

APPENDIX 1

Data Used to Derive Regression and Artificial
Neural Network Models

The following table lists the 1297 compounds dataset used to derive the regression and neural network models in this study. The following abbreviations are used as column headings:

ID number of the compound
CAS Chemical Abstract Service Registry number of compound if found
Compound name of the compound
set train - compounds in the training set
 test1 - compounds in the test set 1
 test2 - compounds in the test set 2
log S experimental aqueous solubility value (in mol/L)
Calc calculated aqueous solubility value by ANNs
Resid the difference between logS and Calc

ID	CAS	Compound	set	log S	Calc	Resid
1	60-35-5	Acetamide	train	1.58	0.85	0.73
2	60-34-4	Methyl_hydrazine	train	1.34	1.08	0.26
3	64-19-7	Acetic_acid	train	1.22	0.95	0.27
4	123-75-1	Pyrrolidine	train	1.15	0.93	0.22
5	56-81-5	Glycerol	train	1.12	0.97	0.16
6	127-07-1	Hydroxyurea	train	1.12	0.49	0.63
7	127-19-5	N,N-Dimethylacetamide	train	1.11	0.67	0.44
8	289-80-5	Pyridazine	train	1.10	0.82	0.28
9	289-95-2	Pyrimidine	train	1.10	0.86	0.24
10	50-70-4	Sorbitol	train	1.09	0.67	0.42
11	541-48-0	beta-Aminobutyric acid	train	1.08	0.13	0.95
12	110-85-0	Piperazine	train	1.07	1.19	-0.12
13	110-89-4	Piperidine	train	1.07	0.59	0.48
14	626-64-2	4-Hydroxypyridine	train	1.02	0.44	0.58
15	142-08-5	2-Hydroxypyridine	train	1.02	0.39	0.63
16	110-94-1	Glutaric_acid	train	1.00	0.00	1.00
17	109-02-4	N-methylmorpholine	train	1.00	0.73	0.27
18	598-55-0	O-Methyl_carbamate	train	0.97	0.63	0.34
19	694-85-9	N-Methyl-2-pyridone	train	0.96	-0.10	1.06
20	79-11-8	Chloroacetic_acid	train	0.93	0.04	0.89
21	51-79-6	O-Ethyl_carbamate	train	0.85	0.23	0.62
22	63-75-2	Arecoline	train	0.81	-0.26	1.07
23	108-46-3	1,3-Benzenediol	train	0.81	-0.14	0.95
24	110-86-1	Pyridine	train	0.76	0.51	0.25
25	109-07-9	2-Methylpiperazine	train	0.74	0.79	-0.05
26	107-43-7	Betaine	train	0.72	0.86	-0.14
27	57-48-7	Fructose	train	0.64	0.71	-0.07
28	120-80-9	1,2-Benzenediol	train	0.62	-0.17	0.79
29	98-92-0	Nicotinamide	train	0.61	-0.41	1.02
30	51953-17-4	4(3H)-Pyrimidone	train	0.59	-0.04	0.62
31	123-38-6	Propanal	train	0.58	0.35	0.23
32	107-31-3	Methyl_formate	train	0.58	0.80	-0.22
33	107-02-8	Acrolein	train	0.57	0.64	-0.07
34	109-99-9	Tetrahydrofuran	train	0.56	0.38	0.18
35	78-93-3	2-Butanone	train	0.52	0.15	0.37
36	2815-34-1	2,5-Dimethylpiperazine	train	0.49	0.35	0.13
37	109-87-5	Dimethoxymethane	train	0.48	0.46	0.02

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38 108-48-5	2,6-Dimethylpyridine	train	0.45	-0.25	0.70
39 589-93-5	2,5-Dimethylpyridine	train	0.40	-0.27	0.67
40 87-72-9	L-Arabinose	train	0.39	0.68	-0.29
41 108-47-4	2,4-Dimethylpyridine	train	0.38	-0.29	0.67
42 583-61-9	2,3-Dimethylpyridine	train	0.38	-0.29	0.67
43 485-35-8	Cytisine	train	0.36	-0.58	0.94
44 643-12-9	D-Inositol	train	0.35	0.49	-0.14
45 123-73-9	2-Butenal	train	0.32	-0.18	0.50
46 80-60-4	alpha-Aminobutyric_acid	train	0.31	0.02	0.29
47 123-56-8	Succinimide	train	0.30	0.23	0.07
48 79-31-2	Isobutyric_acid	train	0.28	0.21	0.07
49 626-67-5	N-methylpiperidine	train	0.23	0.06	0.17
50 123-54-6	2,4-Pentanedione	train	0.22	-0.09	0.31
51 109-94-4	Ethyl_formate	train	0.15	0.34	-0.19
52 107-13-1	Acrylonitrile	train	0.15	0.27	-0.12
53 96-47-9	2-Methyltetrahydrofuran	train	0.11	-0.16	0.27
54 4248-19-5	O-t-Butyl_carbamate	train	0.10	-0.32	0.42
55 75-85-4	2-Ethyl-2-propanol	train	0.08	-0.07	0.15
56 100-63-0	Phenyl_hydrazine	train	0.07	-0.51	0.58
57 597-35-3	Diethyl_Sulfone	train	0.04	-0.30	0.34
58 78-83-1	2-Methylpropanol	train	0.04	0.25	-0.21
59 91-18-9	Pteridine	train	0.02	-0.47	0.49
60 54-85-3	Isoniazid	train	0.01	-0.76	0.77
61 108-95-2	Phenol	train	0.00	-0.32	0.32
62 123-72-8	Butanal	train	-0.01	-0.23	0.22
63 481-37-8	Ecgonine	train	-0.02	-0.27	0.25
64 142-68-7	Tetrahydropyran	train	-0.03	-0.18	0.15
65 ?	5-Ethylhydantoin	train	-0.06	-0.42	0.36
66 10004-44-1	3-Hydroxy-5-methylisoxazole	train	-0.07	-0.20	0.13
67 72-19-5	Threonine	train	-0.09	0.18	-0.27
68 60-29-7	Diethyl_ether	train	-0.09	-0.25	0.16
69 98-01-1	Furfural	train	-0.10	-1.15	1.05
70 ?	2-Methylpteridine	train	-0.12	-0.81	0.70
71 52-67-5	Pencillamine	train	-0.13	-0.20	0.07
72 121-44-8	Triethylamine	train	-0.14	-0.12	-0.02
73 109-97-7	Pyrrole	train	-0.17	0.81	-0.98
74 100-75-4	N-Nitrosopiperidine	train	-0.17	-0.31	0.14
75 488-73-3	d-Quercitol	train	-0.17	0.46	-0.63
76 479-18-5	Dyphylline	train	-0.17	-0.36	0.19
77 107-87-9	2-Pentanone	train	-0.19	-0.44	0.25
78 107-92-6	Butyric_acid	train	-0.19	0.08	-0.27
79 110-15-6	Succinic_acid	train	-0.20	0.30	-0.50
80 598-75-4	3-Methyl-2-butanol	train	-0.20	-0.11	-0.09
81 1596-84-5	Daminozide	train	-0.20	-0.51	0.30
82 96-33-3	Methyl_acrylate	train	-0.22	0.21	-0.43
83 584-02-1	3-Pentanol	train	-0.24	-0.33	0.09
84 145-73-3	Endothall	train	-0.27	-0.60	0.33
85 6032-29-7	2-Pentanol	train	-0.29	-0.34	0.05
86 542-76-7	3-Chloropropionitrile	train	-0.29	-1.01	0.72
87 90-01-7	Salicyl_alcohol	train	-0.29	-0.44	0.15
88 2385-74-2	l-Camphoronic_acid	train	-0.29	-0.50	0.21
89 543-28-2	O-Isobutyl_carbamate	train	-0.30	-0.49	0.19
90 461-58-5	2-Cyanoguanidine	train	-0.31	-0.18	-0.13
91 77-74-7	3-Methyl-3-pentanol	train	-0.38	-0.63	0.25
92 624-18-0	1,4-Benzenediamine	train	-0.38	-0.42	0.04
93 557-17-5	Methyl_propyl_ether	train	-0.39	-0.29	-0.10
94 19550-30-2	2,3-Dimethylbutanol	train	-0.39	-0.63	0.24

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95 100-51-6	Phenylmethanol	train	-0.40	-1.14	0.74
96 63-68-3	Methionine	train	-0.42	-1.07	0.65
97 95-54-5	1,2-Benzenediamine	train	-0.42	-0.44	0.02
98 299-42-3	Ephedrine	train	-0.42	-1.63	1.21
99 108-93-0	Cyclohexanol	train	-0.44	-0.39	-0.05
100 4396-01-4	Pelletierine	train	-0.45	-0.75	0.30
101 109-00-2	3-Hydroxypyridine	train	-0.46	0.43	-0.88
102 93-60-7	Methyl_nicotinate	train	-0.46	-0.69	0.23
103 ?	4-Methylpteridine	train	-0.47	-0.78	0.32
104 7568-93-6	Phenylethanolamine	train	-0.48	-1.05	0.58
105 51-34-3	Scopolamine	train	-0.48	-1.78	1.30
106 110-74-7	Propyl_formate	train	-0.49	-0.20	-0.29
107 624-95-3	3,3-Dimethyl-1-butanol	train	-0.50	-0.65	0.15
108 37517-28-5	Amikacin	train	-0.50	-0.43	-0.07
109 71-00-1	Histidine	train	-0.53	-0.97	0.44
110 94-96-2	2-Ethyl-1,3-hexanediol	train	-0.54	-1.16	0.62
111 56-85-9	Glutamine	train	-0.55	-0.39	-0.16
112 75-56-9	Propylene_oxide	train	-0.59	0.83	-1.42
113 108-94-1	Cyclohexanone	train	-0.60	-0.50	-0.10
114 102-76-1	Glyceryl_triacetate	train	-0.60	-0.69	0.09
115 464-07-3	3,3-Dimethyl-2-butanol	train	-0.62	-0.45	-0.17
116 58-15-1	Aminopyrine	train	-0.63	-0.81	0.18
117 75-09-2	Dichloromethane	train	-0.63	-0.56	-0.07
118 592-35-8	O-Butyl_carbamate	train	-0.66	-0.76	0.10
119 628-32-0	Ethyl_propyl_ether	train	-0.66	-0.91	0.25
120 105-37-3	Ethyl_propionate	train	-0.66	-0.41	-0.25
121 108-39-4	m-Cresol	train	-0.68	-0.84	0.16
122 103-70-8	Formanilide	train	-0.68	-1.14	0.46
123 106-48-9	4-Chlorophenol	train	-0.70	-1.32	0.62
124 108-43-0	3-Chlorophenol	train	-0.70	-1.33	0.63
125 106-44-5	p-Cresol	train	-0.70	-0.85	0.15
126 565-67-3	2-Methyl-3-pentanol	train	-0.70	-0.65	-0.05
127 122-99-6	2-Phenoxyethanol	train	-0.71	-1.07	0.36
128 565-60-6	3-Methyl-2-pentanol	train	-0.72	-0.68	-0.04
129 109-60-4	Propyl_acetate	train	-0.72	-0.47	-0.25
130 594-83-2	2,3,3-Trimethyl-2-butanol	train	-0.72	-0.77	0.05
131 95-55-6	2-Aminophenol	train	-0.72	-0.29	-0.43
132 120-07-0	N-Phenyldiethanolamine	train	-0.73	-1.00	0.26
133 140-88-5	Ethyl_acrylate	train	-0.74	-0.24	-0.50
134 100-02-7	4-Nitrophenol	train	-0.74	-1.44	0.70
135 100-65-2	Phenylhydroxylamine	train	-0.74	-0.49	-0.25
136 70-47-3	L-Asparagine	train	-0.74	-0.13	-0.61
137 672-72-0	Amygdalin	train	-0.77	-1.01	0.25
138 629-14-1	1,2-Diethoxyethane	train	-0.77	-1.13	0.36
139 95-14-7	Benzotriazole	train	-0.78	-1.09	0.31
140 ?	tert-Amyl_carbamate	train	-0.80	-0.78	-0.02
141 123-30-8	4-Aminophenol	train	-0.80	-0.26	-0.54
142 615-77-0	1-Methyluracil	train	-0.80	-0.31	-0.49
143 623-37-0	3-Hexanol	train	-0.80	-0.91	0.11
144 80-62-6	Methyl_methacrylate	train	-0.80	0.02	-0.82
145 105-53-3	Diethyl_malonate	train	-0.82	-0.74	-0.08
146 110-00-9	Furan	train	-0.82	-0.54	-0.28
147 623-42-7	Methyl_butyrate	train	-0.82	-0.48	-0.34
148 1629-60-3	1-Hexen-3-one	train	-0.83	-0.73	-0.10
149 539-86-6	Allicin	train	-0.83	-0.90	0.07
150 59-67-6	Nicotinic_acid	train	-0.84	-0.47	-0.37
151 110-62-3	Pentanal	train	-0.85	-0.85	0.00

