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	*****	*****	*****	*****	*****	*****	*****