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