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152 684-93-5	1-Nitroso-1-methylurea	train	-0.85	-0.26	-0.59
153 109-92-2	Ethyl_vinyl_ether	train	-0.85	0.08	-0.93
154 108-44-1	3-Methylaniline	train	-0.85	-1.14	0.29
155 597-49-9	3-Ethyl-3-pentanol	train	-0.85	-1.20	0.35
156 138-52-3	Salicin	train	-0.85	-0.75	-0.10
157 90-02-8	Salicylaldehyde	train	-0.86	-0.93	0.07
158 ?	7-Chloropteridine	train	-0.87	-1.63	0.75
159 ?	3-Propyl-2,4-pentadione	train	-0.88	-1.44	0.56
160 589-91-3	4-Methylcyclohexanol	train	-0.88	-0.91	0.03
161 74-97-5	Bromochloromethane	train	-0.89	-0.94	0.05
162 103-82-2	Phenylacetic_acid	train	-0.89	-1.47	0.58
163 591-07-1	1-Acetylurea	train	-0.90	-0.15	-0.75
164 ?	7-Methoxypteridine	train	-0.91	-1.02	0.11
165 1517-66-7	1-Phenylethanol	train	-0.92	-1.29	0.37
166 625-06-9	2,4-Dimethyl-2-pentanol	train	-0.92	-0.93	0.01
167 123-25-1	Diethyl_succinate	train	-0.96	-1.05	0.09
168 16529-66-1	3-Pentenitrile	train	-0.96	-1.19	0.23
169 55-21-0	Benzamide	train	-0.96	-1.29	0.33
170 123-08-0	p-Hydroxybenzaldehyde	train	-0.96	-0.92	-0.04
171 58-08-2	Caffeine	train	-0.97	-1.37	0.40
172 122-80-5	4-Aminoacetanilide	train	-0.98	-1.35	0.37
173 106-51-4	2,5-Cyclohexadiene-1,4-dione	train	-0.99	-0.89	-0.10
174 628-28-4	Methyl_butyl_ether	train	-0.99	-0.98	-0.01
175 74-88-4	Iodomethane	train	-1.00	-0.77	-0.23
176 597-96-6	3-Methyl-3-hexanol	train	-1.00	-1.20	0.20
177 542-55-2	Isobutyl_formate	train	-1.01	-0.45	-0.56
178 103-90-2	4-Hydroxyacetanilide	train	-1.03	-1.25	0.22
179 496-15-1	Indoline	train	-1.04	-0.95	-0.09
180 51-21-8	5-Fluorouracil	train	-1.07	-1.17	0.10
181 625-23-0	2-Methyl-2-hexanol	train	-1.08	-1.21	0.13
182 106-41-2	4-Bromophenol	train	-1.09	-1.57	0.48
183 74-96-4	Bromoethane	train	-1.09	-0.79	-0.30
184 108-20-3	Diisopropyl_ether	train	-1.10	-0.84	-0.26
185 122-59-8	Phenoxyacetic_acid	train	-1.10	-1.33	0.23
186 ?	2-Methoxypteridine	train	-1.11	-0.98	-0.13
187 ?	4-Methoxypteridine	train	-1.11	-1.03	-0.08
188 51-67-2	Tyramine	train	-1.12	-1.16	0.04
189 66-81-9	Cycloheximide	train	-1.13	-2.54	1.41
190 1320-98-5	4-Methyl-1-pentanol	train	-1.14	-0.90	-0.24
191 71-30-7	Cytosine	train	-1.14	-0.11	-1.03
192 273-53-0	Benzoxazole	train	-1.16	-1.39	0.23
193 ?	bis-(2-Chloroethyl)-sulfoxide	train	-1.16	-1.03	-0.14
194 97-95-0	2-Ethyl-1-butanol	train	-1.17	-0.92	-0.25
195 67-66-3	Chloroform	train	-1.17	-1.32	0.15
196 105-67-9	2,4-Xylenol	train	-1.19	-1.37	0.18
197 100-52-7	Benzaldehyde	train	-1.19	-1.38	0.19
198 589-18-4	p-Methylbenzyl_alcohol	train	-1.20	-1.31	0.11
199 39589-98-5	Dimethyl_carbate	train	-1.20	-1.87	0.67
200 106-63-8	Isobutyl_acrylate	train	-1.21	-1.02	-0.19
201 600-36-2	2,4-Dimethyl-3-pentanol	train	-1.22	-0.96	-0.26
202 18559-94-9	Salbutamol	train	-1.22	-1.92	0.70
203 63-91-2	L-Tryptophan	train	-1.23	-1.76	0.53
204 144-80-9	Sulfanilacetamide	train	-1.23	-1.98	0.75
205 123-86-4	Butyl_acetate	train	-1.24	-1.05	-0.19
206 111-27-3	1-Hexanol	train	-1.24	-1.23	-0.01
207 50-71-5	Alloxan	train	-1.25	-1.28	0.03
208 7294-05-5	2,2,3-Trimethyl-3-pentanol	train	-1.27	-1.31	0.04

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209 98-86-2	Acetophenone	train	-1.28	-1.79	0.51
210 105-54-4	Ethyl_butyrate	train	-1.28	-0.95	-0.33
211 ?	m-Aminoacetophenone	train	-1.28	-1.52	0.24
212 75-34-3	1,1-Dichloroethane	train	-1.29	-1.08	-0.21
213 51-66-1	4-Methoxyacetanilide	train	-1.30	-1.73	0.43
214 91-22-5	Quinoline	train	-1.30	-1.46	0.16
215 66-25-1	Hexanal	train	-1.30	-1.49	0.19
216 50-59-9	Cephaloridine	train	-1.32	-1.40	0.08
217 107-04-0	1-Chloro-2-bromoethane	train	-1.32	-1.57	0.25
218 103-84-4	Acetanilide	train	-1.33	-1.46	0.13
219 110-12-3	5-Methyl-2-hexanone	train	-1.33	-1.38	0.05
220 90-00-6	o-Ethylphenol	train	-1.36	-1.41	0.05
221 624-24-8	Methyl_valerate	train	-1.36	-1.06	-0.30
222 108-42-9	3-Chloroaniline	train	-1.37	-1.66	0.29
223 556-88-7	Nitroguanidine	train	-1.37	-1.15	-0.22
224 122-97-4	3-Phenylpropanol	train	-1.38	-1.90	0.52
225 627-59-8	5-Methyl-2-hexanol	train	-1.38	-1.22	-0.16
226 57-44-3	Barbital	train	-1.39	-1.70	0.31
227 108-68-9	3,5-Xylenol	train	-1.40	-1.37	-0.03
228 59-46-1	Procaine	train	-1.40	-1.91	0.51
229 533-17-5	2-Chloroacetanilide	train	-1.40	-2.36	0.96
230 589-55-9	4-Heptanol	train	-1.40	-1.48	0.08
231 501-52-0	Hydrocinnamic_acid	train	-1.41	-1.92	0.52
232 110-43-0	2-Heptanone	train	-1.42	-1.71	0.29
233 366-18-7	2,2'-Bipyridine	train	-1.42	-1.23	-0.19
234 526-75-0	2,3-Xylenol	train	-1.43	-1.38	-0.05
235 111-92-2	n-Dibutylamine	train	-1.44	-1.81	0.37
236 110-02-1	Thiophene	train	-1.45	-0.74	-0.71
237 119-65-3	Isoquinoline	train	-1.45	-1.59	0.14
238 88-13-1	Thiophene-3-carboxylic_acid	train	-1.47	-1.17	-0.30
239 540-54-5	1-Chloropropane	train	-1.47	-0.95	-0.52
240 79-00-5	1,1,2-Trichloroethane	train	-1.48	-1.80	0.32
241 123-11-5	p-Methoxybenzaldehyde	train	-1.49	-1.79	0.30
242 ?	Bis-(2-chloroethyl)-sulfone	train	-1.50	-1.37	-0.14
243 352-97-6	Guanidinoacetic_acid	train	-1.51	-0.62	-0.89
244 120-72-9	Indole	train	-1.52	-1.72	0.20
245 2370-12-9	2,2-Dimethyl-1-pentanol	train	-1.52	-1.26	-0.26
246 118-92-3	2-Aminobenzoic_acid	train	-1.52	-1.10	-0.42
247 76-57-3	Codeine	train	-1.52	-2.27	0.75
248 100-46-9	Benzylamine	train	-1.53	-1.12	-0.41
249 95-87-4	2,5-Xylenol	train	-1.54	-1.36	-0.17
250 553-26-4	4,4'-Bipyridine	train	-1.54	-1.55	0.01
251 96-88-8	d,l-Mepivacaine	train	-1.55	-2.74	1.19
252 3121-79-7	4,4-Dimethyl-1-pentanol	train	-1.55	-1.25	-0.30
253 65-85-0	Benzoic_acid	train	-1.55	-1.14	-0.41
254 120-83-2	2,4-Dichlorophenol	train	-1.55	-2.21	0.66
255 543-49-7	2-Heptanol	train	-1.55	-1.54	-0.01
256 ?	7-Methylthiopteridine	train	-1.55	-1.79	0.23
257 ?	2,4-Octadione	train	-1.56	-1.56	0.00
258 97-53-0	Eugenol	train	-1.56	-1.89	0.33
259 708-79-2	1-Methyluric_acid	train	-1.56	-1.42	-0.15
260 59-50-7	3-Methyl-4-chlorophenol	train	-1.57	-1.85	0.28
261 6988-21-2	Dioxacarb	train	-1.57	-2.01	0.44
262 122-85-0	4-Formylacetanilide	train	-1.58	-1.89	0.31
263 619-45-4	Methyl-4-aminobenzoate	train	-1.59	-1.57	-0.02
264 433-97-6	Trifluoro-o-toluic_Acid	train	-1.60	-2.35	0.75
265 96-09-3	Styrene_oxide	train	-1.60	-1.59	-0.01

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266 78-87-5	1,2-Dichloropropane	train	-1.60	-1.66	0.06
267 6305-71-1	2,4-Dimethyl-1-pentanol	train	-1.60	-1.19	-0.41
268 101-42-8	Fenuron	train	-1.60	-1.67	0.07
269 57837-19-1	Metalaxyl	train	-1.60	-2.54	0.94
270 ?	6-Methyl-2,4-heptadione	train	-1.60	-1.27	-0.33
271 22862-76-6	Anisomycin	train	-1.61	-2.31	0.70
272 121-61-9	N-Acetylsulfanilamide	train	-1.61	-1.89	0.28
273 37764-25-3	N,N-Diallyldichloroacetamide	train	-1.62	-2.00	0.38
274 142-28-9	1,3-Dichloropropane	train	-1.62	-1.76	0.14
275 111-43-3	Dipropyl_ether	train	-1.62	-1.58	-0.04
276 39196-18-4	Thiofanox	train	-1.62	-2.29	0.66
277 120-57-0	Piperonal	train	-1.63	-1.30	-0.33
278 71-43-2	Benzene	train	-1.64	-0.79	-0.85
279 75-35-4	1,1-Dichloroethylene	train	-1.64	-0.59	-1.05
280 81-07-2	Saccharin	train	-1.64	-1.82	0.18
281 77-28-1	5-Butyl-5-ethylbarbituric_acid	train	-1.64	-2.18	0.54
282 470-82-6	Eucalyptol	train	-1.64	-2.66	1.01
283 106-47-8	4-Chloroaniline	train	-1.66	-1.65	-0.01
284 81-07-2	1,1-Diox-1,2-benzisothiazol-3-one	train	-1.66	-2.78	1.12
285 57-53-4	Meprobamate	train	-1.67	-1.65	-0.02
286 ?	Cyclohexanol_acetate	train	-1.67	-1.67	0.00
287 121-92-6	3-Nitrobenzoic_acid	train	-1.68	-2.15	0.47
288 106-93-4	1,2-Dibromoethane	train	-1.68	-2.01	0.33
289 1918-00-9	Dicamba	train	-1.70	-2.94	1.24
290 103-69-5	N-Ethylaniline	train	-1.70	-1.37	-0.33
291 111-71-7	Heptanal	train	-1.70	-2.11	0.41
292 151-67-7	Halothane	train	-1.71	-2.23	0.52
293 77-02-1	Aprobarbital	train	-1.71	-2.03	0.32
294 625-25-2	2-Methyl-2-heptanol	train	-1.72	-1.81	0.09
295 31367-46-1	3-Methyl-2-heptanol	train	-1.72	-1.85	0.13
296 106-94-5	1-Bromopropane	train	-1.73	-1.51	-0.22
297 106-34-3	Quinhydrone	train	-1.73	-2.00	0.27
298 88-75-5	2-Nitrophenol	train	-1.74	-1.56	-0.18
299 79-34-5	1,1,2,2-Tetrachloroethane	train	-1.74	-2.38	0.64
300 70-55-3	4-Toluenesulfonamide	train	-1.74	-1.75	0.01
301 539-82-2	Ethyl_valerate	train	-1.75	-1.51	-0.24
302 ?	2-Methylthiopteridine	train	-1.76	-1.81	0.06
303 65-45-2	Salicylamide	train	-1.76	-1.03	-0.73
304 137-58-6	Lidocaine	train	-1.76	-2.52	0.76
305 110-44-1	Sorbic_acid	train	-1.77	-0.86	-0.91
306 103-85-5	1-Phenylthiourea	train	-1.77	-2.00	0.23
307 141-84-4	Rhodanine	train	-1.77	-1.69	-0.09
308 99-76-3	Methyl-4-hydroxybenzoate	train	-1.78	-1.29	-0.49
309 121-79-9	Propyl_gallate	train	-1.78	-1.51	-0.27
310 351-83-7	4-Fluoroacetanilide	train	-1.78	-1.81	0.03
311 98-95-3	Nitrobenzene	train	-1.80	-1.76	-0.04
312 462-06-6	Fluorobenzene	train	-1.80	-1.16	-0.64
313 1129-41-5	m-Tolyl_methylcarbamate	train	-1.80	-1.97	0.17
314 111-70-6	1-Heptanol	train	-1.81	-1.84	0.03
315 69-72-7	Salicylic_acid	train	-1.82	-0.97	-0.85
316 554-57-4	Methazolamide	train	-1.83	-1.39	-0.44
317 93-55-0	Propiophenone	train	-1.83	-2.35	0.52
318 77-06-5	Gibberellic_acid	train	-1.84	-2.56	0.72
319 142-96-1	Dibutyl_ether	train	-1.85	-2.73	0.88
320 100-66-3	Anisole	train	-1.85	-1.33	-0.52
321 99-66-1	Valproic_acid	train	-1.86	-1.68	-0.18
322 591-24-2	3-Methylcyclohexanone	train	-1.87	-1.04	-0.84

