Table 6
First-order groups and their contributions along with sample assignments

	Group	Example	T_{m1i}	T_{b1i}	T_{c1i}	P_{c1i}	V_{c1i}	G_{f1i}	H_{f1i}	H_{v1i}	H_{fus1i}
1	CH_3	*n*-Tetracontane (2)	0.6953	0.8491	1.7506	0.018615	68.35	2.878	−42.479	0.217	1.660
2	CH_2	*n*-Tetracontane (38)	0.2515	0.7141	1.3327	0.013547	56.28	8.064	−20.829	4.910	2.639
3	CH	2-Methylpentane (1)	−0.3730	0.2925	0.5960	0.007259	37.50	8.254	−7.122	7.962	0.134
4	C	2,2-Dimethylbutane (1)	0.0256	−0.0671	0.0306	0.001219	16.01	16.413	8.928	10.730	−1.232
5	CH_2=CH	1-Hexene (1)	1.1728	1.5596	3.2295	0.025745	111.43	95.738	57.509	4.031	1.268
6	CH=CH	2-Hexene (1)	0.9460	1.5597	3.0741	0.023003	98.43	92.656	69.664	9.456	4.441
7	CH_2=C	2-Methyl-1-butene (1)	0.7662	1.3621	2.7717	0.021137	91.40	85.107	61.625	8.602	2.451
8	CH=C	2-Methyl-2-butene (1)	0.1732	1.2971	2.5666	0.019609	83.89	88.691	81.835	14.095	3.032
9	C=C	2,3-Dimethyl-2-butene (1)	0.3928	1.2739	2.6391	0.014114	90.66	93.119	95.710	19.910	2.616
10	CH_2=C=CH	1,2-Butadiene (1)	1.7036	2.6840	5.4330	0.035483	143.57	229.906	198.840	11.310	7.076
11	CH_2=C=C	3-Methyl-1,2-butadiene (1)	1.5453	2.4014	4.8219	0.029678	146.36	226.710	208.490	*****	7.435
12	CH=C=CH	2,3-Pentadiene (1)	1.2850	2.5400	*****	*****	*****	*****	*****	*****	6.000
13	CH≡C	1-Pentyne (1)	2.2276	1.7618	3.7897	0.014010	84.60	230.029	224.902	6.144	−1.548
14	C≡C	3-Decyne (1)	2.0516	1.6767	4.5870	0.010888	74.66	216.013	228.282	12.540	6.128
15	aCH	Benzene (6)	0.5860	0.8365	2.0337	0.007260	42.39	26.732	12.861	3.683	1.948
16	aC fused with aromatic ring	Naphthalene (2)	1.8955	1.7324	5.4979	0.003564	35.71	20.379	20.187	6.631	0.845
17	aC fused with non-aromatic subring	Indane (2)	1.2065	1.1995	3.1058	0.006512	34.65	33.912	30.768	6.152	1.095
18	aC except as above	Benzophenone (1)	0.9176	1.5468	4.5344	0.012859	26.47	23.331	24.701	6.824	−0.531
19	aN in aromatic ring	Pyridine (1)	2.0438	1.3977	4.0954	−0.003339	36.47	89.902	70.862	9.420	2.555
20	aC–CH_3	Toluene (1)	1.0068	1.5653	3.4611	0.020907	97.33	24.919	−19.258	8.279	2.969
21	aC–CH_2	Ethylbenzene (1)	0.1065	1.4925	2.9003	0.018082	87.19	31.663	4.380	11.981	0.948
22	aC–CH	Cumene (1)	−0.5197	0.8665	1.9512	0.011795	73.51	30.393	18.440	13.519	−1.037
23	aC–C	*tert*-Butylbenzene (1)	−0.1041	0.5229	0.8576	0.011298	67.20	40.127	35.297	16.912	−2.856
24	aC–CH=CH_2	Styrene (1)	1.2832	2.4308	5.7861	0.030637	134.69	114.531	77.863	*****	4.013
25	aC–CH=CH	1-Propenylbenzene (1)	1.7744	2.9262	6.5062	0.026282	128.84	111.216	88.084	*****	8.274
26	aC–C=CH_2	α-Methylstyrene (1)	1.2612	2.1472	4.9967	0.026371	110.74	115.728	90.927	*****	3.324
27	aC–C≡CH	Phenylacetylene (1)	1.7495	2.3057	6.4572	0.019507	112.08	263.205	257.448	*****	2.514
28	aC–C≡C	1-Phenyl-1-propyne (1)	*****	2.7341	*****	*****	*****	*****	*****	*****	*****
29	OH	1,4-Butanediol (2)	2.7888	2.5670	5.2188	−0.005401	30.61	−144.051	−178.360	24.214	4.786
30	aC–OH	Phenol (1)	5.1473	3.3205	9.3472	−0.008788	50.77	−131.327	−164.191	34.099	8.427
31	COOH	1,5-Pentanedioic acid (2)	7.4042	5.1108	14.6038	0.009885	90.66	−337.090	−389.931	17.002	10.692
32	aC–COOH	Benzoic acid (1)	12.4296	6.0677	15.4515	0.017100	119.10	−312.422	−361.249	*****	14.649
33	CH_3CO	2-Butanone (1)	2.9588	3.1178	7.0058	0.025227	127.99	−120.667	−180.604	15.195	8.062
34	CH_2CO	3-Pentanone (1)	2.5232	2.6761	5.7157	0.019619	112.79	−120.425	−163.090	19.392	8.826
35	CHCO	2,4-Dimethyl-3-pentanone (1)	1.1565	2.1748	4.4743	0.012487	97.16	−116.799	−139.909	20.350	7.205
36	CCO	2,2,4,4-Tetramethyl-3-pentanone (1)	1.0638	1.7287	*****	*****	*****	*****	*****	*****	*****
37	aC–CO	Acetophenone (1)	2.9157	3.4650	9.4806	0.011007	90.69	−91.812	−106.965	25.036	4.852
38	CHO	1-Hexanal (1)	3.0186	2.5388	5.8013	0.010204	71.08	−100.882	−130.816	12.370	11.325
39	aC–CHO	Benzaldehyde (1)	2.4744	3.5172	9.4795	0.019633	122.91	−80.222	−107.159	*****	7.273
