolamine (neutralized)	9	-1.7941	-1.43	2.971	1.700
387*	616-30-8	(+/-)-3-amino-1,2-propanediol (neutralized)	9	-1.8124	-2.12	2.992	1.700
388*	616-29-5	1,3-diamino-2-hydroxy-propane (neutralized)	9	-1.4275	-2.05	3.006	1.700

389*	534-03-2	2-amino-1,3-pro-panediol (neutralized)	9	-1.6763	-2.15	2.995	1.700
390*	105-59-9	N-methyldiethanol amine (neutralized)	9	-1.8338	-1.04	2.492	1.700
391*	40137-22-2	3-(methylamino)-1,2-propanediol (neutralized)	9	-1.5341	-1.82	2.936	1.700
392	102-71-6	triethanolamine (non-neutralized)	9	-1.7488	-1.00	2.747	1.700
Amines							
393	107-10-8	propylamine	10	-0.7075	0.47	3.588	1.700
394	109-73-9	butylamine	10	-0.5735	0.97	3.529	1.700
395	627-35-0	n-methylpropylamine	10	-0.8087	0.84	3.315	1.700
396	110-58-7	amylamine	10	-0.4848	1.49	3.492	1.700
397	110-68-9	n-methylbutylamine	10	-0.6784	1.33	3.281	1.700
398	111-26-2	hexylamine	10	-0.2197	2.06	3.466	1.700
399	111-68-2	heptylamine	10	0.2109	2.57	3.447	1.700
400	111-86-4	octylamine	10	0.3509	3.04	3.433	1.700

401	112-20-9	nonylamine	10	1.7011	3.57	3.423	1.700
402	2016-57-1	decylamine	10	2.0555	4.10	3.415	1.700
403	7307-55-3	undecylamine	10	2.3279	4.63	3.409	1.700
404	75-31-0	isopropylamine	10	-0.8635	0.26	3.620	1.700
405	78-81-9	isobutylamine	10	-0.2616	0.73	3.564	1.700
406	598-56-1	n,n-dimethylethylamine	10	-0.9083	0.70	3.091	1.700
407	33966-50-6	(+/-)-secbutylamine	10	-0.6708	0.74	3.523	1.700
408	107-85-7	isoamylamine	10	-0.5774	1.32	3.480	1.700
409	625-30-9	1-methylbutylamine	10	-0.6846	1.23	3.583	1.700
410	616-24-0	1-ethylpropylamine	10	-0.8129	1.23	3.583	1.700
411	96-15-1	2-methylbutylamine	10	-0.4774	1.32	3.488	1.700
412	616-39-7	n,n-diethylmethylamine	10	-0.7559	0.95	2.991	1.700
413	75-64-9	tert-butylamine	10	-0.8973	0.40	3.531	1.700
414	594-39-8	tert-amylamine	10	-0.6978	1.10	3.552	1.700
415	598-74-3	(+/-)-1,2-dimethyl-propylamine	10	-0.7095	1.10	3.617	1.700
416	2450-71-7	propargylamine	10	-0.8260	-0.43	1.712	1.700
417	35161-71-8	n-methylpro-	10	-0.9818	0.08	1.727	1.700

		pargylamine					
418	7223-38-3	1-dimethylamino-2-propyne	10	-1.1451	-0.01	1.771	1.700
419	2978-58-7	1,1-dimethylpropargylamine	10	-0.9104	0.64	1.909	1.700
420	109-85-3	2-methoxyethylamine (neutralized)	10	-1.7903	-0.67	3.078	1.700
421	5332-73-0	3-methoxypropylamine (neutralized)	10	-1.7725	-1.02	2.894	1.700
422	6291-85-6	3-ethoxypropylamine (neutralized)	10	-1.7027	-0.49	2.804	1.700
423	37143-54-7	(+/-)-2-amino-1-methoxy propane (non-neutralized)	10	-0.8332	-0.36	3.051	1.700
424*	109-76-2	1,3-diaminopropane	10	-0.7045	-1.43	3.310	1.700
Carboxylic acids							
425	79-09-4	propionic acid (non-neutralized)	11	-0.5123	0.33	1.023	1.023
426	107-92-6	butyric acid	11	-0.5720	0.79	1.028	1.028