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323 467-98-1	Thebainone_A	train	-1.87	-2.52	0.64
324 57-42-1	Meperidine	train	-1.89	-2.85	0.97
325 90-39-1	Sparteine	train	-1.89	-1.56	-0.33
326 628-63-7	Amyl_acetate	train	-1.89	-1.65	-0.24
327 569-31-3	Meconin	train	-1.89	-2.05	0.16
328 123-99-9	Azelaic_acid	train	-1.89	-1.50	-0.40
329 124-48-1	Chlorodibromomethane	train	-1.90	-1.81	-0.09
330 101-31-5	Hyoscyamine	train	-1.91	-2.40	0.50
331 2623-33-8	p-Acetoxy-acetanilide	train	-1.91	-2.09	0.18
332 75-25-2	Bromoform	train	-1.91	-2.11	0.20
333 620-71-3	Propionanilide	train	-1.92	-1.84	-0.08
334 105-66-8	Propyl_butyrat	train	-1.92	-1.48	-0.44
335 121-69-7	N,N-Dimethylaniline	train	-1.92	-1.09	-0.83
336 123-92-2	Isoamyl_acetate	train	-1.92	-1.29	-0.63
337 ?	n-Hexyl_carbamate	train	-1.92	-1.81	-0.11
338 519-05-1	Opianic_acid	train	-1.92	-1.83	-0.10
339 492-70-6	Hydrobenzoin	train	-1.93	-2.61	0.67
340 65-86-1	Orotic_acid	train	-1.93	-1.27	-0.67
341 94-19-9	Sulfaethidole	train	-1.94	-3.11	1.17
342 93-37-8	2,7-Dimethylquinoline	train	-1.94	-2.35	0.40
343 23103-98-2	Pirimicarb	train	-1.95	-1.97	0.03
344 91-23-6	2-Nitroanisole	train	-1.96	-2.15	0.19
345 78-86-4	2-Chlorobutane	train	-1.96	-1.40	-0.56
346 88-74-4	2-Nitroaniline	train	-1.96	-1.70	-0.26
347 104-98-3	Urocanic_acid	train	-1.96	-1.05	-0.92
348 628-41-1	1,4-Cyclohexadiene	train	-1.97	-2.22	0.25
349 38304-91-5	Minoxidil	train	-1.98	-1.91	-0.07
350 1125-78-6	5,6,7,8-Tetrahydro-2-naphthol	train	-1.99	-2.31	0.32
351 71-55-6	1,1,1-Trichloroethane	train	-2.00	-1.86	-0.14
352 88-19-7	2-Toluenesulfonamide	train	-2.02	-1.74	-0.28
353 109-69-3	1-Chlorobutane	train	-2.03	-1.64	-0.39
354 111-13-7	2-Octanone	train	-2.05	-2.34	0.29
355 114-26-1	Propoxur	train	-2.05	-2.29	0.24
356 968-81-0	Acetohexamide	train	-2.06	-3.33	1.28
357 492-38-6	Atropic_acid	train	-2.06	-1.68	-0.37
358 99-49-0	L-Carvone	train	-2.06	-1.57	-0.49
359 118-90-1	o-Toluic_acid	train	-2.06	-1.57	-0.49
360 486-64-6	Vasicinone	train	-2.07	-1.64	-0.42
361 87-51-4	Indole-3-acetic_acid	train	-2.07	-1.36	-0.71
362 499-75-2	Carvacrol	train	-2.08	-2.38	0.30
363 87-47-8	Pyrolan	train	-2.09	-2.40	0.31
364 537-92-8	3-Methylacetanilide	train	-2.09	-1.86	-0.23
365 75-30-9	2-Iodopropane	train	-2.09	-2.06	-0.03
366 591-93-5	1,4-Pentadiene	train	-2.09	-1.80	-0.29
367 123-96-6	2-Octanol	train	-2.09	-2.14	0.05
368 357-57-3	Brucine	train	-2.09	-2.05	-0.04
369 15258-73-8	2,6-Dichlorobenzyl_alcohol	train	-2.10	-2.55	0.45
370 104-76-7	2-Ethyl-1-hexanol	train	-2.11	-2.09	-0.02
371 88-99-3	o-Phthalic_acid	train	-2.11	-1.64	-0.47
372 73-24-5	Adenine	train	-2.12	-0.57	-1.54
373 51-55-8	Atropine	train	-2.12	-2.40	0.28
374 108-98-5	Thiophenol	train	-2.12	-2.25	0.13
375 533-74-4	Dazomet	train	-2.13	-1.74	-0.39
376 99-04-7	m-Toluic_acid	train	-2.14	-1.58	-0.56
377 59-31-4	2-(1H)Quinolinone	train	-2.14	-1.61	-0.53
378 544-25-2	Cycloheptatriene	train	-2.15	-2.26	0.11
379 30979-48-7	Isocarbamid	train	-2.15	-1.42	-0.74

380 580-16-5	6-Hydroxyquinoline	train	-2.16	-1.31	-0.85
381 614-61-9	2-Chlorophenoxyacetic_acid	train	-2.16	-2.14	-0.02
382 52-31-3	Cyclobarbitol	train	-2.17	-2.32	0.15
383 150-69-6	Dulcin	train	-2.17	-1.83	-0.35
384 115-43-5	Phenallymal	train	-2.18	-2.94	0.76
385 339-43-5	Carbutamide	train	-2.18	-2.62	0.44
386 630-20-6	1,1,1,2-Tetrachloroethane	train	-2.18	-2.39	0.21
387 6236-05-1	Nifuroxime	train	-2.19	-2.57	0.38
388 99-09-2	3-Nitroaniline	train	-2.19	-1.65	-0.54
389 76-76-6	Probarbital	train	-2.21	-1.93	-0.28
390 108-88-3	Toluene	train	-2.21	-1.48	-0.73
391 76-93-7	Benzilic_acid	train	-2.21	-2.79	0.58
392 55-63-0	Nitroglycerin	train	-2.22	-2.44	0.22
393 90-15-3	1-Naphthol	train	-2.22	-2.41	0.19
394 89-83-8	Thymol	train	-2.22	-2.37	0.15
395 76466-16-5	DL-2-(2-Chlorophenoxy)propionic_acid	train	-2.22	-2.53	0.31
396 50-11-3	Metharbital	train	-2.23	-1.65	-0.58
397 94-74-6	(4-Chloro-2-methylphenoxy)acetic_acid	train	-2.23	-2.47	0.24
398 515-64-0	Sulfisomidine	train	-2.24	-2.87	0.63
399 614-80-2	2-Hydroxyacetanilide	train	-2.24	-1.29	-0.95
400 5221-53-4	Dimethirimol	train	-2.24	-2.14	-0.10
401 141-90-2	2-Thiouracil	train	-2.26	-1.92	-0.34
402 135-19-3	2-Naphthol	train	-2.28	-2.50	0.22
403 480-68-2	5-Nitrobarbituric acid	train	-2.28	-2.13	-0.16
404 107-08-4	1-Iodopropane	train	-2.29	-2.43	0.14
405 124-07-2	Caprylic_acid	train	-2.30	-1.98	-0.32
406 115-90-2	Fensulfothion	train	-2.30	-2.31	0.01
407 2367-82-0	1,2,3,5-Tetrafluorobenzene	train	-2.31	-2.14	-0.17
408 56-23-5	Tetrachloromethane	train	-2.31	-2.01	-0.30
409 93-89-0	Ethyl_benzoate	train	-2.32	-2.31	-0.01
410 526-08-9	Sulfaphenazole	train	-2.32	-3.22	0.90
411 507-70-0	Borneol	train	-2.32	-2.05	-0.27
412 94-12-2	Risocaine	train	-2.33	-2.39	0.06
413 537-47-3	4-Phenylsemicarbazide	train	-2.33	-1.50	-0.84
414 119-36-8	Methyl_salicylate	train	-2.34	-1.32	-1.01
415 88-06-2	2,4,6-Trichlorophenol	train	-2.34	-2.95	0.61
416 77-21-4	Glutethimide	train	-2.34	-3.12	0.78
417 579-66-8	2,6-Diethylaniline	train	-2.35	-3.00	0.66
418 84-66-2	Diethyl_phthalate	train	-2.35	-2.96	0.61
419 120-47-8	Ethyl-p-hydroxybenzoate	train	-2.35	-1.62	-0.73
420 124-13-0	Octanal	train	-2.36	-2.72	0.36
421 693-02-7	1-Hexyne	train	-2.36	-2.85	0.49
422 2163-69-1	Cycluron	train	-2.36	-1.90	-0.46
423 ?	2-Mercaptopteridine	train	-2.36	-2.72	0.36
424 ?	4-Methylthiopteridine	train	-2.36	-1.78	-0.59
425 62-44-2	Phenacetin	train	-2.37	-2.07	-0.30
426 109-65-9	1-Bromobutane	train	-2.37	-2.21	-0.16
427 108-90-7	Chlorobenzene	train	-2.38	-1.95	-0.43
428 96-12-8	1,2-Dibromo-3-chloropropane	train	-2.38	-2.81	0.43
429 91-15-6	Phthalonitrile	train	-2.38	-2.69	0.31
430 315-30-0	Allopurinol	train	-2.38	-0.65	-1.73
431 100-44-7	alfa-Chlorotoluene	train	-2.39	-2.56	0.17
432 90-43-7	2-Phenylphenol	train	-2.39	-3.19	0.80
433 100-68-5	Thioanisole	train	-2.39	-2.46	0.07
434 541-33-3	1,1-Dichlorobutane	train	-2.40	-2.31	-0.09
435 144-82-1	Sulfamethiazole	train	-2.41	-2.90	0.49
436 100-17-4	4-Nitroanisole	train	-2.41	-2.11	-0.30

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437	121-98-2	Methyl-4-methoxybenzoate	train	-2.41	-2.12	-0.29
438	83-34-1	3-Methylindole	train	-2.42	-2.10	-0.32
439	56-04-2	Methylthiouracil	train	-2.43	-2.21	-0.21
440	78-77-3	1-Bromo-2-methylpropane	train	-2.43	-1.90	-0.53
441	72-14-0	Sulfathiazole	train	-2.43	-2.43	0.00
442	5259-88-1	Oxycarboxin	train	-2.43	-2.52	0.09
443	99-08-1	3-Nitrotoluene	train	-2.44	-2.22	-0.22
444	729-99-7	Sulfamoxole	train	-2.44	-2.85	0.41
445	636-26-0	5-Methyl-2-thiouracil	train	-2.45	-2.21	-0.23
446	120-36-5	Dichlorprop	train	-2.45	-3.19	0.73
447	133-90-4	Chloramben	train	-2.47	-2.61	0.14
448	5902-51-2	Terbacil	train	-2.48	-2.24	-0.24
449	140-10-3	Cinnamic_acid	train	-2.48	-2.12	-0.36
450	1918-16-7	Propachlor	train	-2.48	-2.83	0.35
451	94-75-7	2,4-D	train	-2.51	-2.80	0.28
452	76-74-4	Pentobarbital	train	-2.52	-2.40	-0.12
453	127-33-3	Demeclocycline	train	-2.52	-3.22	0.69
454	2460-49-3	4,5-Dichloroquaiacol	train	-2.53	-2.50	-0.03
455	109-68-2	Trans-2-pentene	train	-2.54	-2.79	0.25
456	352-11-4	p-Fluorobenzyl_chloride	train	-2.54	-2.77	0.23
457	578-67-6	5-Hydroxyquinoline	train	-2.54	-1.31	-1.23
458	3772-76-7	Sulfamethomidine	train	-2.54	-2.95	0.41
459	93-65-2	Mecoprop	train	-2.55	-2.86	0.30
460	24691-76-7	Pyracarbolid	train	-2.56	-2.52	-0.04
461	57-43-2	Amobarbital	train	-2.57	-2.38	-0.19
462	651-06-9	Sulfameter	train	-2.58	-2.78	0.20
463	821-55-6	2-Nonanone	train	-2.58	-2.95	0.37
464	110-83-8	Cyclohexene	train	-2.59	-2.70	0.11
465	535-80-8	m-Chlorobenzoic_acid	train	-2.59	-2.03	-0.56
466	872-55-9	2-Ethylthiophene	train	-2.59	-2.10	-0.49
467	12771-68-5	Ancymidol	train	-2.60	-2.45	-0.15
468	76-01-7	Pentachloroethane	train	-2.60	-3.01	0.41
469	91-75-8	Antazoline	train	-2.60	-3.14	0.54
470	3813-05-6	Benazolin	train	-2.61	-2.71	0.10
471	?	n-Heptyl_carbamate	train	-2.62	-2.34	-0.28
472	723-46-6	Sulfamethoxazole	train	-2.62	-2.69	0.07
473	58-93-5	Hydrochlorthiazide	train	-2.62	-2.56	-0.06
474	70-69-9	p-Aminopropiophenone	train	-2.63	-1.99	-0.64
475	625-29-6	2-Chloropentane	train	-2.63	-2.08	-0.55
476	87-33-2	Isosorbide_dinitrate	train	-2.63	-2.05	-0.59
477	91-80-5	Methapyrilene	train	-2.64	-2.48	-0.16
478	287-92-3	Cyclopentane	train	-2.64	-2.50	-0.14
479	91-81-6	Tripelenamine	train	-2.64	-2.53	-0.11
480	86-87-3	1-Naphthaceneacetic_acid	train	-2.65	-3.32	0.67
481	592-42-7	1,5-Hexadiene	train	-2.68	-2.31	-0.37
482	109-67-1	1-Pentene	train	-2.68	-2.49	-0.19
483	230-46-6	1,7-Phenantroline	train	-2.68	-2.99	0.31
484	25057-89-0	Bentazon	train	-2.68	-2.36	-0.32
485	104-04-1	4-Nitroacetanilide	train	-2.69	-2.28	-0.41
486	549-36-5	2,3-Dichloro-2-methylbutane	train	-2.69	-2.76	0.07
487	7581-97-7	2,3-Dichlorobutane	train	-2.70	-2.19	-0.51
488	92-87-5	p-Benzidine	train	-2.70	-3.34	0.64
489	2432-99-7	11-Aminoundecanoic_acid	train	-2.70	-3.02	0.32
490	106-30-9	Ethyl_heptylate	train	-2.71	-2.66	-0.05
491	94-23-5	Parethoxycaine	train	-2.71	-2.37	-0.35
492	94-26-8	Butyl-p-hydroxybenzoate	train	-2.72	-2.46	-0.26
493	51218-45-2	Metolachlor	train	-2.73	-3.67	0.94