40	CH_3COO	Butyl acetate (1)	2.1657	3.1228	6.3179	0.033812	148.91	−306.733	−387.458	19.342	7.910
41	CH_2COO	Methyl Butyrate (1)	1.6329	2.9850	5.9619	0.026983	132.89	−298.332	−364.204	21.100	9.479
42	CHCOO	Ethyl isobutyrate (1)	1.0668	2.2869	4.7558	0.021990	125.52	−301.414	−352.057	24.937	9.317
43	CCOO	Ethyl 2,2-dimethylpropionate (1)	0.3983	1.6918	*****	*****	*****	*****	*****	23.739	*****
44	HCOO	Propyl formate (1)	2.0223	2.5972	5.6064	0.015249	93.29	−276.878	−327.678	15.422	8.115

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_3O	Methyl butyl ether (1)	1.3643	1.7703	3.4393	0.020084	88.20	−90.329	−156.062	5.783	5.089
50	CH_2O	Di-*n*-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	*tert*-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_2NH_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	*tert*-Butylamine (1)	11.7400	1.6525	2.8546	0.010790	80.01	55.202	2.019	17.257	*****
57	CH_3NH	Dimethylamine (1)	2.4034	2.2514	4.5529	0.015863	77.04	88.512	24.740	11.831	4.490
58	CH_2NH	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_3N	Methyldiethylamine (1)	0.9607	1.3841	3.0106	0.021186	94.94	125.906	55.024	9.493	6.008
61	CH_2N	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	*N*-methyl aniline (1)	1.4837	2.9230	8.4081	−0.005596	86.37	98.195	53.274	23.026	0.624
64	aC–N	*N*,*N*-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_2CN	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_2NCO	Ethyl isocyanate (1)	4.2256	3.4891	*****	*****	*****	*****	*****	*****	*****
74	CHNCO	Isopropyl isocyanate (1)	*****	3.1220	*****	*****	*****	*****	*****	*****	*****
75	CNCO	*tert*-Butyl isocyanate (1)	9.1492	*****	*****	*****	*****	*****	*****	*****	*****
76	aC–NCO	Phenyl isocyanate (1)	2.2327	3.1853	6.5884	0.025065	141.24	*****	*****	*****	*****
77	CH_2NO_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	*n*-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	$CONCH_3CH_2$	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	*****	*****	*****	*****	*****	*****	*****

Table 6 (*Continued*)

	Group	Example	T_{m1i}	T_{b1i}	T_{c1i}	P_{c1i}	V_{c1i}	G_{f1i}	H_{f1i}	H_{v1i}	H_{fus1i}
94	aC–$CONH_2$	Benzamide	12.8071	8.3775	*****	*****	*****	*****	*****	*****	16.811
95	aC–NH(CO)H	*N*-phenylformamide (1)	5.6631	7.3497	19.8979	0.023447	162.08	−44.595	−125.052	*****	8.658
96	aC–N(CO)H	*N*-methyl-*N*-phenylmethanamide (1)	3.3602	5.1373	*****	*****	*****	*****	*****	*****	*****
97	aC–CONH	*N*-methylbenzamide (1)	6.5160	7.5850	*****	*****	*****	*****	*****	*****	10.959
98	aC–NHCO	*N*-(2-methylphenyl)acetamide (1)	9.8204	7.4955	*****	*****	*****	*****	*****	*****	4.370
99	aC–NCO	Phenylmethylacetamide (1)	7.2552	*****	*****	*****	*****	*****	*****	*****	*****
100	NHCONH	*N*,*N*′-dimethylurea (1)	9.3110	8.9406	*****	*****	*****	*****	*****	*****	9.862
101	NH_2CONH	Methylurea (1)	14.2020	16.3539	*****	*****	*****	*****	*****	*****	12.845
102	NH_2CON	*N*,*N*-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	*N*,*N*′-diphenylurea	23.2570	1.1633	*****	*****	*****	*****	*****	*****	18.460
107	NHCO except as above	*N*-chloroacetamide (1)	3.0882	*****	*****	*****	*****	*****	*****	*****	*****
108	CH_2Cl	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_2F	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_2F	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_2CH_2OH	2-Ethoxyethanol (1)	2.3651	4.8721	10.4579	0.025986	159.33	−233.335	−343.903	31.493	8.454
135	$OCHCH_2OH$	2-Ethoxy-1-propanol (1)	*****	4.2329	*****	*****	*****	*****	*****	*****	*****
136	OCH_2CHOH	1-Methoxy-2-propanol (1)	1.5791	3.6653	*****	0.018783	147.66	−239.423	−333.385	*****	12.594
137	–O–OH	*tert*-Butylhydroperoxide (1)	4.8181	3.1669	5.8307	−0.002815	58.01	−75.568	−125.111	*****	*****
138	CH_2SH	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