		(non-neutralized)					
427	109-52-4	valeric acid (non-neutralized)	11	-0.2674	1.39	1.030	1.030
428	142-62-1	hexanoic acid (non-neutralized)	11	-0.2083	1.92	1.030	1.030
429	111-14-8	heptanoic acid (non-neutralized)	11	-0.1126	2.41	1.029	1.029
430	124-07-2	octanoic acid (non-neutralized)	11	0.0807	3.05	1.029	1.029
431	112-50-0	nonanoic acid (non-neutralized)	11	0.3509	3.47	1.029	1.029
432	334-48-5	decanoic acid (non-neutralized)	11	0.5063	4.09	1.028	1.028
433	112-37-8	undecanoic acid (non-neutralized)	11	0.8983	4.53	1.028	1.028
434	79-31-2	isobutyric acid (non-neutralized)	11	-0.3334	0.60	1.082	1.082
435	503-74-2	isovaleric acid (non-neutralized)	11	-0.3415	1.16	1.049	1.049

436	75-98-9	trimethylacetic acid (non-neutralized)	11	-0.2543	1.47	1.118	1.118
437	105-43-1	3-methylvaleric acid (non-neutralized)	11	-0.2331	1.75	1.052	1.052
438	646-07-1	4-methylvaleric acid (non-neutralized)	11	-0.2724	1.75	1.039	1.039
439	88-09-5	2-ethylbutyric acid (non-neutralized)	11	-0.1523	1.68	1.120	1.120
440	99-66-1	2-propylpentanoic acid	11	0.0258	2.75	1.122	1.122
441	149-57-5	2-ethylhexanoic acid (non-neutralized)	11	0.0756	2.64	1.109	1.109
442	625-38-7	vinylacetic acid	11	-0.6424	0.34	0.836	0.836
443	1577-18-0	trans-3-hexenoic acid (non-neutralized)	11	-0.2222	1.40	0.816	0.816
444	141-82-2	malonic acid (non-neutralized)	11	-0.7087	-0.81	0.566	0.566
445	110-15-6	succinic acid (non-neutralized)	11	-0.9395	-0.59	0.713	0.713
446	110-94-1	glutaric acid	11	-0.6387	-0.29	0.846	0.846

		(non-neutralized)					
447	124-04-9	adipic acid (non-neutralized)	11	-0.6060	0.08	0.892	0.892
448	111-16-0	pimelic acid (non-neutralized)	11	-0.5845	0.42	0.940	0.940
449	4839-46-7	3,3-dimethylglutaric acid (non-neutralized)	11	-0.6643	0.16	0.789	0.789
450	505-48-6	suberic acid (non-neutralized)	11	-0.5116	0.95	0.957	0.957
451	111-20-6	sebacic acid (non-neutralized)	11	-0.2676	2.01	0.986	0.986
452	693-23-2	1,10-decanedicarboxylic acid (non-neutralized)	11	-0.0863	3.07	1.001	1.001
453	107-93-7	crotonic acid (non-neutralized)	11	-0.5448	0.72	-0.101	-0.101
454	13991-37-2	trans-2-pentenoic acid (non-neutralized)	11	-0.2774	1.41	-0.081	-0.081

455	13419-69-7	trans-2-hexenoic acid (non-neutralized)	11	-0.1279	1.94	-0.080	-0.080
456	1871-67-6	2-octenoic acid (non-neutralized)	11	0.2089	3.00	-0.080	-0.080
457	3760-11-0	trans-2-nonenoic acid (non-neutralized)	11	0.5995	3.53	-0.080	-0.080
458	471-25-0	propiolic acid (non-neutralized)	11	-0.2942	-0.52	-0.033	-0.033
459	5663-96-7	2-octynoic acid (non-neutralized)	11	-0.0570	2.12	0.055	0.055
460	1846-70-4	α-nonynoic acid (non-neutralized)	11	0.7138	2.65	0.055	0.055
Isothiocyanates							
461	542-85-8	ethylisothiocyanate	12	1.6271	1.47	-0.133	-0.133
462	628-30-8	propylisothiocyanate	12	1.6925	2.42	-0.123	-0.123
463	592-82-5	butyl isothiocyanate	12	1.7212	2.92	-0.110	-0.110
464	629-12-9	amylisothiocyanate	12	1.7055	3.48	-0.122	-0.122
465	4404-45-9	hexylisothiocyanate	12	1.7496	4.01	-0.115	-0.115
466	597-97-7	tert-amylisothio-	12	0.3529	3.13	-0.158	-0.158