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494 543-59-9	1-Chloropentane	train	-2.73	-2.31	-0.42
495 88-67-5	o-Iodobenzoic_acid	train	-2.73	-2.61	-0.12
496 56-29-1	Hexabarital	train	-2.74	-2.35	-0.39
497 112-05-0	Pelargonic_acid	train	-2.75	-2.48	-0.26
498 *1918-02-1	Picloram	train	-2.75	-3.43	0.68
499 130-95-0	Quinine	train	-2.76	-3.46	0.71
500 ?	4-Mercaptopteridine	train	-2.77	-2.69	-0.08
501 229-87-8	Phenanthridine	train	-2.78	-3.66	0.89
502 88-04-0	4-Chloro-3,5-dimethylphenol	train	-2.80	-2.36	-0.44
503 95-47-6	o-Xylene	train	-2.80	-2.23	-0.57
504 22994-85-0	Benznidazole	train	-2.81	-3.17	0.36
505 80-08-0	Dapsone	train	-2.82	-2.70	-0.11
506 108-38-3	m-Xylene	train	-2.82	-2.21	-0.61
507 20354-26-1	Methazole	train	-2.82	-3.42	0.59
508 4360-12-7	Ajmaline	train	-2.82	-2.12	-0.71
509 539-03-7	4-Chloroacetanilide	train	-2.84	-2.32	-0.52
510 127-79-7	Sulfamerazine	train	-2.85	-2.69	-0.16
511 66-02-4	3,5-Diiodotyrosine	train	-2.86	-3.09	0.23
512 738-70-5	Trimethoprim	train	-2.86	-2.44	-0.42
513 564-25-0	Doxycycline	train	-2.87	-2.91	0.05
514 1698-60-8	Pyrazon	train	-2.87	-2.86	-0.01
515 57-62-5	Chlortetracycline	train	-2.88	-3.39	0.51
516 150-68-5	Monuron	train	-2.89	-2.37	-0.52
517 107-82-4	1-Bromo-3-methylbutane	train	-2.89	-2.58	-0.31
518 127-69-5	Sulfisoxazole	train	-2.91	-2.85	-0.06
519 83-56-7	Naphthalene-1,5-diol	train	-2.92	-1.73	-1.19
520 140-67-0	Estragole	train	-2.92	-2.82	-0.10
521 88-96-0	Phthalamide	train	-2.92	-1.84	-1.08
522 4849-32-5	Karbutilate	train	-2.93	-2.69	-0.24
523 437-50-3	Gentisin	train	-2.93	-2.06	-0.87
524 542-69-8	1-Iodobutane	train	-2.96	-3.10	0.14
525 122-11-2	Sulfadimethoxine	train	-2.96	-3.01	0.05
526 957-51-7	Diphenamid	train	-2.98	-3.99	1.01
527 103-36-6	Ethyl_cinnamate	train	-3.00	-3.30	0.30
528 709-98-8	Propanil	train	-3.00	-3.26	0.26
529 509-86-4	Heptabarbital	train	-3.00	-2.53	-0.47
530 143-08-8	1-Nonanol	train	-3.01	-3.00	-0.01
531 28805-78-9	Isonoruron	train	-3.01	-1.99	-1.02
532 628-71-7	1-Heptyne	train	-3.01	-3.42	0.41
533 23947-60-6	Ethirimol	train	-3.02	-2.42	-0.60
534 91-66-7	N,N-Diethylaniline	train	-3.03	-1.92	-1.11
535 834-12-8	Ametryn	train	-3.04	-3.49	0.45
536 53648-05-8	Ibuproxam	train	-3.04	-3.18	0.13
537 3149-00-6	Phenbutamide	train	-3.05	-2.75	-0.30
538 58-94-6	Chlorothiazide	train	-3.05	-2.82	-0.23
539 95-50-1	1,2-Dichlorobenzene	train	-3.05	-3.00	-0.05
540 110-53-2	1-Bromopentane	train	-3.07	-2.89	-0.18
541 485-71-2	Cinchonidine	train	-3.07	-3.44	0.37
542 480-16-0	Morin	train	-3.08	-2.45	-0.63
543 118-10-5	Cinchonine	train	-3.09	-3.44	0.35
544 481-06-1	Santonin	train	-3.09	-2.84	-0.25
545 622-96-8	1-Ethyl-4-methylbenzene	train	-3.11	-3.00	-0.11
546 53-06-5	Cortisone	train	-3.11	-3.39	0.28
547 102-82-9	Tributylamine	train	-3.12	-3.08	-0.03
548 544-10-5	1-Chlorohexane	train	-3.12	-2.96	-0.16
549 60-54-8	Tetracycline	train	-3.12	-2.77	-0.35
550 76-14-2	1,2-Dichlorotetrafluoroethane	train	-3.12	-2.56	-0.56

551 104-46-1	Anethole	train	-3.13	-3.28	0.15
552 131-17-9	Diallyl_phthalate	train	-3.13	-3.04	-0.09
553 352-34-1	1-Fluoro-4-iodobenzene	train	-3.13	-3.25	0.12
554 128-62-1	Noscapine	train	-3.14	-2.91	-0.23
555 79-57-2	Oxytetracycline	train	-3.14	-2.54	-0.60
556 558-13-4	Tetrabromomethane	train	-3.14	-2.92	-0.22
557 5234-68-4	Carboxin	train	-3.14	-2.68	-0.46
558 21725-46-2	Cyanazine	train	-3.15	-4.30	1.15
559 118-55-8	Phenyl_salicylate	train	-3.15	-2.81	-0.34
560 102-07-8	Carbanilide	train	-3.15	-2.98	-0.17
561 364-62-5	Metoclopramide	train	-3.18	-2.62	-0.56
562 149-30-4	2-Mercaptobenzothiazole	train	-3.18	-3.06	-0.12
563 109-66-0	n-Pentane	train	-3.18	-3.28	0.10
564 526-73-8	1,2,3-Trimethylbenzene	train	-3.20	-2.98	-0.22
565 108-37-2	1-Bromo-3-chlorobenzene	train	-3.21	-3.29	0.08
566 611-14-3	1-Ethyl-2-methylbenzene	train	-3.21	-3.01	-0.20
567 117-34-0	Diphenylacetic_acid	train	-3.22	-3.63	0.41
568 20244-70-6	1,2-Diiodoethylene	train	-3.22	-3.09	-0.13
569 592-41-6	1-Hexene	train	-3.23	-3.06	-0.17
570 53780-34-0	Mefluidide	train	-3.24	-3.40	0.16
571 95-76-1	3,4-Dichloroaniline	train	-3.24	-2.61	-0.63
572 622-50-4	4-Iodoacetanilide	train	-3.25	-2.90	-0.35
573 15972-60-8	Alachlor	train	-3.26	-3.59	0.33
574 13110-37-7	Pentyl-4-aminobenzoate	train	-3.26	-3.39	0.13
575 7286-84-2	Chloramben_methyl_ester	train	-3.26	-3.19	-0.08
576 618-51-9	m-Iodobenzoic_acid	train	-3.27	-2.66	-0.61
577 2188-67-2	Naepaine	train	-3.27	-3.03	-0.24
578 591-49-1	1-Methylcyclohexene	train	-3.27	-3.13	-0.14
579 98-82-8	Isopropylbenzene	train	-3.27	-2.87	-0.40
580 80-35-3	Sulfamethoxypyridazine	train	-3.28	-2.78	-0.50
581 63-25-2	Carbaryl	train	-3.28	-3.33	0.05
582 96-37-7	Methylcyclopentane	train	-3.30	-3.16	-0.14
583 24691-80-3	Fenfuram	train	-3.30	-3.25	-0.06
584 133-91-5	3,5-Diiodosalicylic_acid	train	-3.31	-2.98	-0.32
585 74-11-3	p-Chlorobenzoic_acid	train	-3.31	-2.02	-1.29
586 693-54-9	2-Decanone	train	-3.31	-3.53	0.22
587 95-63-6	1,2,4-Trimethylbenzene	train	-3.31	-2.96	-0.35
588 57-24-9	Strychnine	train	-3.32	-2.34	-0.98
589 1689-84-5	Bromoxynil	train	-3.33	-3.01	-0.32
590 5131-24-8	Ditalimfos	train	-3.35	-3.93	0.58
591 85-02-9	Benzo(f)quinoline	train	-3.36	-3.71	0.35
592 76-75-5	Thiopental	train	-3.36	-3.42	0.06
593 56-54-2	Quinidine	train	-3.37	-3.53	0.16
594 81-25-4	Cholic_acid	train	-3.37	-3.94	0.57
595 389-08-2	Nalidixic_acid	train	-3.37	-2.47	-0.90
596 103-65-1	n-Propylbenzene	train	-3.37	-3.04	-0.33
597 76674-21-0	Flutriafol	train	-3.37	-3.72	0.35
598 95-06-7	Sulfallate	train	-3.39	-3.38	-0.01
599 111-11-5	Methyl_caprylate	train	-3.39	-2.83	-0.56
600 64-77-7	Tolbutamide	train	-3.39	-2.89	-0.51
601 1668-19-5	Doxepin	train	-3.40	-4.38	0.98
602 112-38-9	Undecylenic_acid	train	-3.40	-2.90	-0.50
603 108-67-8	1,3,5-Trimethylbenzene	train	-3.40	-2.95	-0.45
604 26225-79-6	Ethofumesate	train	-3.42	-2.98	-0.44
605 127-31-1	Fludrocortisone	train	-3.43	-3.47	0.04
606 2164-17-2	Fluometuron	train	-3.43	-2.78	-0.65
607 334-48-5	Caprinic_acid	train	-3.44	-2.97	-0.47

608 77-27-0	Thiamylal	train	-3.46	-3.41	-0.05
609 136-60-7	Butyl_benzoate	train	-3.48	-3.42	-0.06
610 92-69-3	p-Phenylphenol	train	-3.48	-3.34	-0.14
611 382-45-6	Adrenosterone	train	-3.48	-3.76	0.27
612 583-53-9	1,2-Dibromobenzene	train	-3.50	-3.70	0.20
613 122-39-4	Diphenylamine	train	-3.51	-2.78	-0.73
614 68-35-9	Sulfadiazine	train	-3.51	-2.48	-1.03
615 291-64-5	Cycloheptane	train	-3.52	-3.80	0.28
616 330-55-2	Linuron	train	-3.52	-3.10	-0.42
617 591-17-3	m-Bromotoluene	train	-3.52	-3.10	-0.42
618 95-49-8	o-Chlorotoluene	train	-3.52	-2.68	-0.84
619 86-57-7	1-Nitronaphthalene	train	-3.54	-3.55	0.01
620 75-83-2	2,2-Dimethylbutane	train	-3.55	-3.69	0.14
621 15299-99-7	Napropamide	train	-3.57	-4.05	0.48
622 80-74-0	Acetyl_sulfisoxazole	train	-3.59	-3.45	-0.14
623 120-82-1	1,2,4-Trichlorobenzene	train	-3.59	-3.82	0.23
624 87-17-2	Salicylanilide	train	-3.59	-2.61	-0.98
625 73-48-3	Bendroflumethiazide	train	-3.59	-3.80	0.21
626 91-20-3	Naphthalene	train	-3.60	-3.46	-0.14
627 846-49-1	Lorazepam	train	-3.60	-4.00	0.40
628 1689-83-4	Ioxynil	train	-3.61	-3.92	0.31
629 43121-43-3	Triadimefon	train	-3.61	-3.47	-0.14
630 112-30-1	1-Decanol	train	-3.63	-3.54	-0.09
631 106-39-8	1-Bromo-4-chlorobenzene	train	-3.63	-3.29	-0.34
632 50-02-2	Dexamethasone	train	-3.64	-3.74	0.10
633 474-25-9	Chenodeoxycholic_acid	train	-3.64	-4.45	0.81
634 50-47-5	Desipramine	train	-3.66	-4.12	0.47
635 629-05-0	1-Octyne	train	-3.66	-3.98	0.32
636 67-72-1	Hexachloroethane	train	-3.67	-3.57	-0.10
637 94-82-6	2,4-DB	train	-3.67	-3.31	-0.36
638 83-88-5	Riboflavin	train	-3.68	-3.50	-0.18
639 1156-19-0	Tolazamide	train	-3.68	-3.02	-0.66
640 124-94-7	Triamcinolone	train	-3.69	-3.28	-0.41
641 63-05-8	Androstenedione	train	-3.69	-4.39	0.70
642 116-44-9	Sulfapyrazine	train	-3.70	-2.51	-1.19
643 22071-15-4	Ketoprofen	train	-3.70	-3.94	0.24
644 56030-54-7	Sufentanil	train	-3.71	-4.02	0.31
645 129-20-4	Oxyphenbutazone	train	-3.73	-3.26	-0.47
646 107-83-5	2-Methylpentane	train	-3.74	-3.66	-0.08
647 105-05-5	1,4-Diethylbenzene	train	-3.75	-3.76	0.01
648 86-30-6	Diphenylnitrosamine	train	-3.75	-3.23	-0.52
649 14437-17-3	Chlorfenprop-methyl	train	-3.77	-4.28	0.51
650 91-57-6	2-Methylnaphthalene	train	-3.77	-4.06	0.29
651 17560-51-9	Metolazone	train	-3.78	-3.52	-0.26
652 14293-44-8	Xipamide	train	-3.79	-3.38	-0.41
653 2011-67-8	Nimetazepam	train	-3.80	-3.79	-0.01
654 452-35-7	Ethoxyzolamide	train	-3.81	-2.83	-0.98
655 50-33-9	Phenylbutazone	train	-3.81	-3.85	0.04
656 111-25-1	1-Bromohexane	train	-3.81	-3.54	-0.27
657 83-49-8	Hyodeoxycholic_acid	train	-3.82	-4.45	0.63
658 3772-43-8	Stadacaine	train	-3.84	-3.14	-0.70
659 135-98-8	2-Butylbenzene	train	-3.89	-3.64	-0.25
660 90-13-1	1-Chloronaphthalene	train	-3.93	-4.31	0.38
661 013476-55-6	Hexyl-4-aminobenzoate	train	-3.95	-3.91	-0.04
662 97-23-4	Dichlorphen	train	-3.95	-3.49	-0.46
663 208-96-8	Acenaphthylene	train	-3.96	-4.26	0.30
664 53-16-7	Estrone	train	-3.96	-4.61	0.65