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_3S	Dimethylsulfide (1)	1.7150	2.9892	6.9733	0.018013	122.03	35.845	−3.337	14.296	7.497
144	CH_2S	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	*****	*****	*****	*****	*****	19.038	*****
146	CS	di-*tert*-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_2H_3O	Ethyl oxirane (1)	1.3135	2.8451	6.6418	0.021238	125.43	11.149	−52.241	*****	*****
166	C_2H_2O	2,2-Dimethyl oxirane (1)	*****	2.6124	6.0159	0.010678	194.36	1.890	−51.390	*****	*****
167	C_2O	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)	*N*-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

Table 7
Second-order groups and their contributions along with sample assignments

	Group	Example	T_{m2j}	T_{b2j}	T_{c2j}	P_{c2j}	V_{c2j}	G_{f2j}	H_{f2j}	H_{v2j}	H_{fus2j}
1	$(CH_3)_2CH$	2-Methylpentane (1)	0.1175	−0.0035	−0.0471	0.000473	1.71	−0.418	−0.419	−0.399	0.396
2	$(CH_3)_3C$	2,2,4,4-Tetramethylpentane (2)	−0.1214	0.0072	−0.1778	0.000340	3.14	−2.776	−1.967	−0.417	0.554
3	$CH(CH_3)CH(CH_3)$	2,3,4-Trimethylpentane (2)	0.2390	0.3160	0.5602	−0.003207	−3.75	6.996	6.065	0.532	−1.766
4	$CH(CH_3)C(CH_3)_2$	2,2,3,4,4-Pentamethylpentane (2)	−0.3276	0.3976	0.8994	−0.008733	−10.06	8.938	8.078	0.623	0.351
5	$C(CH_3)_2C(CH_3)_2$	2,2,3,3,4,4-Hexamethylpentane (2)	3.3297	0.4487	1.5535	−0.016852	−8.70	10.735	10.535	5.086	−1.089
6	$CH_n{=}CH_m{-}CH_p{=}CH_k$ (k, m, n, p in 0..2)	1,3-Butadiene (1)	0.7451	0.1097	0.4214	0.000792	−7.88	−6.562	−11.786	1.632	1.408
7	$CH_3{-}CH_m{=}CH_n$ (m, n in 0..2)	2-Methyl-2-butene (3)	0.0524	0.0369	−0.0172	−0.000101	0.50	−0.120	−0.048	0.064	0.070
8	$CH_2{-}CH_m{=}CH_n$ (m, n in 0..2)	1,4-Pentadiene (2)	−0.1077	−0.0537	0.0262	0.000815	0.14	1.006	1.449	−0.060	−0.632
9	$CH_p{-}CH_m{=}CH_n$ (m, n in 0..2; p in 0..1)	3-Methyl-1-butene (1)	−0.2485	−0.0093	−0.1526	−0.000163	−2.67	3.857	3.964	0.004	−0.368
10	CHCHO or CCHO	2-Methylbutyraldehyde (1)	0.5715	−0.1286	−1.0434	0.005789	10.36	−0.525	1.514	−0.550	−0.369
11	CH_3COCH_2	2-Pentanone (1)	−0.0968	−0.0215	−0.0338	−0.000111	−4.08	−1.543	0.033	−0.403	0.105
12	CH_3COCH or CH_3COC	3-Methyl-2-pentanone (1)	−0.6024	−0.0803	−0.3658	−0.001892	3.02	2.202	4.994	0.723	1.005
13	CHCOOH or CCOOH	2-Methyl butanoic acid (1)	−3.1734	−0.3203	−4.7275	0.006916	10.56	3.920	1.121	7.422	5.475
14	CH_3COOCH or CH_3COOC	Isopropyl acetate (1)	0.2114	−0.2066	−0.5537	−0.000569	4.28	−11.779	−12.295	−1.871	1.208
15	CO–O–CO	Propanoic anhydride (1)	−1.2441	−0.0500	−0.3576	0.001812	2.98	−16.075	−14.140	*****	−2.666
16	CHOH	2-Butanol (1)	−0.3489	−0.2825	−0.6768	0.000246	−3.04	−5.614	−4.422	−0.206	−0.599
17	COH	2-Methyl-2-butanol (1)	0.3695	−0.5325	−1.5224	0.003224	13.98	−25.382	−25.929	−1.579	−0.459
18	CH_3COCH_nOH (n in 0..2)	3-Hydroxy-2-butanone (1)	0.9886	−0.2987	−0.3940	−0.002912	5.17	6.621	8.244	*****	*****
19	NCCHOH or NCCOH	2-Hydroxypropionitrile (1)	−1.1810	0.2981	0.3414	−0.000516	0.68	4.833	0.000	*****	−0.149
20	$OH{-}CH_n{-}COO$ (n in 0..2)	Ethyl lactate (1)	−0.1526	−0.2310	*****	*****	*****	*****	*****	*****	*****
21	$CH_m(OH)CH_n(OH)$ (m, n in 0..2)	Ethylene glycol (1)	−0.0414	0.8854	1.9395	−0.004712	7.54	−1.051	−0.592	−6.611	−0.306
22	$CH_m(OH)CH_n(-)$ (m, n, p in 0..2)	2-Amino-1-butanol (1)	−0.5941	0.5082	1.2342	0.002581	5.58	−1.506	−0.959	*****	−0.041
23	$CH_m(NH_2)CH_n(NH_2)$ (m, n in 0..2)	Ethylenediamine (1)	0.3258	−0.0064	−3.3555	0.000726	20.82	0.344	−1.443	2.384	−1.575
24	$CH_m(NH)CH_n(NH_2)$ (m, n in 1..2)	Diethylenetriamine (1)	−1.8403	0.2318	−1.1598	0.000157	−26.31	3.848	3.608	*****	*****
25	$H_2NCOCH_nCH_mCONH_2$ (m, n in 1..2)	Butanediamide (1)	11.5351	*****	*****	*****	*****	*****	*****	*****	*****
26	$CH_m(NH_n){-}COOH$ (m, n in 0..2)	L-Alanine (1)	12.3481	*****	62.4740	−0.002696	17.78	3.145	6.598	*****	7.032
