

141	aC-SH	Benzenethiol (1)	2.8464	3.2675	9.5115	0.010086	95.08	48.905	41.648	17.413	4.513
142	-SH (except as above)	Cyclohexanethiol (1)	0.9600	2.3323	7.7987	0.006399	57.89	15.818	11.339	9.813	5.829
143	CH ₃ S	Dimethylsulfide (1)	1.7150	2.9892	6.9733	0.018013	122.03	35.845	-3.337	14.296	7.497
144	CH ₂ S	Diethylsulfide (1)	1.0063	2.6524	6.4871	0.015254	106.60	42.684	21.492	16.965	4.096
145	CHS	Diisopropylsulfide (1)	0.7892	2.0965	*****	*****	*****	*****	*****	*****	*****
146	CS	di- <i>tert</i> -Butylsulfide (1)	1.1170	1.6412	*****	*****	*****	*****	*****	19.996	*****
147	aC-S-	Phenyl methyl sulfide (1)	0.9646	2.9731	*****	*****	*****	*****	*****	*****	*****
148	SO	Dimethyl sulfoxide (1)	5.3663	6.2796	19.8953	-0.005534	82.36	-52.231	-71.050	*****	13.403
149	SO ₂	Dimethyl sulfone (1)	7.0778	7.0976	17.2586	-0.000784	89.95	-257.608	-305.498	*****	17.748
150	SO ₃ (sulfite)	Dimethyl sulfite (1)	*****	3.9199	8.6910	0.004240	115.80	*****	-430.833	*****	*****
151	SO ₃ (sulfonate)	Dimethyl sulfonate (1)	5.8426	6.7785	*****	*****	*****	*****	*****	*****	*****
152	SO ₄ (sulfate)	Dimethyl sulfate (1)	3.6976	5.5627	18.9366	-0.027208	144.58	-519.853	-621.412	*****	*****
153	aC-SO	Phenyl methyl sulfoxide (1)	3.9911	6.1185	*****	*****	*****	*****	*****	*****	*****
154	aC-SO ₂	Diphenyl sulfone (1)	5.2948	8.4333	*****	*****	135.47	-314.643	-370.493	*****	3.281
155	PH (phosphine)	Dimethylphosphine (1)	*****	2.0536	*****	*****	*****	*****	*****	*****	*****
156	P (phosphine)	Trimethylphosphine (1)	*****	1.0984	*****	*****	*****	*****	*****	*****	*****
157	PO ₃ (phosphite)	Triethylphosphite (1)	1.0306	2.7900	*****	*****	*****	*****	*****	*****	*****
158	PHO ₃ (phosphonate)	Dimethylphosphonate (1)	*****	5.6433	*****	*****	*****	*****	*****	*****	*****
159	PO ₃ (phosphonate)	Trimethylphosphonate (1)	*****	4.5468	*****	*****	*****	*****	*****	*****	*****
160	PHO ₄ (phosphate)	Diethylphosphate (1)	2.7461	5.1567	*****	*****	*****	*****	*****	*****	*****
161	PO ₄ (phosphate)	Trimethylphosphate (1)	2.0330	3.7657	16.9914	-0.029036	85.59	*****	-1060.325	*****	*****
162	aC-PO ₄	Triphenylphosphate (1)	-1.7840	2.3522	*****	*****	*****	*****	-1005.161	*****	4.256
163	aC-P	Triphenylphosphine (1)	0.2337	2.9272	38.6148	-0.126108	-142.79	*****	72.339	*****	-5.654
164	CO ₃ (carbonate)	Diethylcarbonate (1)	3.6593	2.8847	6.6804	0.007235	93.56	-447.186	-516.282	21.613	8.363
165	C ₂ H ₃ O	Ethyl oxirane (1)	1.3135	2.8451	6.6418	0.021238	125.43	11.149	-52.241	*****	*****
166	C ₂ H ₂ O	2,2-Dimethyl oxirane (1)	*****	2.6124	6.0159	0.010678	194.36	1.890	-51.390	*****	*****
167	C ₂ O	Trimethyl oxirane (1)	*****	2.2036	*****	*****	*****	*****	*****	*****	*****
168	CH ₂ (cyclic)	Cyclopentane (5)	0.5699	0.8234	1.8815	0.009884	49.24	13.287	-18.575	3.341	1.069
169	CH (cyclic)	Methylcyclopentane (1)	0.0335	0.5946	1.1020	0.007596	44.95	6.107	-12.464	6.416	2.511
170	C (cyclic)	1,1-Dimethylcyclohexane (1)	0.1695	0.0386	-0.2399	0.003268	33.32	-0.193	-2.098	7.017	-0.921
171	CH=CH (cyclic)	Cyclobutene (1)	1.1936	1.5985	3.6426	0.013815	83.91	86.493	59.841	7.767	1.185
172	CH=C (cyclic)	1-Methylcyclopentene (1)	0.4344	1.2529	3.5475	0.010576	70.98	67.056	64.295	7.171	2.559
173	C=C (cyclic)	1,2-Dimethylcyclopentene (1)	0.3048	1.1975	*****	*****	*****	*****	*****	*****	*****
174	CH ₂ =C (cyclic)	Methylene cyclohexane (1)	0.2220	1.5109	4.4913	0.019101	83.96	*****	*****	*****	5.351
175	NH (cyclic)	Cyclopentimine (1)	3.4814	2.1634	5.9726	-0.003678	51.80	72.540	23.138	13.700	8.655
176	N (cyclic)	<i>N</i> -methylpyrrolidine (1)	0.6040	1.6541	4.3905	-0.001179	31.41	83.779	65.622	*****	0.269
177	CH=N (cyclic)	Imidazole (1)	5.5779	6.5230	*****	*****	*****	*****	*****	*****	3.993
178	C=N (cyclic)	2-Methyl-1H-imidazole (1)	6.6382	6.6710	*****	*****	*****	*****	*****	*****	*****
179	O (cyclic)	Tetrahydropyran (1)	1.3828	1.0245	2.7409	-0.000387	17.69	-114.062	-137.353	6.877	3.806
180	CO (cyclic)	Cyclobutanone (1)	3.2119	2.8793	12.6396	-0.000207	57.38	-156.672	-180.166	17.124	6.137
181	S (cyclic)	2-Methyl-thiophene (1)	1.6023	2.3256	5.5523	0.001540	45.45	12.020	15.453	12.262	5.170
182	SO ₂ (cyclic)	Cyclobutadiene sulfone (1)	6.1006	*****	24.3995	0.002487	96.66	-241.601	-283.839	*****	9.934