665 3248-05-3	4,7-Dimethyl-1,10-phenanthroline	train	-3.97	-3.69	-0.28
666 2622-26-6	Pericyazine	train	-3.98	-4.05	0.07
667 15687-27-1	Ibuprofen	train	-3.99	-3.58	-0.41
668 886-50-0	Terbutryne	train	-4.00	-3.77	-0.23
669 138-86-3	D-Limonene	train	-4.00	-3.84	-0.16
670 2539-17-5	Tetrachloroguaiacol	train	-4.02	-3.94	-0.08
671 27314-13-2	Norflurazon	train	-4.04	-4.36	0.32
672 1912-26-1	Trietazine	train	-4.06	-3.62	-0.44
673 2303-16-4	Diallate	train	-4.08	-3.10	-0.98
674 28911-01-5	Triazolam	train	-4.08	-4.18	0.10
675 110-38-3	Ethyl_capriate	train	-4.10	-4.25	0.15
676 426-13-1	Fluoromethasone	train	-4.10	-4.02	-0.08
677 83-26-1	Pindone	train	-4.11	-3.58	-0.53
678 1982-49-6	Siduron	train	-4.11	-3.28	-0.84
679 538-93-2	Isobutylbenzene	train	-4.12	-3.59	-0.53
680 53-43-0	Prasterone	train	-4.12	-4.02	-0.11
681 571-58-4	1,4-Dimethylnaphthalene	train	-4.14	-4.66	0.52
682 91-58-7	2-Chloronaphthalene	train	-4.14	-4.30	0.16
683 2049-95-8	t-Amylbenzene	train	-4.15	-4.41	0.26
684 69-23-8	Fluphenazine	train	-4.15	-4.40	0.25
685 14214-32-5	Difenoxuron	train	-4.16	-3.07	-1.08
686 481-29-8	Epiandrosterone	train	-4.16	-4.41	0.25
687 41483-43-6	Bupirimate	train	-4.16	-3.46	-0.70
688 22204-53-1	Naprosyn	train	-4.16	-3.83	-0.33
689 58-39-9	Perphenazine	train	-4.16	-4.04	-0.12
690 1127-76-0	1-Ethyl-naphthalene	train	-4.17	-4.69	0.52
691 101-81-5	Diphenylmethane	train	-4.17	-4.30	0.13
692 2464-37-1	Chlorflurecol-methyl	train	-4.18	-3.62	-0.56
693 50-49-7	Imipramine	train	-4.19	-4.04	-0.15
694 26644-46-2	Triforine	train	-4.19	-4.47	0.28
695 23184-66-9	Butachlor	train	-4.19	-4.48	0.29
696 741-58-2	Bensulide	train	-4.20	-4.36	0.16
697 15310-01-7	Benodanil	train	-4.21	-4.36	0.16
698 664-95-9	Tolcyclamide	train	-4.21	-3.25	-0.96
699 60-99-1	Methotrimeprazine	train	-4.22	-3.92	-0.29
700 578-06-3	1-Aminoacridine	train	-4.22	-3.24	-0.98
701 298-04-4	Disulfoton	train	-4.23	-4.35	0.12
702 1194-65-6	2,6-Dichlorobenzonitrile	train	-4.24	-3.74	-0.50
703 3452-09-3	1-Nonyne	train	-4.24	-4.51	0.27
704 2655-19-8	Butacarb	train	-4.24	-4.30	0.06
705 1678-91-7	Ethylcyclohexane	train	-4.25	-4.38	0.13
706 108-08-7	2,4-Dimethylpentane	train	-4.26	-4.04	-0.22
707 27195-67-1	cis-1,2-Dimethylcyclohexane	train	-4.27	-4.30	0.02
708 575-41-7	1,3-Dimethylnaphthalene	train	-4.29	-4.65	0.36
709 50-04-4	Hydrocortisone_acetate	train	-4.30	-4.06	-0.24
710 1002-84-2	Pentadecanoic_acid	train	-4.31	-5.04	0.74
711 484-12-8	Osthole	train	-4.31	-4.04	-0.27
712 92-52-4	Biphenyl	train	-4.31	-4.38	0.07
713 6876-23-9	trans-1,2-Dimethylcyclohexane	train	-4.33	-4.30	-0.04
714 90-11-9	1-Bromonaphthalene	train	-4.35	-4.53	0.18
715 547-75-1	Hyochoic_acid	train	-4.35	-4.03	-0.32
716 56-53-1	DES	train	-4.35	-3.83	-0.52
717 530-78-9	Flufenamic_acid	train	-4.36	-4.11	-0.25
718 52-21-1	Prednisolone_acetate	train	-4.37	-3.85	-0.52
719 101-27-9	Barbane	train	-4.37	-3.51	-0.86
720 58-38-8	Prochlorperazine	train	-4.40	-4.52	0.12
721 580-13-2	2-Bromonaphthalene	train	-4.40	-4.52	0.12

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722 84-74-2	Dibutyl_phthalate	train	-4.40	-4.64	0.24
723 53-41-8	Androsterone	train	-4.40	-4.41	0.01
724 57-83-0	Progesterone	train	-4.43	-5.06	0.63
725 139-40-2	Propazine	train	-4.43	-3.93	-0.50
726 59756-60-4	Fluridone	train	-4.44	-4.97	0.53
727 111-66-0	1-Octene	train	-4.44	-4.16	-0.28
728 103-33-3	Azobenzene	train	-4.45	-4.25	-0.20
729 853-23-6	5,6-Dehydroisoandrosterone_acetate	train	-4.46	-4.96	0.50
730 3380-34-5	Triclosan	train	-4.46	-4.53	0.07
731 589-90-2	1,4-Dimethylcyclohexane	train	-4.47	-4.28	-0.18
732 5104-49-4	Flurbiprofen	train	-4.49	-4.41	-0.08
733 615-54-3	1,2,4-Tribromobenzene	train	-4.50	-4.72	0.22
734 319-86-8	delta-Hexachlorocyclohexane	train	-4.51	-4.65	0.14
735 142-82-5	n-Heptane	train	-4.53	-4.49	-0.04
736 2051-60-7	2-Chlorobiphenyl	train	-4.54	-5.13	0.59
737 122-34-9	Simazine	train	-4.55	-3.48	-1.07
738 634-66-2	1,2,3,4-Tetrachlorobenzene	train	-4.57	-4.56	-0.01
739 68-22-4	Norethisterone	train	-4.57	-3.86	-0.71
740 58-89-9	gamma-Hexachlorocyclohexane	train	-4.59	-4.65	0.06
741 014309-40-1	Heptyl-4-aminobenzoate	train	-4.60	-4.43	-0.17
742 551-06-4	1-Naphthyl_isothiocyanate	train	-4.60	-4.65	0.05
743 132-64-9	Dibenzofuran	train	-4.60	-4.98	0.38
744 126-07-8	Griseofulvin	train	-4.61	-4.51	-0.10
745 53-86-1	Indomethacin	train	-4.62	-4.59	-0.03
746 143-07-7	Vulvic_acid	train	-4.62	-3.87	-0.75
747 110-42-9	Methyl_caprate	train	-4.63	-3.92	-0.71
748 634-90-2	1,2,3,5-Tetrachlorobenzene	train	-4.63	-4.54	-0.09
749 83-32-9	Acenaphthene	train	-4.63	-4.44	-0.19
750 538-68-1	n-Pentylbenzene	train	-4.64	-4.54	-0.10
751 84-69-5	Diisobutyl_phthalate	train	-4.66	-4.16	-0.50
752 112-53-8	Dodecanol	train	-4.67	-4.53	-0.14
753 111-82-0	Methyl_laurate	train	-4.69	-4.89	0.21
754 84-06-0	Thiopropazate	train	-4.70	-4.72	0.02
755 50-65-7	Niclosamide	train	-4.70	-4.31	-0.39
756 68-96-2	17-a-Hydroxyprogesterone	train	-4.71	-4.15	-0.56
757 2152-44-5	Betamethasone-17-valerate	train	-4.71	-5.15	0.44
758 571-61-9	1,5-Dimethylnaphthalene	train	-4.74	-4.66	-0.08
759 ?	n-Propylcyclopentane	train	-4.74	-4.37	-0.37
760 60-89-9	Mepazine	train	-4.74	-4.18	-0.57
761 555-37-3	Neburon	train	-4.77	-3.63	-1.14
762 4282-40-0	1-Iodoheptane	train	-4.81	-4.84	0.03
763 28299-41-4	Ditolyl_ether	train	-4.85	-4.66	-0.19
764 97-77-8	Disulfiram	train	-4.86	-4.88	0.02
765 2051-61-8	3-Chlorobiphenyl	train	-4.88	-5.12	0.24
766 1177-87-3	Dexamethasone-17-acetate	train	-4.90	-4.46	-0.44
767 86-73-7	Fluorene	train	-4.91	-4.74	-0.17
768 91-94-1	3,3'-Dichlorobenzidine	train	-4.92	-4.54	-0.38
769 2131-41-1	1,4,5-Trimethylnaphthalene	train	-4.92	-5.21	0.29
770 18181-80-1	Bromopropylate	train	-4.93	-5.12	0.18
771 13698-49-2	Delmadinone_acetate	train	-4.95	-5.42	0.47
772 84-17-3	Dienestrol	train	-4.95	-3.60	-1.35
773 86-74-8	Carbazole	train	-4.97	-3.26	-1.71
774 ?	4,5,7-Trichloro-2,1,3-benzothiadiazole	train	-4.98	-4.23	-0.75
775 50-53-3	Chlorpromazine	train	-5.01	-4.50	-0.51
776 27541-88-4	Quinonamid	train	-5.03	-4.62	-0.41
777 608-21-9	1,2,3-Tribromobenzene	train	-5.04	-4.74	-0.30
778 124-11-8	1-Nonene	train	-5.05	-4.68	-0.37

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779	111-83-1	1-Bromooctane	train	-5.06	-4.71	-0.35
780	36330-85-5	Fenbufen	train	-5.06	-4.32	-0.74
781	10238-21-8	Glyburide	train	-5.09	-5.26	0.16
782	78-48-8	DEF	train	-5.14	-5.17	0.03
783	475-31-0	Glycocholic_acid	train	-5.15	-4.38	-0.77
784	613-13-8	2-Aminoanthracene	train	-5.17	-4.85	-0.32
785	77-47-4	Hexachlorocyclopentadiene	train	-5.18	-4.47	-0.71
786	84-65-1	Anthraquinone	train	-5.19	-4.04	-1.15
787	40596-69-8	Methoprene	train	-5.19	-5.29	0.10
788	33146-45-1	2,6-PCB	train	-5.21	-5.73	0.52
789	6893-02-3	Liothyronine	train	-5.22	-5.31	0.10
790	1730-37-6	1-Methylfluorene	train	-5.22	-5.28	0.06
791	111-65-9	n-Octane	train	-5.24	-5.04	-0.20
792	33284-50-3	2,4-PCB	train	-5.25	-5.73	0.48
793	977-79-7	Medrogestone	train	-5.27	-5.41	0.14
794	13029-08-8	2,2'-PCB	train	-5.27	-5.72	0.45
795	474-86-2	Equilin	train	-5.28	-4.29	-0.99
796	34883-43-7	2,4'-PCB	train	-5.28	-5.71	0.43
797	146-54-3	Triflupromazine	train	-5.30	-5.04	-0.26
798	262-12-4	Dibenzo-p-dioxine	train	-5.31	-5.20	-0.11
799	544-63-8	Tetradecanoic_acid	train	-5.33	-4.69	-0.64
800	595-33-5	Megestrol_acetate	train	-5.35	-5.08	-0.27
801	57-85-2	Testosterone_propionate	train	-5.37	-5.34	-0.02
802	2425-06-1	Captafol	train	-5.40	-4.52	-0.88
803	014309-41-2	Octyl-4-aminobenzoate	train	-5.40	-4.96	-0.44
804	119-91-5	Biquinoline	train	-5.40	-5.57	0.17
805	2363-58-8	Epitiostanol	train	-5.41	-5.24	-0.17
806	3495-42-9	Chlorquinox	train	-5.43	-4.95	-0.48
807	1836-75-5	Nitrofen	train	-5.46	-5.16	-0.30
808	29091-05-2	Dinitramine	train	-5.47	-5.32	-0.14
809	33089-61-1	Amitraz	train	-5.47	-5.22	-0.25
810	508-96-3	Hydrocortisone_Tebutate	train	-5.51	-4.74	-0.77
811	1861-40-1	Benfluralin	train	-5.53	-5.62	0.09
812	563-12-2	Ethion	train	-5.54	-5.59	0.05
813	20168-99-4	Cinmetacin	train	-5.54	-4.61	-0.93
814	13121-70-5	Cyhexatin	train	-5.59	-5.32	-0.26
815	85-68-7	Benzyl_butyl_phthalate	train	-5.64	-5.46	-0.18
816	3734-48-3	Chlordene	train	-5.64	-5.89	0.24
817	608-93-5	Pentachlorobenzene	train	-5.65	-5.22	-0.43
818	434-03-7	Ethisterone	train	-5.66	-4.34	-1.32
819	57-11-4	Stearic_acid	train	-5.68	-6.13	0.45
820	19666-30-9	Oxadiazon	train	-5.69	-5.16	-0.53
821	36378-49-1	Androstane-17-one	train	-5.70	-5.84	0.14
822	299-84-3	Ronnel	train	-5.72	-5.82	0.10
823	82-68-8	Quintozone	train	-5.82	-6.06	0.23
824	206-44-0	Fluoranthene	train	-6.00	-6.53	0.53
825	38444-81-4	2,3',5-PCB	train	-6.01	-6.24	0.23
826	35367-38-5	Difluron	train	-6.02	-5.41	-0.60
827	112-72-1	Myristyl_alcohol	train	-6.05	-5.50	-0.55
828	35693-92-6	2,4,6-PCB	train	-6.14	-6.27	0.13
829	129-00-0	Pyrene	train	-6.19	-6.51	0.32
830	2642-98-0	6-Aminochrysene	train	-6.20	-6.42	0.22
831	16606-02-3	2,4',5-PCB	train	-6.25	-6.23	-0.02
832	38444-85-8	2,3,4'-PCB	train	-6.26	-6.26	0.00
833	15862-07-4	2,4,5-PCB	train	-6.27	-6.28	0.01
834	60-57-1	Dieldrin	train	-6.29	-6.49	0.20
835	38444-86-9	2',3,4-PCB	train	-6.29	-6.26	-0.03