27	$HOOC{-}CH_n{-}COOH$ (n in 1..2)	Malonic acid (1)	0.9327	−0.1222	1.9595	−0.001479	12.46	−5.217	−6.058	*****	4.264
28	$HOOC{-}CH_n{-}CH_m{-}COOH$ (n, m in 1..2)	Succinic acid (1)	7.5057	*****	0.7686	0.000090	15.17	−4.281	−6.929	*****	29.245
29	$HO{-}CH_n{-}COOH$ (n in 1..2)	2-Hydroxyisobutyric acid (1)	−0.4531	−0.4625	*****	*****	*****	*****	*****	*****	*****
30	$NH_2{-}CH_n{-}CH_m{-}COOH$ (n, m in 1..2)	β-Alanine (1)	14.1593	*****	*****	*****	*****	*****	*****	*****	*****
31	$CH_3{-}O{-}CH_n{-}COOH$ (n in 1..2)	Methoxyacetic acid (1)	−2.3026	0.9198	0.4750	−0.001445	7.91	−2.678	−1.727	*****	*****
32	HS–CH–COOH	2-Mercaptopropionic acid (1)	−2.1535	*****	*****	*****	*****	*****	*****	*****	*****
33	$HS{-}CH_n{-}CH_m{-}COOH$ (n, m in 1..2)	β-Thiolactic acid (1)	−2.7514	*****	−0.2697	0.000655	20.43	−7.376	7.292	*****	−3.623
34	$NC{-}CH_n{-}CH_m{-}CN$ (n, m in 1..2)	1,2-Dicyanoethane (1)	4.0747	1.8957	1.9699	0.002330	24.82	18.974	5.661	*****	−8.038
35	$OH{-}CH_n{-}CH_m{-}CN$ (n, m in 1..2)	3-Hydroxypropanenitrile (1)	−0.9493	1.3434	0.2311	−0.001022	14.54	0.558	−3.906	*****	−4.371
36	$HS{-}CH_n{-}CH_m{-}SH$ (n, m in 1..2)	1,2-Ethanedithiol (1)	0.2232	0.1815	2.1272	0.001321	−10.31	6.728	0.794	−0.683	−0.931
37	$COO{-}CH_n{-}CH_m{-}OOC$ (n, m in 1..2)	Ethylene glycol diacetate (1)	−0.5946	0.3401	1.5418	−0.003385	−2.33	1.306	4.025	1.203	*****
38	$OOC{-}CH_m{-}CH_m{-}COO$ (n, m in 1..2)	Dimethylsuccinate (1)	2.5962	0.5794	*****	*****	*****	*****	*****	*****	2.303
39	$NC{-}CH_n{-}COO$ (n in 1..2)	Methylcyanoacetate (1)	−0.2509	1.2171	2.7051	−0.001999	−0.73	*****	*****	*****	1.100
40	$COCH_nCOO$ (n in 1..2)	Methylacetoacetate (1)	0.6304	0.2427	0.7502	−0.000231	1.69	10.556	−7.261	*****	*****
41	$CH_m{-}O{-}CH_n{=}CH_p$ (m, n, p in 0..3)	Ethyl viny ether (1)	−0.0811	0.1399	0.2900	−0.000432	−4.54	−10.098	−9.411	0.372	3.169
42	$CH_m{=}CH_n{-}F$ (m, n in 0..2)	1-Fluoro-1-propene (1)	−0.2568	0.0591	*****	*****	*****	*****	*****	*****	2.823
43	$CH_m{=}CH_n{-}Br$ (m, n in 0..2)	1-Bromo-1-propene (1)	−0.4329	−0.3192	*****	−0.010021	2.63	14.470	17.014	*****	2.212
44	$CH_m{=}CH_n{-}I$ (m, n in 0..2)	1-Iodo-1-propene (1)	*****	−0.3486	*****	*****	*****	*****	*****	*****	*****
45	$CH_m{=}CH_n{-}Cl$ (m, n in 0..2)	1-Chloro-2-methylpropene (1)	0.0446	−0.0268	−0.0188	0.000152	2.80	8.207	9.715	*****	−0.480
46	$CH_m{=}CH_n{-}CN$ (m, n in 0..2)	Acrylonitrile (1)	0.1027	0.0653	−1.1249	0.000893	3.82	−8.304	−16.903	*****	−0.405

47	$CH_n{=}CH_m{-}COO{-}CH_p$ (m, n, p in 0..3)	Ethyl Acrylate (1)	0.2117	−0.0430	−0.0880	0.000044	0.21	−12.085	−12.509	*****	−0.014
48	$CH_m{=}CH_n{-}CHO$ (m, n in 0..2)	Propenaldehyde (1)	−0.7191	0.1102	*****	*****	*****	*****	*****	*****	*****
49	$CH_m{=}CH_n{-}COOH$ (m, n in 0..2)	Acrylic Acid (1)	2.4103	0.0667	−1.7762	−0.000763	4.36	10.194	9.090	*****	1.291
50	$aC{-}CH_n{-}X$ (n in 1..2) X: Halogen	Benzyl bromide (1)	0.8092	0.4537	2.2630	0.002464	−4.88	−8.081	−8.570	*****	*****
51	$aC{-}CH_n{-}NH_m$ (n in 1..2; m in 0..2)	Benzyl amine (1)	−1.0802	0.2590	1.4069	−0.000034	2.50	−2.044	−3.447	4.608	−0.639
52	$aC{-}CH_n{-}O{-}$ (n in 1..2)	Benzyl ethyl ether (1)	0.8607	−0.0425	0.2698	−0.000417	−7.49	6.043	5.486	*****	0.969
53	$aC{-}CH_n{-}OH$ (n in 1..2)	Benzyl alcohol (1)	0.8981	0.1005	−1.0107	0.002944	−0.25	*****	*****	*****	−2.754
54	$aC{-}CH_n{-}CN$ (n in 1..2)	Benzyl cyanide (1)	0.1088	1.0587	2.4950	−0.000796	−11.01	25.157	16.950	*****	*****
55	$aC{-}CH_n{-}CHO$ (n in 1..2)	Phenyl acetaldehyde (1)	1.9470	−0.0177	*****	*****	*****	*****	*****	*****	*****
56	$aC{-}CH_n{-}SH$ (n in 1..2)	Phenyl methanethiol (1)	1.2057	0.1702	0.8705	0.000183	2.00	16.725	7.568	*****	0.890
57	$aC{-}CH_n{-}COOH$ (n in 1..2)	Phenyl acetic acid (1)	0.3666	0.1584	*****	*****	*****	*****	*****	*****	−4.086
58	$aC{-}CH_n{-}CO{-}$ (n in 1..2)	Phenyl acetone (1)	−0.2363	0.3094	*****	*****	*****	*****	*****	*****	*****
