

Table 6 (Continued)

	Group	Example	T_{mli}	T_{bli}	T_{cli}	P_{cli}	V_{cli}	G_{fli}	H_{fli}	H_{vli}	H_{fusli}
94	aC–CONH ₂	Benzamide	12.8071	8.3775	*****	*****	*****	*****	*****	*****	16.811
95	aC–NH(CO)H	<i>N</i> -phenylformamide (1)	5.6631	7.3497	19.8979	0.023447	162.08	–44.595	–125.052	*****	8.658
96	aC–N(CO)H	<i>N</i> -methyl- <i>N</i> -phenylmethanamide (1)	3.3602	5.1373	*****	*****	*****	*****	*****	*****	*****
97	aC–CONH	<i>N</i> -methylbenzamide (1)	6.5160	7.5850	*****	*****	*****	*****	*****	*****	10.959
98	aC–NHCO	<i>N</i> -(2-methylphenyl)acetamide (1)	9.8204	7.4955	*****	*****	*****	*****	*****	*****	4.370
99	aC–NCO	Phenylmethylacetamide (1)	7.2552	*****	*****	*****	*****	*****	*****	*****	*****
100	NHCONH	<i>N,N'</i> -dimethylurea (1)	9.3110	8.9406	*****	*****	*****	*****	*****	*****	9.862
101	NH ₂ CONH	Methylurea (1)	14.2020	16.3539	*****	*****	*****	*****	*****	*****	12.845
102	NH ₂ CON	<i>N,N</i> -dimethylurea (1)	13.0856	2.0796	*****	*****	*****	*****	*****	*****	10.958
103	NHCON	Trimethylurea (1)	8.4447	7.1529	*****	*****	*****	*****	*****	*****	12.098
104	NCON	Tetramethylurea (1)	3.5041	4.1459	*****	*****	*****	*****	*****	*****	9.557
105	aC–NHCONH ₂	Phenylurea (1)	13.4695	5.7604	*****	*****	*****	*****	*****	*****	16.703
106	aC–NHCONH	<i>N,N'</i> -diphenylurea	23.2570	1.1633	*****	*****	*****	*****	*****	*****	18.460
107	NHCO except as above	<i>N</i> -chloroacetamide (1)	3.0882	*****	*****	*****	*****	*****	*****	*****	*****
108	CH ₂ Cl	1-Chlorobutane (1)	1.9253	2.6364	6.2561	0.021419	112.12	–19.484	–65.056	11.754	6.353
109	CHCl	2-Chloropropane (1)	1.0224	2.0246	4.3756	0.015640	100.78	–31.933	–65.127	12.048	*****
110	CCl	2-Chloro-2-methylpropane (1)	1.8424	1.7049	3.7063	0.009187	87.01	–37.848	–62.881	16.597	–0.082
111	CHCl ₂	1,1-Dichloroethane (1)	2.5196	3.3420	7.8956	0.028236	159.79	–24.214	–80.812	17.251	6.781
112	CCl ₂	2,2-Dichloropropane (1)	3.6491	2.9609	*****	*****	*****	*****	*****	20.473	1.823
113	CCl ₃	1,1,1-Trichloroethane	4.4493	3.9093	8.8073	0.036746	204.71	–44.122	–105.369	20.550	3.492
114	CH ₂ F	1-Fluorobutane (1)	1.5597	1.5022	3.3179	0.023315	87.71	–180.212	–227.469	8.238	7.139
115	CHF	2-Fluorobutane (1)	1.1289	1.3738	2.6702	0.020040	78.08	–228.239	–261.901	*****	3.917
116	CF	2-Fluoro-2-methylpropane (1)	2.5398	1.0084	2.1633	–0.010120	*****	*****	*****	6.739	*****
117	CHF ₂	1,1-Difluoroethane (1)	2.1689	2.2238	3.5702	0.031524	102.71	–411.239	–463.901	*****	7.011
118	CF ₂	Perfluorohexane (4)	0.1312	0.5142	0.8543	0.018572	95.09	*****	*****	1.621	*****
119	CF ₃	Hexafluoroethane (2)	1.4828	1.1916	1.7737	0.048565	108.85	–615.333	–673.875	7.352	2.526
120	CCl ₂ F	Tetrachloro-1,2-difluoroethane (2)	3.2035	2.5053	5.1653	0.037948	171.04	–249.020	–306.765	8.630	3.114
121	HCClF	1-Chloro-1,2,2,2-tetrafluoroethane (1)	*****	2.0542	*****	*****	*****	*****	*****	*****	*****
122	CClF ₂	1,2-Dichlorotetrafluoroethane (2)	1.7510	1.7227	3.0593	0.041641	146.01	–396.814	–458.074	8.086	2.156
123	aC–Cl	Chlorobenzene (1)	1.7134	2.0669	5.7046	0.016033	92.67	1.985	–17.002	11.224	4.435
124	aC–F	Hexafluorobenzene (6)	0.9782	0.7945	1.5491	0.014037	54.36	–141.306	–160.965	3.965	2.003
125	aC–I	Iodobenzene (1)	2.1905	3.7739	12.4470	0.014403	131.08	91.505	95.048	*****	2.814
126	aC–Br	Bromobenzene (1)	2.4741	2.8414	8.4199	0.010199	104.12	42.977	38.917	14.393	5.734
127	I [–] except as above	Iodoethane (1)	1.9444	3.1778	8.5775	–0.004637	104.28	43.910	47.632	14.171	6.103
128	Br [–] except as above	Bromoethane (1)	1.7641	2.4231	4.5036	–0.001460	77.99	5.528	–1.703	9.888	4.826
129	F [–] except as above	Benzyl fluoride (1)	1.2308	0.8504	0.8976	0.012034	24.62	–182.973	–201.968	*****	3.096
130	Cl [–] except as above	Ethyl chloroacetate (1)	1.5454	1.5147	4.0947	0.007923	57.77	–29.876	–46.963	*****	5.181
131	CHNOH	Propionaldehyde oxime (1)	3.9813	4.5721	*****	*****	*****	*****	*****	*****	*****
132	CNOH	Diethyl ketoxime (1)	3.5484	4.0142	*****	*****	*****	*****	*****	*****	*****
133	aC–CHNOH	Phenyl oxime (1)	10.5579	*****	*****	*****	*****	*****	*****	*****	*****
134	OCH ₂ CH ₂ OH	2-Ethoxyethanol (1)	2.3651	4.8721	10.4579	0.025986	159.33	–233.335	–343.903	31.493	8.454
135	OCHCH ₂ OH	2-Ethoxy-1-propanol (1)	*****	4.2329	*****	*****	*****	*****	*****	*****	*****
136	OCH ₂ CHOH	1-Methoxy-2-propanol (1)	1.5791	3.6653	*****	0.018783	147.66	–239.423	–333.385	*****	12.594
137	–O–OH	<i>tert</i> -Butylhydroperoxide (1)	4.8181	3.1669	5.8307	–0.002815	58.01	–75.568	–125.111	*****	*****
138	CH ₂ SH	Ethanethiol (1)	2.2992	3.1974	7.7300	0.017299	105.68	27.469	–8.021	16.815	10.068
139	CHSH	2-Propanethiol (1)	0.9704	2.5910	5.8527	0.008968	109.36	27.030	3.510	17.098	4.266
140	CSH	2-Methyl-2-propanethiol (1)	4.2329	2.0902	4.6431	0.005118	94.01	27.338	12.589	18.397	–0.623