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836	10311-84-9	Dialifos	train	-6.34	-5.43	-0.91
837	120-12-7	Anthracene	train	-6.35	-5.50	-0.85
838	3424-82-6	o,p'-DDE	train	-6.36	-6.88	0.52
839	2974-92-7	3,4-PCB	train	-6.39	-5.74	-0.65
840	41464-39-5	2,2',3,5'-PCB	train	-6.47	-6.79	0.32
841	53-19-0	o,p'-DDD	train	-6.51	-7.09	0.58
842	2050-68-2	4,4'-PCB	train	-6.56	-5.71	-0.85
843	41464-40-8	2,2',4,5'-PCB	train	-6.57	-6.76	0.19
844	781-43-1	9,10-Dimethylanthracene	train	-6.57	-6.31	-0.26
845	18181-70-9	Iodofenphos	train	-6.62	-6.30	-0.32
846	238-84-6	Benzo(a)fluorene	train	-6.68	-6.44	-0.24
847	217-59-4	Triphenylene	train	-6.74	-7.20	0.46
848	41464-41-9	2,2',5,6'-PCB	train	-6.80	-6.77	-0.03
849	52251-71-5	2-Ethylanthracene	train	-6.89	-6.32	-0.57
850	72-55-9	p,p'-DDE	train	-6.90	-6.82	-0.08
851	613-12-7	2-Methylanthracene	train	-6.96	-5.89	-1.07
852	57-97-6	7,12-Dimethylbenz(a)anthracene	train	-7.02	-7.73	0.71
853	92-94-4	p-Terphenyl	train	-7.11	-6.88	-0.23
854	72-54-8	p,p'-DDD	train	-7.20	-7.05	-0.15
855	55312-69-1	2,2',3,4,5-PCB	train	-7.21	-7.45	0.24
856	32598-11-1	2,3',4',5-PCB	train	-7.25	-6.78	-0.47
857	38444-93-8	2,2',3,3'-PCB	train	-7.28	-6.81	-0.47
858	512-04-9	Diosgenin	train	-7.32	-6.79	-0.53
859	56558-16-8	2,2,4,6,6'-PCB	train	-7.32	-7.36	0.04
860	31508-00-6	2,3',4,4',5-PCB	train	-7.39	-7.37	-0.02
861	15968-05-5	2,2',6,6'-PCB	train	-7.39	-6.79	-0.60
862	239-64-5	13H-Dibenzo(a,i)carbazole	train	-7.42	-7.34	-0.08
863	52663-63-2	2,2',3,5,5',6-PCB	train	-7.42	-8.03	0.61
864	55215-17-3	2,2',3,4,6-PCB	train	-7.43	-7.42	-0.01
865	74472-42-7	2,3,3',4,4',6-PCB	train	-7.66	-8.06	0.40
866	52712-04-6	2,2',3,4,5,5'-PCB	train	-7.68	-8.06	0.38
867	32598-10-0	2,3',4,4'-PCB	train	-7.80	-6.82	-0.98
868	38380-08-4	2,3,3',4,4',5-PCB	train	-7.82	-8.08	0.26
869	18259-05-7	2,3,4,5,6-PCB	train	-7.92	-7.52	-0.40
870	52663-69-1	2,2',3,4,4',5',6-PCB	train	-7.92	-8.76	0.84
871	56-49-5	3-Methylcholanthrene	train	-7.92	-7.89	-0.03
872	205-82-3	Benzo(j)fluoranthene	train	-8.00	-8.22	0.22
873	38380-07-3	2,2',3,3',4,4'-PCB	train	-8.01	-8.08	0.07
874	50-32-8	Benzo(a)pyrene	train	-8.19	-8.20	0.01
875	205-99-2	Benzo(b)fluoranthene	train	-8.23	-8.22	-0.01
876	31251-03-3	Fluotrimazole	train	-8.40	-7.85	-0.55
877	35065-27-1	2,2',4,4',5,5'-PCB	train	-8.56	-8.01	-0.55
878	52704-70-8	2,2',3,3',5',6-PCB	train	-8.60	-8.01	-0.59
879	33970-03-2	2,2',4,4',6,6'-PCB	train	-8.71	-8.00	-0.71
880	198-55-0	Perylene	train	-8.80	-8.22	-0.58
881	52712-05-7	2,2',3,4,5,5',6-PCB	train	-8.94	-8.82	-0.12
882	2136-99-4	2,2',3,3',5,5',6,6'-PCB	train	-9.15	-9.54	0.39
883	35694-08-7	2,2',3,3',4,4',5,5'-PCB	train	-9.16	-9.57	0.41
884	2051-24-3	2,2',3,3',4,4',5,5',6,6'-PCB	train	-11.62	-11.07	-0.55
885	598-50-5	N-Methylurea	test1	1.13	0.52	0.61
886	96-48-0	gamma-Butyrolactone	test1	1.07	0.41	0.66
887	616-45-5	Pyrrolidone	test1	1.07	0.62	0.45
888	110-91-8	Morpholine	test1	1.06	0.87	0.19
889	453-20-3	3-Hydroxytetrahydrofuran	test1	1.05	0.69	0.37
890	872-50-4	N-Methylpyrrolidone	test1	1.00	0.45	0.55
891	100-55-0	3-Pyridinemethanol	test1	0.96	0.17	0.79
892	57-13-6	Urea	test1	0.96	0.89	0.07

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893	79-06-1	Acrylamide	test1	0.96	0.53	0.43
894	632-22-4	Tetramethylurea	test1	0.94	0.85	0.09
895	75-50-3	Trimethylamine	test1	0.84	1.20	-0.36
896	54-11-5	Nicotine	test1	0.79	-1.30	2.09
897	50-99-7	Glucose	test1	0.74	0.57	0.17
898	149-32-6	Erythritol	test1	0.70	0.81	-0.11
899	79-20-9	Methyl_acetate	test1	0.52	0.53	-0.01
900	77-92-9	Citric_acid	test1	0.51	0.43	0.08
901	78-40-0	Triethyl_phosphate	test1	0.43	-0.63	1.06
902	78-92-2	2-Butanol	test1	0.43	0.22	0.21
903	144-62-7	Oxalic_acid	test1	0.38	0.45	-0.07
904	591-22-0	3,5-Dimethylpyridine	test1	0.38	-0.30	0.68
905	583-58-4	3,4-Dimethylpyridine	test1	0.36	-0.33	0.69
906	62-56-6	Thiourea	test1	0.32	-0.54	0.86
907	374-01-6	1,1,1-Trifluoro-2-propanol	test1	0.30	-0.48	0.78
908	?	7-Methylpteridine	test1	0.06	-0.79	0.84
909	79-41-4	Methacrylic_acid	test1	0.01	0.43	-0.42
910	71-36-3	1-Butanol	test1	0.00	-0.03	0.03
911	79-07-2	Chloroacetamide	test1	-0.02	-0.17	0.15
912	141-78-6	Ethyl_acetate	test1	-0.04	0.07	-0.11
913	598-53-8	Methyl_isopropyl_ether	test1	-0.06	0.05	-0.11
914	96-23-1	1,3-Dichloro-2-propanol	test1	-0.11	-1.02	0.91
915	554-12-1	Methyl_propionate	test1	-0.14	0.05	-0.19
916	123-31-9	1,4-Benzenediol	test1	-0.17	-0.13	-0.04
917	52-68-8	Trichlorfon	test1	-0.22	-2.03	1.81
918	1634-04-4	Methyl_t-butyl_ether	test1	-0.24	-0.31	0.07
919	621-84-1	O-Benzyl_carbamate	test1	-0.35	-1.78	1.43
920	96-50-4	2-Aminothiazole	test1	-0.36	0.19	-0.55
921	461-72-3	Hydantoin	test1	-0.40	0.27	-0.67
922	75-84-3	2,2-Dimethyl-1-propanol	test1	-0.40	-0.08	-0.32
923	150-13-0	4-Aminobenzoic_acid	test1	-0.40	-1.06	0.66
924	120-89-8	Parabanic_acid	test1	-0.40	-0.54	0.14
925	62-53-3	Aniline	test1	-0.41	-0.57	0.16
926	594-60-5	2,3-Dimethyl-2-butanol	test1	-0.41	-0.41	0.00
927	111-76-2	2-Butoxyethanol	test1	-0.42	-0.89	0.47
928	105-57-7	1,1-Diethoxyethane	test1	-0.43	-0.86	0.43
929	141-76-4	beta-Iodopropionic_acid	test1	-0.43	-1.18	0.75
930	142-84-7	Dipropylamine	test1	-0.46	-0.87	0.41
931	137-32-6	2-Methyl-1-butanol	test1	-0.47	-0.33	-0.14
932	88-14-2	2-Furoic_acid	test1	-0.48	-1.15	0.67
933	590-36-3	2-Methyl-2-pentanol	test1	-0.49	-0.63	0.14
934	123-51-3	Isopentanol	test1	-0.52	-0.31	-0.21
935	108-21-4	Isopropyl_acetate	test1	-0.55	-0.24	-0.31
936	625-54-7	Ethyl_isopropyl_ether	test1	-0.55	-0.53	-0.02
937	75-08-1	Ethanethiol	test1	-0.60	0.13	-0.73
938	71-41-0	1-Pentanol	test1	-0.60	-0.62	0.02
939	83-07-8	Aminophenazone	test1	-0.62	-1.23	0.61
940	79-46-9	2-Nitropropane	test1	-0.62	-0.13	-0.49
941	95-48-7	o-Cresol	test1	-0.62	-0.84	0.22
942	96-45-7	Ethylenethiourea	test1	-0.71	-0.30	-0.41
943	60-12-8	2-Phenylethanol	test1	-0.74	-1.30	0.56
944	108-03-2	1-Nitropropane	test1	-0.80	-0.23	-0.57
945	108-11-2	4-Methyl-2-pentanol	test1	-0.80	-0.64	-0.16
946	591-78-6	2-Hexanone	test1	-0.80	-1.07	0.27
947	88-09-5	2-Ethylbutyric_acid	test1	-0.81	-0.73	-0.08
948	124-04-9	Adipic_acid	test1	-0.82	-0.35	-0.47
949	106-57-0	2,5-Piperazinedione	test1	-0.83	0.17	-1.00

950 122-15-6	Dimetan	test1	-0.85	-1.34	0.49
951 95-53-4	2-Methylaniline	test1	-0.85	-1.14	0.29
952 595-41-5	2,3-Dimethyl-3-pentanol	test1	-0.85	-0.96	0.11
953 4911-70-0	2,3-Dimethyl-2-pentanol	test1	-0.89	-0.98	0.09
954 626-93-7	2-Hexanol	test1	-0.89	-0.94	0.05
955 98-96-4	2-Pyrazinecarboxamide	test1	-0.91	-0.24	-0.67
956 529-64-6	DL-Tropic_acid	test1	-0.93	-1.40	0.47
957 ?	2-Methylcyclohexanone	test1	-0.94	-1.06	0.12
958 538-32-9	Benzylurea	test1	-0.95	-1.60	0.65
959 579-10-2	N-Methylacetanilide	test1	-0.95	-1.59	0.64
960 759-73-9	1-Nitroso-1-ethylurea	test1	-0.96	-0.51	-0.45
961 100-47-0	Benzonitrile	test1	-1.00	-1.76	0.76
962 554-84-7	3-Nitrophenol	test1	-1.01	-1.48	0.47
963 1185-33-7	2,2-Dimethyl-1-butanol	test1	-1.04	-0.67	-0.37
964 107-06-2	1,2-Dichloroethane	test1	-1.06	-1.16	0.10
965 78-59-1	Isophorone	test1	-1.06	-1.64	0.58
966 95-57-8	2-Chlorophenol	test1	-1.06	-1.34	0.28
967 142-62-1	Caproic_acid	test1	-1.06	-0.94	-0.12
968 111-26-2	Hexylamine	test1	-1.10	-1.65	0.55
969 105-30-6	2-Methyl-1-pentanol	test1	-1.11	-0.92	-0.19
970 111-44-4	bis-(2-Chloroethyl)_ether	test1	-1.12	-1.90	0.78
971 3970-62-5	2,2-Dimethyl-3-pentanol	test1	-1.15	-0.99	-0.16
972 149-91-7	Gallic_acid	test1	-1.16	-1.14	-0.02
973 74-95-3	Dibromomethane	test1	-1.17	-1.37	0.20
974 607-67-0	4-Hydroxy-2-methylquinoline	test1	-1.20	-1.57	0.37
975 106-49-0	4-Methylaniline	test1	-1.21	-1.15	-0.06
976 58-63-9	Inosine	test1	-1.23	-2.60	1.37
977 99-24-1	Methyl_gallate	test1	-1.24	-1.12	-0.12
978 626-48-2	6-Methyluracil	test1	-1.26	-0.31	-0.95
979 443-48-1	Metronidazole	test1	-1.26	-1.53	0.27
980 461-98-3	2,6-Dimethyl-4-pyrimidinamine	test1	-1.28	0.00	-1.28
981 100-61-8	N-Methylaniline	test1	-1.28	-0.89	-0.39
982 123-19-3	4-Heptanone	test1	-1.30	-1.61	0.31
983 156-59-2	1,2-Dichloroethylene	test1	-1.30	-1.09	-0.21
984 576-26-1	2,6-Xylenol	test1	-1.31	-1.36	0.05
985 590-12-5	1,2-Dibromoethylene	test1	-1.32	-1.66	0.34
986 627-08-7	Propyl_isopropyl_ether	test1	-1.34	-1.19	-0.15
987 51481-61-9	Cimetidine	test1	-1.35	-3.34	1.99
988 107-05-1	3-Chloropropylene	test1	-1.36	-0.42	-0.94
989 63-74-1	Sulfanilamide	test1	-1.36	-1.27	-0.09
990 85-44-9	Phthalic_anhydride	test1	-1.39	-2.49	1.10
991 95-65-8	3,4-Xylenol	test1	-1.41	-1.39	-0.02
992 75-29-6	2-Chloropropane	test1	-1.41	-0.69	-0.72
993 99-96-7	p-Hydroxybenzoic_acid	test1	-1.41	-0.91	-0.50
994 108-10-1	4-Methyl-2-pentanone	test1	-1.42	-0.77	-0.65
995 124-83-4	d-Camphoric_acid	test1	-1.42	-1.26	-0.16
996 751-97-3	Rolitetracycline	test1	-1.42	-2.74	1.32
997 98-89-5	Cyclohexanecarboxylic_acid	test1	-1.45	-0.97	-0.48
998 105-55-5	1,3-Diethylthiourea	test1	-1.46	-1.64	0.18
999 ?	n-Amyl_carbamate	test1	-1.47	-1.28	-0.18
1000 98-16-8	3-Trifluoromethylaniline	test1	-1.47	-2.02	0.55
1001 589-82-2	3-Heptanol	test1	-1.47	-1.50	0.03
1002 66-22-8	Uracil	test1	-1.48	-0.17	-1.31
1003 106-95-6	3-Bromopropylene	test1	-1.50	-0.84	-0.66
1004 95-16-9	Benzothiazole	test1	-1.50	-1.68	0.18
1005 1484-80-6	Coniine	test1	-1.50	-0.35	-1.15
1006 95-51-2	2-Chloroaniline	test1	-1.52	-1.68	0.16