59	$aC{-}CH_n{-}S{-}$ (n in 1..2)	Benzyl methyl sulfide (1)	0.4506	0.1030	*****	*****	*****	*****	*****	*****	*****
60	$aC{-}CH_n{-}OOC{-}H$ (n in 1..2)	Benzyl formate (1)	*****	0.2238	1.7860	0.004195	−3.40	3.020	4.145	*****	*****
61	$aC{-}CH_m{-}NO_2$ (n in 1..2)	Phenyl nitromethane (1)	*****	0.5390	*****	*****	*****	*****	*****	*****	*****
62	$aC{-}CH_n{-}CONH_2$ (n in 1..2)	Phenyl ethanamide (1)	2.2421	−0.2197	*****	*****	*****	*****	*****	*****	*****
63	$aC{-}CH_n{-}OOC$ (n in 1..2)	Benzyl acetate (1)	−0.6997	0.0886	1.1629	−0.000384	−7.02	1.556	4.066	*****	*****
64	$aC{-}CH_n{-}COO$ (n in 1..2)	Methyl phenyl acetate (1)	−0.2636	0.0352	*****	*****	*****	*****	*****	*****	*****
65	$aC{-}SO_2{-}OH$	Benzenesulfonic acid (1)	−1.1057	*****	*****	*****	*****	*****	*****	*****	*****
66	$aC{-}CH(CH_3)_2$	Cumene (1)	0.0642	0.0196	0.1565	−0.001446	−2.04	1.238	−0.751	1.030	−0.270
67	$aC{-}C(CH_3)_3$	*tert*-Butylbenzene (1)	0.0790	0.0494	0.8016	−0.006495	−5.70	0.354	−0.192	*****	−0.878
68	$aC{-}CF_3$	Perfluorotoluene (1)	−10.8058	−1.5974	*****	*****	*****	*****	*****	*****	*****
69	$(CH_n{=}C)$(cyclic)–CHO (n in 0..2)	Furfural (1)	−1.0516	0.4267	2.4070	−0.002650	0.39	−6.438	−12.517	*****	−1.670
70	$(CH_n{=}C)_{cyc}{-}COO{-}CH_m$ (n, m in 0..3)	Methyl furanyrate (1)	−6.9427	0.0879	*****	*****	*****	*****	*****	*****	*****
71	$(CH_n{=}C)_{cyc}{-}CO{-}$ (n in 0..2)	2-Acetylfuran (1)	0.6572	0.6115	*****	*****	*****	*****	*****	*****	*****
72	$(CH_n{=}C)_{cyc}{-}CH_3$ (n in 0..2)	1,2-Dimethylcyclopentene (2)	0.0416	0.0173	−0.2509	−0.000624	0.03	28.972	24.560	*****	2.235
73	$(CH_n{=}C)_{cyc}{-}CH_2$ (n in 0..2)	2-Ethylfuran (1)	−0.3151	−0.0504	−1.1019	0.003921	−4.43	−22.533	−12.044	*****	0.961
74	$(CH_n{=}C)_{cyc}{-}CN$ (n in 0..2)	3-Cyanofuran (1)	1.5819	−0.2474	*****	*****	*****	*****	*****	*****	*****
75	$(CH_n{=}C)_{cyc}{-}Cl$ (n in 0..2)	2-Chlorofuran (1)	−0.8604	−0.5736	*****	*****	*****	*****	*****	*****	*****
76	$CH_{cyc}{-}CH_3$	Methylcyclopentane (1)	−0.1326	−0.1210	−0.1233	0.000779	2.79	4.178	4.452	0.096	0.033
77	$CH_{cyc}{-}CH_2$	Ethylcyclohexane (1)	−0.4669	−0.0148	0.3816	0.001694	−2.95	5.332	4.428	−0.428	−1.137
78	$Ch_{cyc}{-}CH$	Isopropylcyclopentane (1)	−0.3548	0.1395	0.1093	0.000124	6.19	6.084	−4.128	0.153	2.421
79	$Ch_{cyc}{-}C$	*tert*-Butylcyclohexane (1)	−0.1727	0.1829	*****	*****	*****	*****	*****	*****	*****
80	$Ch_{cyc}{-}CH{=}CH_n$ (n in 1..2)	Vinylcyclopentane (1)	0.6817	−0.1192	*****	*****	*****	*****	*****	*****	*****
81	$Ch_{cyc}{-}C{=}CH_n$ (n in 1..2)	Limonene (1)	−1.0631	−0.0455	−0.2832	0.002114	−16.97	6.768	10.390	*****	*****
82	$Ch_{cyc}{-}Cl$	Chloro cyclopentane (1)	0.5124	0.2667	*****	*****	*****	*****	*****	*****	*****
83	$Ch_{cyc}{-}F$	Fluoro cyclohexane (1)	2.8497	−0.1899	*****	*****	*****	*****	*****	*****	*****
84	$Ch_{cyc}{-}OH$	Cyclohexanol (1)	1.3691	−0.3179	0.8973	0.004640	−7.73	−3.024	−8.050	2.134	*****
85	$Ch_{cyc}{-}NH_2$	Cyclohexylamine (1)	1.5069	−0.3576	−0.9610	0.000039	−2.50	2.046	3.446	−4.607	0.328
86	$Ch_{cyc}{-}NH{-}CH_n$ (n in 0..3)	*N*-methylcyclohexylamine (1)	0.0370	−0.7458	−2.0833	−0.014535	−51.50	−11.965	14.531	*****	0.402
87	$Ch_{cyc}{-}N{-}CH_n$ (n in 0..3)	*N*,*N*-dimethylcyclohexanamine (1)	*****	0.1218	*****	*****	*****	*****	*****	*****	*****
88	$Ch_{cyc}{-}SH$	Cyclohexanethiol (1)	−0.3312	−0.0569	−0.6447	−0.000199	−2.00	−16.723	−7.569	*****	−0.878
89	$Ch_{cyc}{-}CN$	Cyanocyclopentane (1)	*****	0.4649	*****	*****	*****	*****	*****	*****	*****
90	$Ch_{cyc}{-}COOH$	Cyclopropanecarboxylic acid (1)	−2.0822	0.1506	*****	*****	*****	*****	*****	*****	*****
91	$Ch_{cyc}{-}CO$	Methyl cyclohexyl ketone (1)	0.7743	0.1300	*****	*****	*****	*****	*****	−0.616	*****
92	$Ch_{cyc}{-}NO_2$	Nitrocyclohexane (1)	−0.8578	0.6540	*****	*****	*****	*****	*****	*****	*****
