

45	aC-COO	Methyl benzoate (1)	1.3348	3.1952	6.7311	0.018948	105.53	-291.662	-307.727	25.206	8.149
46	aC-OOCH	Phenyl formate (1)	*****	0.4621	*****	*****	*****	*****	*****	*****	*****
47	aC-OOC	Phenyl acetate (1)	4.8044	3.0854	*****	*****	*****	*****	*****	*****	5.875
48	COO except as above	Ethyl acrylate (1)	1.5038	2.1903	4.7346	0.013087	81.17	-299.803	-331.397	*****	10.573
49	CH ₃ O	Methyl butyl ether (1)	1.3643	1.7703	3.4393	0.020084	88.20	-90.329	-156.062	5.783	5.089
50	CH ₂ O	Di- <i>n</i> -butyl ether (1)	0.8733	1.3368	2.4217	0.017954	74.03	-105.579	-152.239	9.997	4.891
51	CH-O	sec-Butyl ether (1)	0.2461	0.8924	0.7889	0.014487	60.06	-101.207	-147.709	14.620	4.766
52	C-O	<i>tert</i> -Butylether (1)	-0.4446	0.4983	0.2511	0.005613	52.96	-92.804	-121.608	13.850	2.458
53	aC-O	Methyl phenyl ether (1)	1.3045	1.8522	3.6588	0.005115	47.27	-83.354	-101.783	16.151	-0.118
54	CH ₂ NH ₂	Ethylamine (1)	3.2742	2.7987	8.1745	0.011413	117.62	68.812	-10.703	15.432	13.482
55	CHNH ₂	sec-Butylamine (1)	30.8394	2.0948	4.2847	0.013049	76.36	61.452	0.730	16.048	6.283
56	CNH ₂	<i>tert</i> -Butylamine (1)	11.7400	1.6525	2.8546	0.010790	80.01	55.202	2.019	17.257	*****
57	CH ₃ NH	Dimethylamine (1)	2.4034	2.2514	4.5529	0.015863	77.04	88.512	24.740	11.831	4.490
58	CH ₂ NH	Dipropylamine (1)	1.7746	1.8750	3.2422	0.020482	95.15	88.874	23.610	13.067	7.711
59	CHNH	Diisopropylamine (1)	1.7577	1.2317	2.0057	0.005329	99.16	73.101	21.491	14.048	2.561
60	CH ₃ N	Methyldiethylamine (1)	0.9607	1.3841	3.0106	0.021186	94.94	125.906	55.024	9.493	6.008
61	CH ₂ N	Triethylamine (1)	0.0442	1.1222	2.1673	0.027454	74.05	121.247	65.331	12.636	1.756
62	aC-NH ₂	Aniline (1)	3.9889	3.8298	10.2155	0.005335	81.40	66.470	17.501	23.335	6.542
63	aC-NH	<i>N</i> -methyl aniline (1)	1.4837	2.9230	8.4081	-0.005596	86.37	98.195	53.274	23.026	0.624
64	aC-N	<i>N,N</i> -dimethyl aniline (1)	1.7618	2.1918	5.8536	-0.000838	108.39	143.280	115.606	22.249	-2.576
65	NH ₂ except as above	Cyclobutylamine	3.3478	2.0315	4.7420	0.000571	63.39	42.687	-8.556	13.425	6.158
66	CH=N	Acetaldazine (2)	8.8492	1.5332	*****	*****	*****	*****	*****	*****	*****
67	C=N	Ketazine (2)	1.4621	1.4291	*****	*****	*****	*****	*****	*****	*****
68	CH ₂ CN	Propionitrile (1)	2.5760	4.5871	12.9827	0.036523	133.62	134.997	99.245	21.923	7.303
69	CHCN	Isobutyronitrile (1)	2.1393	3.9774	8.4309	0.029034	134.73	142.475	151.390	24.963	9.464
70	CCN	2,2-Dimethylpropionitrile (1)	3.3807	2.8870	5.8829	0.024654	120.74	142.295	124.770	24.967	4.166
71	aC-CN	Benzonitrile (1)	5.1346	4.1424	10.4124	0.020978	119.08	162.175	148.968	*****	6.788
72	CN except as above	Acrylonitrile (1)	3.2747	3.0972	8.1381	0.024346	94.91	130.986	124.917	16.639	6.867
73	CH ₂ NCO	Ethyl isocyanate (1)	4.2256	3.4891	*****	*****	*****	*****	*****	*****	*****
74	CHNCO	Isopropyl isocyanate (1)	*****	3.1220	*****	*****	*****	*****	*****	*****	*****
75	CNCO	<i>tert</i> -Butyl isocyanate (1)	9.1492	*****	*****	*****	*****	*****	*****	*****	*****
76	aC-NCO	Phenyl isocyanate (1)	2.2327	3.1853	6.5884	0.025065	141.24	*****	*****	*****	*****
77	CH ₂ NO ₂	1-Nitropropane (1)	3.2131	4.5311	10.9507	0.021056	157.57	25.783	-65.620	29.640	10.989
78	CHNO ₂	2-Nitropropane (1)	0.7812	3.8069	9.5487	0.014899	143.36	16.407	-60.750	29.173	*****
79	CNO ₂	2-Methyl-2-nitropropane (1)	5.6280	3.3059	*****	*****	*****	*****	*****	*****	-4.187
80	aC-NO ₂	Nitrobenzene (1)	4.3531	4.5750	12.1243	0.018311	133.06	57.352	-22.931	24.863	7.572
81	NO ₂ except as above	Nitrocyclohexane (1)	3.0376	3.2069	*****	*****	*****	*****	*****	*****	6.302
82	ONO	Butyl nitrite (1)	*****	1.8896	*****	*****	*****	*****	*****	*****	*****
83	ONO ₂	<i>n</i> -Butyl nitrate (1)	2.5974	3.2656	*****	*****	*****	*****	*****	*****	9.353
84	HCON(CH ₂) ₂	Diethylformamide (1)	*****	5.8779	*****	*****	*****	*****	*****	*****	*****
85	HCONHCH ₂	Ethylformamide (1)	*****	7.4566	*****	*****	*****	*****	*****	*****	46.490
86	CONH ₂	Butyramide (1)	13.2124	6.5652	25.1184	0.001467	138.71	-127.512	-201.369	44.240	16.840
87	CONHCH ₃	Methylacetamide (1)	5.4720	5.0724	20.5590	0.023455	190.71	-102.912	-203.069	*****	17.429
88	CONHCH ₂	Ethylacetamide (1)	5.8825	6.6810	*****	*****	*****	*****	-183.613	52.723	*****
89	CON(CH ₃) ₂	Dimethylacetamide (1)	4.1720	6.0070	15.4603	0.043090	244.71	-56.412	-188.069	38.290	11.553
90	CONCH ₃ CH ₂	Methylethylacetamide (1)	*****	*****	*****	*****	*****	*****	-48.210	*****	*****
91	CON(CH ₂) ₂	Diethylacetamide (1)	*****	5.0664	*****	*****	*****	*****	*****	*****	*****
92	CONHCO	Diacetamide (1)	9.1763	7.6172	*****	*****	*****	*****	*****	*****	*****
93	CONCO	Methyldiacetamide	3.2657	5.6487	*****	*****	*****	*****	*****	*****	*****