1007 65-71-4	5-Methyluracil	test1	-1.52	-0.38	-1.14
1008 75-27-4	Bromodichloromethane	test1	-1.54	-1.54	0.00
1009 98-10-2	Benzenesulfonamide	test1	-1.56	-1.39	-0.17
1010 75-26-3	2-Bromopropane	test1	-1.59	-1.19	-0.40
1011 59-92-7	Levodopa	test1	-1.60	-1.36	-0.24
1012 97-59-6	Allantoin	test1	-1.60	-1.25	-0.35
1013 75-03-6	Iodoethane	test1	-1.60	-1.71	0.11
1014 598-06-1	3-Methyl-3-heptanol	test1	-1.60	-1.77	0.17
1015 99-92-3	p-Aminoacetophenone	test1	-1.61	-1.52	-0.09
1016 7307-04-2	5,5-Dimethyl-2,4-hexadione	test1	-1.63	-1.13	-0.50
1017 627-19-0	1-Pentyne	test1	-1.64	-2.27	0.63
1018 3337-71-1	Asulam	test1	-1.66	-2.01	0.35
1019 131-11-3	Dimethyl_phthalate	test1	-1.66	-2.45	0.79
1020 495-69-2	Hippuric_acid	test1	-1.68	-1.94	0.26
1021 104-75-6	2-Ethylhexylamine	test1	-1.71	-2.57	0.86
1022 16118-49-3	Carbetamide	test1	-1.83	-2.66	0.83
1023 15879-93-3	Chloralose	test1	-1.84	-1.71	-0.14
1024 111-68-2	Heptylamine	test1	-1.85	-2.29	0.44
1025 93-58-3	Methyl_benzoate	test1	-1.85	-1.85	0.00
1026 109-70-6	1-Bromo-3-chloropropane	test1	-1.85	-2.18	0.33
1027 4695-62-9	D-Fenchone	test1	-1.85	-2.24	0.38
1028 106-99-0	1,3-Butadiene	test1	-1.87	-1.31	-0.56
1029 91-64-5	Coumarin	test1	-1.89	-2.22	0.33
1030 118-91-2	o-Chlorobenzoic_acid	test1	-1.89	-2.05	0.16
1031 552-32-9	2-Nitroacetanilide	test1	-1.91	-2.37	0.46
1032 96-18-4	1,2,3-Trichloropropane	test1	-1.92	-2.24	0.32
1033 134-32-7	1-Naphthylamine	test1	-1.92	-2.91	0.99
1034 1198-37-4	2,4-Dimethylquinoline	test1	-1.94	-2.37	0.43
1035 69-33-0	Tubercidin	test1	-1.95	-2.47	0.52
1036 615-15-6	2-Methylbenzimidazole	test1	-1.96	-1.17	-0.79
1037 90-05-1	Guaiacol	test1	-1.96	-0.74	-1.22
1038 79-01-6	Trichloroethylene	test1	-1.96	-1.74	-0.22
1039 540-36-3	p-Difluorobenzene	test1	-1.97	-1.46	-0.51
1040 78-70-6	Linalool	test1	-1.99	-1.85	-0.14
1041 76-22-2	Camphor	test1	-1.99	-2.26	0.27
1042 57-67-0	Sulfaguanidine	test1	-1.99	-2.13	0.14
1043 106-70-7	Methyl_capronate	test1	-2.00	-1.66	-0.34
1044 513-36-0	1-Chloro-2-methylpropane	test1	-2.00	-1.36	-0.64
1045 372-18-9	m-Difluorobenzene	test1	-2.00	-1.48	-0.52
1046 78-79-5	2-Methyl-1,3-butadiene	test1	-2.03	-1.62	-0.41
1047 121-34-6	Vanillic_acid	test1	-2.05	-1.14	-0.91
1048 5392-40-5	Citral	test1	-2.06	-2.39	0.34
1049 52-43-7	Allobarbitol	test1	-2.06	-1.84	-0.22
1050 41814-78-2	Tricyclazole	test1	-2.07	-3.11	1.04
1051 109-64-8	1,3-Dibromopropane	test1	-2.08	-2.64	0.56
1052 15271-41-7	Tranid	test1	-2.08	-2.72	0.64
1053 29973-13-5	Ethiofencarb	test1	-2.09	-3.14	1.05
1054 53808-87-0	Tetroxoprim	test1	-2.10	-2.74	0.64
1055 142-29-0	Cyclopentene	test1	-2.10	-2.14	0.04
1056 56-75-7	Chloramphenicol	test1	-2.11	-3.41	1.30
1057 78-75-1	1,2-Dibromopropane	test1	-2.15	-2.46	0.31
1058 51-52-5	Propylthiouracil	test1	-2.15	-2.03	-0.12
1059 271-44-3	Indazole	test1	-2.16	-0.67	-1.49
1060 109-75-5	Butanethiol	test1	-2.18	-0.81	-1.37
1061 619-02-3	l-Dihydrocarvone	test1	-2.18	-1.83	-0.35
1062 95-95-4	2,4,5-Trichlorophenol	test1	-2.21	-2.95	0.74
1063 76-24-4	Alloxanthin	test1	-2.23	-3.08	0.85

1064 50-36-2	Cocaine	test1	-2.23	-2.59	0.36
1065 57-68-1	Sulfamethazine	test1	-2.27	-2.88	0.61
1066 614-28-8	Dibenzamid	test1	-2.27	-3.57	1.30
1067 102-69-2	Tripropylamine	test1	-2.28	-1.64	-0.64
1068 482-05-3	Diphenic_acid	test1	-2.28	-3.12	0.83
1069 68-94-0	Hypoxanthine	test1	-2.29	-1.36	-0.93
1070 122-88-3	4-Chlorophenoxyacetic_acid	test1	-2.29	-2.12	-0.17
1071 108-85-0	Bromocyclohexane	test1	-2.30	-2.69	0.39
1072 101-77-9	bis-(p-Aminophenyl)-methane	test1	-2.30	-3.34	1.04
1073 123-66-0	Ethyl_capronate	test1	-2.31	-2.09	-0.22
1074 88-72-2	2-Nitrotoluene	test1	-2.33	-2.20	-0.13
1075 103-73-1	Phenetole	test1	-2.33	-1.96	-0.37
1076 22259-30-9	Formetanate	test1	-2.34	-2.20	-0.14
1077 2032-59-9	Aminocarb	test1	-2.36	-1.78	-0.57
1078 59-66-5	Acetazoleamide	test1	-2.36	-2.60	0.24
1079 100-01-6	4-Nitroaniline	test1	-2.37	-1.62	-0.75
1080 327-54-8	1,2,4,5-Tetrafluorobenzene	test1	-2.38	-2.11	-0.27
1081 616-44-4	3-Methylthiophene	test1	-2.39	-1.38	-1.01
1082 111-87-5	1-Octanol	test1	-2.39	-2.43	0.04
1083 82-02-0	Khellin	test1	-2.40	-4.03	1.64
1084 98-54-4	p-t-Butylphenol	test1	-2.41	-2.51	0.10
1085 148-24-3	8-Quinolinol	test1	-2.42	-1.23	-1.19
1086 142-92-7	Hexyl_acetate	test1	-2.46	-2.25	-0.21
1087 99-99-0	4-Nitrotoluene	test1	-2.49	-2.23	-0.26
1088 14073-97-3	L-Menthone	test1	-2.49	-2.44	-0.06
1089 594-36-5	2-Chloro-2-methylbutane	test1	-2.51	-1.95	-0.56
1090 614-29-9	DL-1,2-Diphenylethanol	test1	-2.52	-3.55	1.03
1091 89-78-1	Menthol	test1	-2.53	-2.21	-0.32
1092 127-18-4	Tetrachloroethylene	test1	-2.54	-2.42	-0.12
1093 108-86-1	Bromobenzene	test1	-2.55	-2.37	-0.18
1094 91-01-0	Benzhydrol	test1	-2.55	-3.15	0.60
1095 2235-90-7	Etryptamine	test1	-2.57	-2.73	0.16
1096 1746-81-2	Monolinuron	test1	-2.57	-2.45	-0.12
1097 60-18-4	L-Tyrosine	test1	-2.57	-1.47	-1.10
1098 136-77-6	4-Hexylresorcinol	test1	-2.59	-2.79	0.21
1099 502-56-7	5-Nonanone	test1	-2.59	-2.79	0.20
1100 118-52-5	1,3-Dichloro-5,5-dimethylhydantoin	test1	-2.60	-2.33	-0.27
1101 99-94-5	p-Toluic_acid	test1	-2.60	-1.59	-1.01
1102 85-41-6	Phthalimide	test1	-2.61	-2.19	-0.42
1103 485-65-4	Hydrocinchonine	test1	-2.63	-3.61	0.99
1104 616-20-6	3-Chloropentane	test1	-2.63	-2.10	-0.53
1105 3625-25-0	Reposal	test1	-2.64	-2.61	-0.03
1106 125-33-7	Primidone	test1	-2.64	-2.60	-0.04
1107 2315-68-6	Propyl_benzoate	test1	-2.67	-2.85	0.18
1108 133-67-5	Trichlormethiazide	test1	-2.68	-3.63	0.95
1109 77-65-6	Carbromal	test1	-2.68	-2.16	-0.52
1110 144-83-2	Sulfapyridine	test1	-2.70	-2.33	-0.37
1111 475-25-2	Hematein	test1	-2.70	-2.08	-0.62
1112 ?	7-Mercaptopteridine	test1	-2.71	-2.70	0.00
1113 111-86-4	n-Octylamine	test1	-2.75	-2.91	0.16
1114 100-41-4	Ethylbenzene	test1	-2.77	-2.26	-0.51
1115 106-42-3	p-Xylene	test1	-2.77	-2.21	-0.56
1116 72-48-0	Alizarin	test1	-2.78	-2.63	-0.15
1117 591-50-4	Iodobenzene	test1	-2.78	-3.20	0.42
1118 62-23-7	4-Nitrobenzoic_acid	test1	-2.80	-2.09	-0.71
1119 599-88-2	Sulfaperine	test1	-2.82	-2.69	-0.13
1120 80-05-7	Diphenylolpropane	test1	-2.82	-3.31	0.49

1121	100-42-5	Styrene	test1	-2.82	-1.74	-1.08
1122	579-44-2	Benzoin	test1	-2.85	-3.77	0.92
1123	6164-98-3	Chlordimenform	test1	-2.86	-2.97	0.11
1124	119-68-6	N-Methylantranilic_acid	test1	-2.88	-1.52	-1.36
1125	122-66-7	Hydrazobenzene	test1	-2.92	-2.48	-0.44
1126	4849-32-5	Kasugamycin	test1	-2.93	-2.69	-0.24
1127	93-76-5	2,4,5-T	test1	-2.96	-3.42	0.46
1128	50-23-7	Hydrocortisone	test1	-2.97	-3.23	0.26
1129	51940-44-4	Pipedemic_acid	test1	-2.98	-3.81	0.83
1130	83-43-2	6-Methylprednisolone	test1	-2.99	-3.43	0.44
1131	94-20-2	Chlorpropamide	test1	-3.03	-3.05	0.02
1132	58-27-5	Menadione	test1	-3.03	-2.97	-0.07
1133	76-13-1	1,1,2-Trichlorotrifluoroethane	test1	-3.04	-2.89	-0.15
1134	541-73-1	1,3-Dichlorobenzene	test1	-3.04	-2.98	-0.06
1135	496-11-7	Indane	test1	-3.04	-2.59	-0.45
1136	85-34-7	Chlorfenac	test1	-3.08	-3.57	0.49
1137	103-88-8	4-Bromoacetanilide	test1	-3.08	-2.36	-0.72
1138	106-43-4	p-Chlorotoluene	test1	-3.08	-2.66	-0.42
1139	110-82-7	Cyclohexane	test1	-3.10	-3.15	0.05
1140	119-61-9	Benzophenone	test1	-3.12	-3.83	0.71
1141	3042-84-0	Brompyrazone	test1	-3.12	-2.64	-0.49
1142	87-20-7	Isoamyl_salicylate	test1	-3.16	-2.66	-0.50
1143	124-19-6	Nonanal	test1	-3.17	-3.29	0.12
1144	106-38-7	p-Bromotoluene	test1	-3.19	-3.10	-0.09
1145	694-80-4	1-Bromo-2-chlorobenzene	test1	-3.19	-3.30	0.11
1146	50-24-8	Prednisolone	test1	-3.21	-3.23	0.02
1147	7681-93-8	Natamycin	test1	-3.21	-3.83	0.62
1148	61-57-4	Niridazole	test1	-3.22	-2.77	-0.45
1149	691-37-2	4-Methyl-1-pentene	test1	-3.24	-2.88	-0.36
1150	853-34-9	Kebuzone	test1	-3.27	-3.59	0.32
1151	106-46-7	1,4-Dichlorobenzene	test1	-3.27	-2.97	-0.30
1152	57-27-2	Morphine	test1	-3.28	-2.01	-1.27
1153	73-49-4	Quinethazone	test1	-3.29	-2.90	-0.39
1154	2029-64-3	n-Octyl_carbamate	test1	-3.30	-2.84	-0.46
1155	1114-71-2	Pedulate	test1	-3.35	-2.30	-1.05
1156	88-85-7	Dinoseb	test1	-3.38	-3.61	0.23
1157	101-21-3	Chloropham	test1	-3.38	-2.91	-0.47
1158	106-32-1	Ethyl_caprylate	test1	-3.39	-3.22	-0.17
1159	1134-23-2	Cycloate	test1	-3.40	-2.53	-0.88
1160	94-62-2	Piperine	test1	-3.46	-3.23	-0.22
1161	87-58-1	2,3,4,5-Tetraiodopyrrol	test1	-3.46	-4.89	1.44
1162	108-36-1	1,3-Dibromobenzene	test1	-3.54	-3.68	0.14
1163	34123-59-6	Isoproturon	test1	-3.54	-2.39	-1.15
1164	112-37-8	Undecanoic_acid	test1	-3.55	-3.43	-0.12
1165	514-17-0	Hydroxyisoandrosterone	test1	-3.59	-3.46	-0.13
1166	552-58-9	Eriodictyol	test1	-3.62	-2.04	-1.58
1167	298-81-7	Methoxsalen	test1	-3.66	-3.84	0.19
1168	54-31-9	Furosemide	test1	-3.66	-3.46	-0.20
1169	98-06-6	t-Butylbenzene	test1	-3.66	-3.65	-0.01
1170	548-00-5	Ethyl_biscoumacetate	test1	-3.66	-4.41	0.75
1171	260-94-6	Acridine	test1	-3.67	-3.53	-0.14
1172	96-14-0	3-Methylpentane	test1	-3.68	-3.67	-0.01
1173	298-00-0	Parathion_methyl	test1	-3.68	-3.74	0.06
1174	92-36-4	2-(4-Aminophenyl)-6-methyl-benzothiazole	test1	-3.68	-4.22	0.53
1175	2008-41-5	Butylate	test1	-3.68	-2.01	-1.68
1176	85-79-0	Dibucaine	test1	-3.70	-3.95	0.25
1177	90-12-0	1-Methylnaphthalene	test1	-3.70	-4.08	0.38