93	$Ch_{cyc}{-}S{-}$	Methyl cyclopentyl sulfide (1)	−0.8638	0.0043	*****	*****	*****	*****	*****	*****	*****
94	$Ch_{cyc}{-}CHO$	Cyclohexanecarboxaldehyde (1)	0.5076	−0.2692	*****	*****	*****	*****	*****	*****	*****
95	$Ch_{cyc}{-}O{-}$	Methoxycyclohexane (1)	−0.3978	−0.2787	*****	*****	*****	*****	*****	*****	*****

Table 7 (*Continued*)

	Group	Example	T_{m2j}	T_{b2j}	T_{c2j}	P_{c2j}	V_{c2j}	G_{f2j}	H_{f2j}	H_{v2j}	H_{fus2j}
96	Ch_{cyc}–OOCH	Cyclohexyl ester formic acid (1)	*****	−0.2107	*****	*****	*****	*****	*****	*****	*****
97	Ch_{cyc}–COO	Ethyl cyclobutyrate (1)	*****	0.0926	*****	*****	*****	*****	*****	*****	*****
98	Ch_{cyc}–OOC	Cyclohexyl acetate (1)	−0.4666	−0.4495	−0.3450	−0.000692	−12.03	4.358	−15.751	*****	*****
99	C_{cyc}–CH_3	1,1-Dimethyl-cyclohexane (2)	0.1737	0.0722	0.1607	0.001235	1.95	0.107	0.238	0.808	−1.237
100	C_{cyc}–CH_2	1-Ethyl-1-methyl-cyclopentane (1)	−1.9233	0.0319	0.1090	−0.000610	−5.17	18.755	21.498	0.585	*****
101	C_{cyc}–OH	1-Methylcyclopentanol (1)	0.7334	−0.6775	−2.1303	−0.004683	−14.40	−18.970	−21.975	*****	0.235
102	>N_{cyc}–CH_3	*N*-methyl-2-pyrrolidone (1)	−0.0383	0.0604	−0.0003	0.000058	*****	*****	*****	*****	*****
103	>N_{cyc}–CH_2	*N*-ethylpyrrole (1)	1.0497	−0.3080	*****	*****	*****	*****	*****	*****	*****
104	AROMRINGs^{1}s^2	2-Methyl-phenol (1), 2-Et-toluene (1)	−0.6388	−0.1590	−0.3161	0.000522	2.86	1.577	1.486	1.164	−1.470
105	AROMRINGs^{1}s^3	3-Methyl-phenol (1), 3-Et-toluene (1)	−0.6218	0.0217	−0.0693	0.001790	6.54	−1.037	0.294	−1.910	−1.059
106	AROMRINGs^{1}s^4	4-Methyl-phenol (1), 4-Et-toluene (1)	0.9840	0.1007	0.0803	0.000467	3.70	−0.709	0.384	0.331	1.244
107	AROMRINGs^{1}s^{2}s^3	1,2,3-Trimethylbenzene (1)	−0.2762	−0.1647	1.0088	−0.005598	−9.58	7.731	5.743	1.433	0.473
108	AROMRINGs^{1}s^{2}s^4	1,2,4-Trihydroxybenzene (1)	−0.3689	−0.1387	0.0908	0.000255	−2.05	−2.767	−0.449	0.313	−0.302
109	AROMRINGs^{1}s^{3}s^5	3,5-Diethyltoluene (1)	−0.3841	−0.1314	−0.6412	0.004090	−7.67	−2.148	−7.538	−0.117	−2.530
110	AROMRINGs^{1}s^{2}s^{3}s^4	3-Ethyl-1,2,4-trimethylbenzene (1)	1.7722	0.2745	2.1116	−0.007612	−7.04	14.226	12.710	*****	−1.736
111	AROMRINGs^{1}s^{2}s^{3}s^5	1,2,3,5-Tetramethylbenzene (1)	0.4553	0.1645	0.9353	−0.001811	−0.04	4.926	5.220	*****	−2.246
112	AROMRINGs^{1}s^{2}s^{4}s^5	1,2,4,5-Tetramethylbenzene (1)	2.0561	0.0754	0.6241	−0.000500	−0.04	−0.474	−1.340	*****	8.034
113	PYRIDINEs^2	2-Methylpyridine (1)	−0.5769	−0.1196	−1.0256	0.007006	8.68	−9.713	−9.644	−1.683	−0.786
114	PYRIDINEs^3	3-Methylpyridine (1)	−0.2556	0.0494	0.5784	0.007006	8.68	−2.523	−2.446	0.277	3.671
115	PYRIDINEs^4	4-Methylpyridine (1)	1.6282	0.1344	0.6595	0.001283	14.28	−4.703	−6.466	0.397	5.975
116	PYRIDINEs^{2}s^3	2,3-Dimethylpyridine (1)	−0.1341	0.0032	*****	*****	*****	*****	*****	−0.939	*****
117	PYRIDINEs^{2}s^4	2,4-Dimethylpyridine (1)	−1.6848	−0.0817	*****	*****	*****	*****	*****	−1.269	*****
118	PYRIDINEs^{2}s^5	2,5-Dimethylpyridine (1)	−0.9802	−0.1564	*****	*****	*****	*****	*****	−1.719	*****
119	PYRIDINEs^{2}s^6	2,6-Dimethylpyridine (1)	0.3018	−0.5176	−2.2773	0.008029	−50.26	−16.570	−17.778	−3.419	−1.487
120	PYRIDINEs^{3}s^4	3,4-Dimethylpyridine (1)	0.1018	0.5477	*****	*****	*****	*****	*****	1.742	*****
121	PYRIDINEs^{3}s^5	3,5-Dimethylpyridine (1)	0.2811	0.3533	*****	*****	*****	*****	*****	0.572	*****
122	PYRIDINEs^{2}s^{3}s^6	2,3,6-Trimethylpyridine (1)	−0.3189	−0.3888	*****	*****	*****	*****	*****	−2.744	*****

Table 8
Third-order groups and their contributions along with sample assignments

	Group	Example	T_{m3k}	T_{b3k}	T_{c3k}	P_{c3k}	V_{c3k}	G_{f3k}	H_{f3k}	H_{fus3k}
1	HOOC–$(CH_n)_m$–COOH ($m > 2$, n in 0..2)	1,5-Pentanedioic acid (1)	−1.5257	1.6498	−1.6986	0.001544	−3.72	−4.708	−6.572	−7.583
2	NH_n–$(CH_n)_m$–COOH ($m > 2$, n in 0..2)	4-Aminobutyric acid (1)	11.2271	*****	*****	*****	*****	*****	*****	*****