		cyanate							
467	57-06-7	allyl isothiocyanate	12	2.0605	1.94	-0.267	-0.267		
468	Not found	1,3-propylene diisothiocyanate	12	2.7212	2.57	-0.378	-0.378		
α-halogenated unsaturates									
469	638-29-9	valeryl chloride	13	-0.3447	2.46	0.254	0.254	0.3517	164.05
470	142-61-0	hexanoyl chloride	13	0.3395	2.99	0.254	0.254	0.3517	177.34
471	2528-61-2	heptanoyl chloride	13	0.4592	3.52	0.254	0.254	0.3517	260.91
472	111-64-8	octanoyl chloride	13	0.4149	4.05	0.253	0.253	0.3269	315.77
473	615-83-8	ethyl-2-bromovalerate	13	0.6985	2.55	-0.064	-0.064	0.3270	490.47
474	615-96-3	ethyl-2-bromohexanoate	13	0.8601	3.08	-0.063	-0.063	0.3275	363.29
475	535-11-5	ethyl-2-bromopropionate	13	1.0570	1.49	-0.105	-0.105	0.3281	487.26
476	3196-15-4	methyl-2-bromobutyrate	13	1.0241	1.49	-0.101	-0.101	0.3304	350.72
477	533-68-6	ethyl-2-bromobutyrate	13	0.7640	2.02	-0.066	-0.066	0.3268	566.76
478	3674-13-3	ethyl 2,3-	13	2.2076	1.98	-0.338	-0.338	0.3260	263.38

		dibromopropionate							
479	609-11-0	ethyl 2,3-dibromobutyrate	13	1.4377	2.5	-0.489	-0.489	0.3268	363.97
480	609-12-1	ethyl 2-bromoisovalerate	13	0.0205	2.42	-0.018	-0.018	0.3270	442.42
481	544-29-4	ethyl 2-bromooctanoate	13	1.4989	4.14	-0.064	-0.064	0.3266	772.70
482	535-13-7	ethyl 2-chloropropionate	13	-0.4312	1.35	0.359	0.359	0.3255	322.65
483	14064-10-9	diethyl chloromalonate	13	0.6345	1.64	-0.170	-0.170	0.3270	278.28
484	600-00-0	ethyl-2-bromoiosbutyrate	13	0.1523	1.8	0.127	0.127	0.3285	339.50
485	513-88-2	1,1-dichloroacetone	13	0.6409	0.97	-0.100	-0.100	0.3254	97.87
486	4091-39-8	3-chloro-2-butanone	13	0.2690	0.43	0.203	0.203	0.3363	111.78
487	5469-26-1	1-bromo-3,3-dimethyl-2-butanone	13	2.3768	1.28	0.347	0.347	0.3364	260.37
488	1694-29-7	3-chloro-2,4-pentanedione	13	1.4437	0.05	-0.269	-0.269	0.3477	118.85
489	6305-43-7	1,4-dibromo-2,3-	13	1.7620	-0.86	-0.770	-0.770	0.2993	455.42

		butanedione							
490	17346-16-6	2,4-dibromo-2,4-dimethyl-3-pentanone	13	0.5130	1.97	-0.055	-0.055	0.3359	207.31
491	39081-91-9	2,5-dibromo-3,4-hexanedione	13	2.1675	0.2	-0.784	-0.784	0.3478	265.12
492	821-06-7	1,4-dibromo-2-butene	13	1.9245	2.03	-0.164	-0.164	0.3443	1264.90
493	1617-17-0	2-chloropropionitrile	13	-0.8631	0.75	0.355	0.355	0.3211	89.07
494	107-14-2	chloroacetonitrile	13	0.8453	0.45	0.337	0.337	0.3619	168.62
495	3018-12-0	dichloroacetonitrile	13	0.9731	0.93	-0.307	-0.307	0.3235	66.42
496	19481-82-4	2-bromopropionitrile	13	0.6256	0.89	-0.199	-0.199	0.3393	147.10
497	534-07-6	1,3-dichloroacetone	13	2.0458	0.02	0.209	0.209	0.4039	249.84
498	545-06-2	Trichloroacetonitrile	13	1.8827	2.09	-0.956	-0.956	0.3185	77.44
499	590-17-0	Bromoacetonitrile	13	2.2291	0.36	-0.200	-0.200	0.3550	246.74
500	3252-43-5	Dibromoacetonitrile	13	2.3979	1.21	-0.868	-0.868	0.3229	154.06

* Excluded because log K_{ow} values are outside the range $-1 < \log K_{ow} < 5$

** E_{lumo}, corrected for the values of the pro-electrophiles (the E_{lumo} of the metabolites are included), and all $E_{lumo} > 1.7$ are replaced with 1.7. This E_{lumo} is used in all the QSARs.

*** Chemical groups, included in the general model ($\log (IGC_{50}^{-1}) = 0.645(0.014) (\log K_{ow}) - 0.342 (0.035) (E_{lumo}) - 1.11(0.05)$.

Groups: 1 – non-polar narcosis; 2 – diester narcosis; 3 – carboxylic salts; 4 – Schiff-bases; 5 – strained ring lactones;
6 – pro-electrophiles; 7 – SN_2 substitution; 8 – miscellaneous; 9 – aminoalcohols; 10 – amine narcosis; 11 – carboxylic acids;
12 – isothiocyanates; 13 – SN_2 - □-halo activation.