1178 535-65-9	Glybuthiazole	test1	-3.74	-3.43	-0.31
1179 64-85-7	Deoxycorticosterone	test1	-3.75	-4.27	0.52
1180 1929-82-4	Nitrapyrin	test1	-3.76	-3.65	-0.11
1181 99-87-6	p-Isopropyltoluene	test1	-3.77	-3.56	-0.21
1182 378-44-9	Betamethasone	test1	-3.77	-3.74	-0.03
1183 61-68-7	Mefenamic_acid	test1	-3.78	-3.33	-0.45
1184 514-10-3	Abietic_acid	test1	-3.80	-4.40	0.60
1185 146-22-5	Nitrazepam	test1	-3.80	-3.63	-0.17
1186 123-29-5	Ethyl_nonanoate	test1	-3.80	-3.75	-0.05
1187 37924-13-3	Perfluidone	test1	-3.80	-4.07	0.27
1188 14686-13-6	trans-2-Heptene	test1	-3.82	-3.87	0.05
1189 110-54-3	n-Hexane	test1	-3.84	-3.90	0.06
1190 52-39-1	Aldosterone	test1	-3.85	-3.40	-0.45
1191 108-87-2	Methylcyclohexane	test1	-3.85	-3.77	-0.08
1192 31431-39-7	Mebendazole	test1	-3.88	-3.77	-0.11
1193 81-81-2	Warfarin	test1	-3.89	-4.14	0.25
1194 3766-60-7	Buturon	test1	-3.90	-2.82	-1.08
1195 137-26-8	Thiram	test1	-3.90	-4.31	0.41
1196 13993-65-2	Metiazinic_acid	test1	-3.94	-3.34	-0.60
1197 83-44-3	Deoxycholic_acid	test1	-3.95	-4.43	0.48
1198 101-84-8	Diphenyl_ether	test1	-3.96	-3.45	-0.51
1199 629-06-1	1-Chloroheptane	test1	-3.99	-3.58	-0.41
1200 58-18-4	17-Methyltestosterone	test1	-3.99	-4.39	0.40
1201 700-12-9	Pentamethylbenzene	test1	-4.00	-4.46	0.46
1202 50-04-4	Cortisone_acetate	test1	-4.00	-4.06	0.06
1203 87-61-6	1,2,3-Trichlorobenzene	test1	-4.00	-3.85	-0.15
1204 122-14-5	Fenitrothion	test1	-4.04	-4.02	-0.02
1205 104-51-8	n-Butylbenzene	test1	-4.06	-3.81	-0.25
1206 106-37-6	1,4-Dibromobenzene	test1	-4.07	-3.68	-0.39
1207 732-11-6	Prometryn	test1	-4.10	-3.87	-0.23
1208 298-02-2	Phorate	test1	-4.11	-4.03	-0.08
1209 118-08-1	Hydrastine	test1	-4.11	-3.25	-0.86
1210 67-78-7	Triamcinolone_diacetate	test1	-4.13	-4.52	0.39
1211 292-64-8	Cyclooctane	test1	-4.15	-4.44	0.29
1212 36322-90-4	Piroxicam	test1	-4.16	-3.42	-0.73
1213 4394-00-7	Niflumic_acid	test1	-4.17	-4.00	-0.17
1214 55880-77-8	Pentachlorobutadiene	test1	-4.23	-3.49	-0.74
1215 60-87-7	Promethazine	test1	-4.26	-3.68	-0.58
1216 52-01-7	Spirolactone	test1	-4.28	-5.66	1.38
1217 87-86-5	Pentachlorophenol	test1	-4.28	-4.34	0.06
1218 128-13-2	Ursodeoxycholic_acid	test1	-4.29	-4.45	0.16
1219 939-27-5	2-Ethylanthracene	test1	-4.29	-4.99	0.70
1220 57-63-6	Ethinyl_estradiol	test1	-4.30	-4.22	-0.08
1221 58-40-2	Promazine	test1	-4.30	-3.77	-0.53
1222 2463-84-5	Dicaphon	test1	-4.31	-4.75	0.44
1223 76-25-5	Triamcinolone_acetonide	test1	-4.32	-4.21	-0.11
1224 132-65-0	Dibenzothiophene	test1	-4.38	-5.22	0.84
1225 60168-88-9	Fenarimol	test1	-4.38	-4.58	0.19
1226 83-79-4	Rotenone	test1	-4.42	-4.86	0.44
1227 52-86-8	Haloperidol	test1	-4.43	-4.44	0.01
1228 629-04-9	1-Bromoheptane	test1	-4.43	-4.14	-0.29
1229 84-16-2	Hexestrol	test1	-4.43	-4.40	-0.03
1230 50-48-6	Amitriptyline	test1	-4.46	-5.24	0.78
1231 2487-01-6	Medinoterb_acetate	test1	-4.47	-4.56	0.09
1232 4516-69-2	1,1,3-Trimethylcyclopentane	test1	-4.48	-4.42	-0.05
1233 108-70-3	1,3,5-Trichlorobenzene	test1	-4.48	-3.81	-0.67
1234 117-89-5	Trifluoperazine	test1	-4.52	-5.08	0.56

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1235 5836-10-2	Chloropropylate	test1	-4.53	-5.22	0.69
1236 55-38-9	Fenthion	test1	-4.57	-4.55	-0.02
1237 1107-99-9	Prednisolone-21-trimethylacetate	test1	-4.58	-4.51	-0.08
1238 1022-46-4	2-Phenyl-3,1-benzoxazin-4-one	test1	-4.61	-4.06	-0.54
1239 103-29-7	Bibenzyl	test1	-4.62	-4.91	0.29
1240 56-47-3	Deoxycorticosterone_acetate	test1	-4.63	-5.14	0.51
1241 145-13-1	Pregnenolone	test1	-4.65	-4.68	0.03
1242 581-40-8	2,3-Dimethylnaphthalene	test1	-4.72	-4.64	-0.08
1243 529-86-2	1-Anthranol	test1	-4.73	-4.14	-0.60
1244 51-98-9	Norethisterone_acetate	test1	-4.79	-4.85	0.06
1245 5598-13-0	Chlorpyrifos_methyl	test1	-4.82	-5.42	0.60
1246 57-91-0	alpha-Estradiol	test1	-4.84	-4.11	-0.74
1247 2303-17-5	Triallate	test1	-4.88	-3.73	-1.15
1248 1982-47-4	Chloroxuron	test1	-4.89	-3.72	-1.17
1249 581-42-0	2,6-Dimethylnaphthalene	test1	-4.89	-4.63	-0.26
1250 87-68-3	Hexachlorobutadiene	test1	-4.91	-4.08	-0.83
1251 19044-88-3	Oryzalin	test1	-5.16	-4.04	-1.12
1252 2051-62-9	4-Chlorobiphenyl	test1	-5.20	-5.12	-0.08
1253 1077-16-3	n-Hexylbenzene	test1	-5.21	-5.23	0.02
1254 517-09-9	Equilenin	test1	-5.24	-4.73	-0.52
1255 26002-80-2	Phenothrin	test1	-5.24	-6.27	1.02
1256 85-01-8	Phenanthrene	test1	-5.26	-5.52	0.26
1257 56-72-4	Coumaphos	test1	-5.38	-5.79	0.41
1258 24009-05-0	1-Hydroxychlorde	test1	-5.46	-5.25	-0.21
1259 1897-45-6	Chlorothalonil	test1	-5.64	-5.92	0.28
1260 1582-09-8	Trifluralin	test1	-5.68	-5.51	-0.17
1261 786-19-6	Carbophenothion	test1	-5.74	-6.06	0.32
1262 2050-67-1	3,3'-PCB	test1	-5.80	-5.71	-0.09
1263 779-02-2	9-Methylanthracene	test1	-5.89	-5.91	0.02
1264 1732-13-4	1,2,3,6,7,8-Hexahydopyrene	test1	-5.96	-6.21	0.25
1265 37680-65-2	2,2',5-PCB	test1	-6.02	-6.24	0.22
1266 2104-96-3	Bromophos	test1	-6.09	-5.43	-0.66
1267 72-20-8	Endrin	test1	-6.18	-6.49	0.31
1268 7012-37-5	2,4,4'-PCB	test1	-6.21	-6.24	0.03
1269 1024-57-3	Heptachlor_epoxide	test1	-6.29	-6.72	0.43
1270 55702-45-9	2,3,6-PCB	test1	-6.29	-6.28	-0.01
1271 52645-53-1	Permethrin	test1	-6.29	-7.22	0.93
1272 76-44-8	Heptachlor	test1	-6.32	-6.55	0.23
1273 2437-79-8	2,2',4,4'-PCB	test1	-6.51	-6.77	0.26
1274 789-02-6	o,p'-DDT	test1	-6.62	-7.74	1.12
1275 1330-78-5	Tricresyl_phosphate	test1	-6.70	-7.00	0.30
1276 57-10-3	Palmitic_acid	test1	-6.81	-5.44	-1.37
1277 72-43-5	Methoxychlor	test1	-6.89	-7.28	0.39
1278 117-81-7	di-(2-Ethylhexyl)-phthalate	test1	-6.96	-7.60	0.64
1279 35693-99-3	2,2',5,5'-PCB	test1	-7.00	-6.76	-0.24
1280 52663-62-4	2,2',3,3',4-PCB	test1	-7.05	-7.41	0.36
1281 33284-53-6	2,3,4,5-PCB	test1	-7.16	-6.88	-0.28
1282 36653-82-4	Cetyl_alcohol	test1	-7.26	-6.18	-1.08
1283 309-00-2	Aldrin	test1	-7.33	-6.37	-0.96
1284 192-97-2	Benzo(e)pyrene	test1	-7.80	-8.22	0.42
1285 38380-02-8	2,2',3,4,5'-PCB	test1	-7.91	-7.38	-0.53
1286 243-17-4	Benzo(b)fluorene	test1	-8.04	-6.43	-1.61
1287 218-01-9	Chrysene	test1	-8.06	-7.18	-0.88
1288 52663-71-5	2,2',3,3',4,4',6-PCB	test1	-8.30	-8.80	0.50
1289 35065-28-2	2,2',3,4,4',5'-PCB	test1	-8.32	-8.05	-0.27
1290 55215-18-4	2,2',3,3',4,5-PCB	test1	-8.42	-8.10	-0.32
1291 207-08-9	Benzo(k)fluoranthene	test1	-8.49	-8.20	-0.29

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1292 92-24-0	Naphthacene	test1	-8.60	-7.26	-1.34
1293 38411-22-2	2,2',3,3',6,6'-PCB	test1	-8.65	-8.02	-0.63
1294 53-70-3	Dibenz(a,h)anthracene	test1	-8.66	-8.76	0.10
1295 191-24-2	Benzo(ghi)perylene	test1	-9.03	-9.28	0.25
1296 40186-72-9	2,2',3,3',4,4',5,5',6-PCB	test1	-10.26	-10.32	0.06
1297 52663-77-1	2,2',3,3',4,5,5',6,6'-PCB	test1	-10.41	-10.31	-0.10
1298 37680-73-2	2,2',4,5,5'-PCB	test2	-7.89	-7.21	-0.68
1299 94-09-7	Benzocaine	test2	-2.32	-1.79	-0.53
1300 50-78-2	Acetylsalicylic_acid	test2	-1.72	-1.69	-0.03
1301 58-55-9	Theophylline	test2	-1.39	-1.71	0.32
1302 60-80-0	Antipyrine	test2	0.39	-1.29	1.68
1303 1912-24-9	Atrazine	test2	-3.85	-3.51	-0.34
1304 50-06-6	Phenobarbital	test2	-2.32	-2.97	0.65
1305 330-54-1	Diuron	test2	-3.80	-2.86	-0.94
1306 67-20-9	Nitrofurantoin	test2	-3.38	-3.42	0.04
1307 57-41-0	Phenytoin	test2	-3.90	-3.40	-0.50
1308 439-14-5	Diazepam	test2	-3.76	-4.05	0.29
1309 58-22-0	Testosterone	test2	-4.09	-3.98	-0.11
1310 58-89-9	Lindane	test2	-4.64	-4.71	0.07
1311 56-38-2	Parathion	test2	-4.66	-4.13	-0.53
1312 333-41-5	Diazinon	test2	-3.64	-4.01	0.37
1313 77-09-8	Phenolphthalein	test2	-2.90	-3.99	1.09
1314 121-75-5	Malathion	test2	-3.37	-3.24	-0.13
1315 2921-88-2	Chlorpyrifos	test2	-5.49	-5.61	0.12
1316 363-24-6	Prostaglandin_E2	test2	-2.47	-3.29	0.82
1317 50-29-3	p,p'-DDT	test2	-8.08	-7.67	-0.41
1318 57-74-9	Chlordane	test2	-6.86	-7.29	0.43