3	NH_2–$(CH_n)_m$–OH ($m > 2$, n in 0..2)	4-Aminobutanol (1)	0.7732	1.0750	0.4950	0.000728	−23.74	3.079	4.171	−4.840
4	OH–$(CH_n)_m$–OH ($m > 2$, n in 0..2)	1,9-Nonanediol (1)	0.6674	0.7193	0.1725	−0.000327	−0.84	7.536	5.411	−0.272
5	OH–$(CH_p)_k$–O–$(CH_n)_m$–OH (m, $k > 0$; p, n in 0..2)	Dipropylene glycol (1)	−0.1073	1.1867	6.6872	0.001937	1.44	−8.397	−8.651	1.661
6	OH–$(CH_p)_k$–S–$(CH_n)_m$–OH (m, $k > 0$; p, n in 0..2)	2,2′-Diethyl-dihydroxy sulfide (1)	−1.3891	*****	2.6769	0.003792	−1.62	10.194	8.164	−3.479
7	OH–$(CH_p)_k$–NHx–$(CH_n)_m$–OH (m, $k > 0$; p, n, x in 0..2)	Diethanolamine (1)	−0.0781	0.2991	*****	0.003254	−0.69	1.662	1.753	0.301
8	CH_p–O–$(CH_n)_m$–OH ($m > 2$; n, p in 0..2)	Butoxypropanol (1)	*****	−0.4605	*****	*****	*****	*****	*****	*****
9	NH_2–$(CH_n)_m$–NH_2 ($m > 2$; n in 0..2)	1,5-Diaminopentane (1)	−0.0604	0.0060	−4.3195	0.006734	6.69	4.100	0.371	5.666
10	NH_k–$(CH_n)_m$–NH_2 ($m > 2$; k in 0..1; n in 0..2)	*N*,*N*-dimethylpropylenediamine (1)	−1.1888	−0.1819	*****	*****	*****	*****	*****	*****
11	SH–$(CH_n)_m$–SH ($m > 2$; n in 0..2)	1,5-Pentanedithiol (1)	0.6669	0.4516	*****	*****	*****	*****	*****	*****
12	NC–$(CH_n)_m$–CN ($m > 2$)	Glutaronitrile (1)	−0.3798	1.3440	0.0834	−0.011090	−36.89	−7.035	7.782	−0.607
13	COO–$(CH_n)_m$–OOC ($m > 2$; n in 0..2)	Glyceryl tridodecanoate (1)	−2.6542	*****	*****	*****	*****	*****	*****	*****
14	aC–$(CH_n{=}CH_m)_{cyc}$ (fused rings) (n, m in 0..1)	Indene (1), Acenaphtylene (2)	0.2479	−0.3741	−0.0185	0.000851	−8.87	−1.601	2.689	−2.703
15	aC–aC (different rings)	Biphenylene (2), Biphenyl (1)	1.1395	−0.4961	6.1894	−0.040100	−26.26	−4.459	−4.558	−0.385
16	aC–$CH_{n,cyc}$ (different rings) (n in 0..1)	Cyclohexylbenzene (1)	0.0570	−0.4574	−0.2474	−0.005826	−8.55	−5.267	−5.914	−0.442
17	aC–$CH_{n,cyc}$ (fused rings) (n in 0..1)	Tetralin (2), Indane (2)	−0.5640	−0.1736	0.5060	−0.003746	−11.56	−4.203	−4.863	−0.143
18	aC–$(CH_n)_m$–aC (different rings) ($m > 1$; n in 0..2)	Bibenzyl (1)	1.9902	0.3138	3.0321	0.003007	9.73	1.318	0.084	5.377
19	aC–$(CH_n)_m$–CH_{cyc} (different rings) ($m > 0$; n in 0..2)	1-Cyclopentyl-3-phenylpropane (1)	*****	0.5928	*****	*****	*****	*****	*****	*****
20	CH_{cyc}–Ch_{cyc} (different rings)	Cyclohexylcyclohexane (1)	0.5460	0.4387	2.1761	0.002745	7.72	−67.517	−66.870	*****
21	CH_{cyc}–$(CH_n)_m$–CH_{cyc} (different rings) ($m > 0$; n in 0..2)	1,2-Dicyclohexylethane (1)	0.4497	0.5632	*****	*****	*****	*****	*****	*****
22	CH multiring	Hexahydroindan (2), Decalin (2)	0.6647	0.1415	0.4963	−0.000985	−3.33	*****	*****	0.223
23	C multiring	Spiropentane (1)	0.0792	*****	*****	*****	*****	*****	*****	*****
24	aC–CH_m–aC (different rings) (m in 0..2)	Diphenylmethane (1)	0.6457	0.2391	0.1174	−0.002673	−4.67	−0.729	0.866	−0.958
25	aC–$(CH_m{=}CH_n)$–aC (different rings) (m, n in 0..2)	1,2-Diphenylethylene (1)	0.9608	0.7192	0.7039	−0.004661	14.31	−0.702	−2.291	3.275
26	$(CH_m{=}C)_{cyc}$–CH=CH–$(C{=}CH_n)_{cyc}$ (different rings)	1,2-Furanyl ethene (1)	16.2235	*****	*****	*****	*****	*****	*****	*****
27	$(CH_m{=}C)_{cyc}$–CH_p–$(C{=}CH_n)_{cyc}$ (different rings)	Difuranyl methane (1)	16.8558	*****	*****	*****	*****	*****	*****	*****
28	aC–CO–aC (different rings)	Benzophenone (1)	−1.0394	1.0171	−0.2678	−0.001837	−7.05	11.125	7.108	−4.091
29	aC–CH_m–CO–aC (different rings) (m in 0..2)	Benzyl phenone (1)	−0.4486	0.9674	*****	*****	*****	*****	*****	*****
30	aC–CO–$(C{=}CH_n)_{cyc}$ (different rings) (n in 0..1)	Phenyl-2-furanyl-methanone (1)	−0.1376	0.1126	*****	*****	*****	*****	*****	*****
31	aC–CO–CO–aC (different rings)	Diphenylethanedione (1)	0.4361	0.9317	*****	*****	*****	*****	*****	−3.687
32	aC–CO_{cyc} (fused rings)	Phenolphthalein (1)	3.6847	0.5031	*****	*****	*****	*****	*****	2.047
