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