33	aC–CO–$(CH_n)_m$–CO–aC (different rings) ($m > 0$; n in 0..2)	1,4-Diphenyl-1,4-butanedione (1)	4.9038	*****	*****	*****	*****	*****	*****	7.327
34	aC–CO–$CH_{n,cyc}$ (different rings) (n in 0..1)	Cyclohexyl phenyl methanone (1)	−7.0038	*****	*****	*****	*****	*****	*****	*****
35	aC–CO–NH_n–aC (different rings) (n in 0..1)	*N*-phenyl benzamide (1)	5.9653	*****	*****	*****	*****	*****	*****	2.510
36	aC–NH_nCONH_m–aC (different rings) (n, m in 0..1)	*N*,*N*′-diphenylurea (1)	1.5629	*****	*****	*****	*****	*****	*****	0.018
37	aC–CO–N_{cyc} (different rings)	*N*-phenonyl-piperidine (1)	−9.1856	*****	*****	*****	*****	*****	*****	*****
38	aC–S_{cyc} (fused rings)	Dibenzothiophene (2)	0.2612	0.2242	3.5541	0.004600	12.60	8.333	9.212	−0.784
39	aC–S–aC (different rings)	Diphenyl sulfide (1)	−1.8403	0.0185	*****	*****	*****	*****	*****	*****
40	aC–PO_n–aC (different rings) (n in 0..4)	Triphenylphosphate (3)	0.0393	*****	*****	*****	*****	*****	*****	*****
41	aC–SO_n–aC (different rings) (n in 1..4)	Diphenyl sulfone (1)	0.9514	−0.0850	*****	*****	*****	*****	*****	−2.485
42	aC–$NH_{n,cyc}$ (fused rings) (n in 0..1)	Carbazole (2)	3.4983	1.1457	3.5541	0.017201	0.44	−2.221	−16.080	0.196
43	aC–NH–aC (different rings)	Diphenylamine (1)	−0.3048	0.5768	0.9519	0.008484	1.42	−0.596	−1.994	1.934
44	aC–$(C{=}N)_{cyc}$ (different rings)	Phenyl-3-pyrazole (1)	−1.3060	−0.5335	*****	*****	*****	*****	*****	*****
45	aC–$(N{=}CH_n)_{cyc}$ (fused rings) (n in 0..1)	Benzoxazole (1)	−4.9289	−5.2736	*****	*****	*****	*****	*****	−0.599
46	aC–$(CH_n{=}N)_{cyc}$ (fused rings) (n in 0..1)	Benzoisoxazole (1)	−10.1007	*****	*****	*****	*****	*****	*****	*****

Table 8 (*Continued*)

	Group	Example	T_{m3k}	T_{b3k}	T_{c3k}	P_{c3k}	V_{c3k}	G_{f3k}	H_{f3k}	H_{fus3k}
47	aC–O–CH_n–aC (different rings) (n in 0..2)	Benzyl phenyl ether (1)	1.0834	0.6571	*****	*****	*****	*****	*****	*****
48	aC–O–aC (different rings)	Diphenyl ether (1)	−0.4803	−0.8252	−0.9785	0.001162	−2.63	2.668	−5.074	1.193
49	aC–CH_n–O–CH_m–aC (different rings) (n, m in 0..2)	Benzyl ether (1)	−3.2676	0.2790	−1.4002	−0.004716	28.42	−4.229	−2.303	−3.971
50	aC–O_{cyc} (fused rings)	Benzoxazole (1)	−0.3545	−0.6848	*****	*****	*****	*****	*****	−1.153
51	AROMFUSED[2]	Naphthalene (2)	0.2825	0.0441	−1.0095	−0.001332	−6.88	1.993	1.904	0.694
52	AROMFUSED[2]s^1	1-Methylnaphtalene (1)	−1.2836	−0.1666	0.1605	−0.002030	−3.17	−2.940	−2.274	−3.699
53	AROMFUSED[2]s^2	2,7-Dimethylnaphtalene (2)	0.3378	−0.2692	−0.6765	−0.002436	−3.85	−1.873	−1.316	2.037
54	AROMFUSED[2]s^2s^3	2,3-Dimethylnaphtalene (1)	1.8941	−0.2807	*****	*****	*****	*****	*****	2.150
55	AROMFUSED[2]s^1s^4	1,4-Dimethylnaphtalene (1)	−2.7585	−0.3294	*****	*****	*****	*****	*****	*****
56	AROMFUSED[2]s^1s^2	1,2-Dimethylnaphtalene (1)	−3.0362	−0.2931	*****	*****	*****	*****	*****	*****
57	AROMFUSED[2]s^1s^3	1,3-Dimethylnaphtalene (1)	−3.2228	−0.3360	*****	*****	*****	*****	*****	*****
58	AROMFUSED[3]	Phenalene (3), Pyrene (2)	1.6600	0.0402	−1.0430	0.004695	35.21	3.896	5.819	1.176
59	AROMFUSED[4a]	Anthracene (1)	7.0402	1.0466	3.3011	0.015244	−6.96	13.843	11.387	5.027
60	AROMFUSED[4a]s^1	9-Methylanthracene (1)	−3.3463	−7.8521	*****	*****	*****	*****	*****	*****
61	AROMFUSED[4a]s^1s^4	9,10-Dimethylanthracene (1)	6.8373	*****	*****	*****	*****	*****	*****	*****
62	AROMFUSED[4p]	Phenanthrene (1), Pyrene (2)	−1.5856	0.9126	2.8885	0.007280	−24.02	−16.040	−19.089	−3.417
63	AROMFUSED[4p]s^3s^4	9,10-Dimethylphenanthrene (1)	2.0821	*****	*****	*****	*****	*****	*****	*****
64	PYRIDINE.FUSED[2]	Quinoline (1)	−4.4725	−0.9432	1.1251	−0.005369	63.29	8.688	13.586	−4.967
65	PYRIDINE.FUSED[2–iso]	Isoquinoline (1)	−2.5898	−0.5844	3.9241	−0.011207	−2.71	−5.112	−0.314	−2.587
66	PYRIDINE.FUSED[4]	Acridine (1)	1.0358	0.1733	7.7134	−0.001275	−12.04	20.073	15.786	−1.365