Table S5. MG method based property models analysed using simultaneous regression method: First-order groups and their contributions [a] for the properties÷ T_b, T_c, P_c, V_c, T_m, G_f, H_f, H_{fus}, $LogK_{ow}$ F_p, and H_v

	Group	T_{b1i}	T_{c1i}	P_{c1i}	V_{c1i}	T_{m1i}	G_{f1i}	H_{f1i}	H_{fus1i}	$LogK_{ow1i}$	F_{p1i}	H_{v1i}
1	CH_3	0.9218	1.0898	0.0100	63.9854	0.7555	-20.4345	-84.0390	1.1420	0.1152	33.0909	1.6141
2	CH_2	0.5780	3.4604	0.0101	56.8278	0.2966	8.1877	-20.6506	2.6516	0.4594	11.4107	4.8014
3	CH	-0.1189	4.6659	0.0107	37.2813	-0.5960	33.2787	37.6525	-0.9254	0.4300	-17.7416	5.7553
4	C	-0.6495	6.6169	0.0075	25.0561	-0.3679	66.0035	96.1819	-2.0279	0.8143	-36.6949	4.9183
5	CH_2=CH	1.4953	5.2031	0.0181	106.7610	1.0430	76.0611	23.7826	1.8927	0.2304	42.4673	-0.4710
6	CH=CH	1.2001	8.2552	0.0194	97.7190	0.6600	95.8888	82.4195	5.4232	0.4297	10.1964	-2.4067
7	CH_2=C	1.0308	7.3554	0.0176	93.6274	0.3327	91.0854	78.1789	3.1782	0.3122	6.0196	-2.9764
8	CH=C	0.7646	10.0135	0.0170	87.2150	-0.3944	114.7548	138.6480	4.3549	0.6026	-15.4082	-5.6340
9	C=C	0.4080	13.5316	0.0209	101.2116	-0.9826	142.3553	201.5682	2.7754	0.5563	-44.0014	-7.2229
10	CH_2=C=CH	2.1764	11.0144	0.0261	140.9994	1.6865	209.8955	161.8935	6.0995	****	****	11.1663
11	CH_2=C=C	1.7104	12.6575	0.0261	148.4107	1.5154	229.8483	213.1922	7.0169	****	****	****
12	C=C=C	****	****	****	****	****	****	****	****	****	****	****
13	CH≡C	1.5883	6.5964	0.0082	81.1724	2.1745	209.8823	187.1424	-1.4111	-0.2171	60.1706	6.3754
14	C≡C	1.2721	11.6977	0.0101	76.6824	1.3372	216.7880	230.2948	5.6768	0.6099	****	11.3710
15	aCH	0.7332	3.7648	0.0046	45.2515	0.6317	19.9241	-0.6732	1.4441	0.1960	18.7143	4.0975
16	aC fused with aromatic ring	1.2531	17.9650	0.0033	4.5530	2.0942	28.3757	20.2301	1.6799	0.2148	18.8824	5.7969
17	aC fused with non-aromatic	1.1611	18.2562	-0.0068	8.4391	1.6734	29.9678	13.1628	1.5330	0.1295	0.5527	5.5248
18	aC except as above	0.8317	21.0902	-0.0001	23.4172	0.9510	36.6009	49.4849	0.2638	0.2487	29.4370	6.3586
19	aN in aromatic ring	1.0507	9.5985	-0.0057	23.7909	2.0185	84.8886	54.1833	4.5449	-0.3810	49.5376	11.8029
20	aC-CH_3	1.2616	7.9731	0.0153	99.8977	1.1155	15.9981	-33.2700	3.0939	0.5432	43.3846	6.9939
21	aC-CH_2	0.8530	11.8624	0.0162	77.4668	-0.1922	43.9629	31.7820	2.3781	0.6971	24.7144	8.9948
22	aC-CH	0.0274	12.1443	0.0183	68.6439	-0.8845	60.0040	82.2207	2.2627	1.0146	-4.5611	9.0081
23	aC-C	-0.6053	7.1924	0.0215	59.4496	-1.2958	103.5315	142.8566	-0.9647	1.3668	-9.6315	13.7692
24	aC-CH=CH_2	1.8860	14.8280	0.0214	110.6358	1.3216	105.9971	64.5454	5.0190	1.2001	60.9284	****
25	aC-CH=CH	1.8784	22.0515	0.0251	100.4258	1.6683	122.8255	123.2564	5.1278	0.7694	41.6313	****
26	aC-C=CH_2	1.4167	16.6802	0.0236	94.0262	0.7823	129.5146	126.2463	4.7422	0.8764	34.6946	****
27	aC-C≡CH	1.8080	16.9729	0.0146	91.0862	1.7154	254.0264	246.7003	3.5090	0.7982	60.5521	****
28	aC-C≡C	2.0510	****	****	****	5.1689	****	****	****	1.1884	****	****
29	OH	2.2476	10.1672	-0.0071	24.4092	3.2424	-161.8492	-213.8185	3.9494	-1.3365	87.6576	23.9705
30	aC-OH	2.5461	24.0543	-0.0100	40.6785	5.1624	-140.7095	-179.2701	9.1184	-0.1125	101.859	35.6554
31	COOH	3.9741	30.6307	0.0060	78.8678	6.6986	-362.2582	-432.9967	6.4971	-1.2021	128.265	15.1359
32	aC-COOH	4.5935	43.9567	0.0112	98.4660	14.0994	-321.7557	-379.2337	20.4443	0.0375	163.982	****
33	CH_3CO	2.6907	14.1929	0.0189	132.0797	3.2535	-149.7355	-213.0782	6.2525	-0.3980	87.7425	12.8497
34	CH_2CO	1.9665	15.1201	0.0178	122.2872	2.8589	-114.0724	-154.6631	8.3352	-0.2250	63.7628	16.7382
35	CHCO	1.1925	14.7945	0.0163	94.3910	1.5650	-90.5148	-91.1938	5.9492	0.2663	****	16.1213
36	CCO	0.5925	****	****	****	1.9597	****	****	****	0.3889	****	14.5913
37	aC-CO	2.2519	29.9384	0.0136	81.0181	2.4974	-79.8262	-85.9307	4.2919	-0.1345	73.3748	22.8491
38	CHO	2.1021	11.2208	0.0045	58.6962	2.9059	-120.2465	-165.7752	9.7013	-0.9687	72.5327	12.7980
39	aC-CHO	2.6711	25.4355	0.0138	98.8795	3.1633	-89.2637	-119.3350	8.4880	-0.1943	91.5521	****
40	CH_3COO	2.6199	12.9819	0.0234	145.4135	2.3902	-323.4199	-421.5642	6.6799	-0.6609	81.5056	20.1649
41	CH_2COO	2.1182	15.6198	0.0223	134.9034	1.4259	-295.3058	-358.6780	8.4006	-0.2896	46.4475	21.0123

42	CHCOO	1.4466	15.3731	0.0238	123.9395	0.9772	-274.3717	-303.2337	7.9878	-0.3449	35.0582	21.8994
43	CCOO	0.5787	****	****	****	0.4546	****	****	****	0.4214	****	18.1851
44	HCOO	2.2249	11.5492	0.0083	90.8410	2.2831	-297.9270	-365.8808	7.3510	-0.9691	66.8687	15.4891
45	aC-COO	2.1193	20.7693	0.0172	88.6432	1.5817	-276.4139	-282.8609	5.1647	-0.0157	54.9432	23.0191
46	aC-OOCH	****	****	****	****	****	****	****	****	-0.4718	****	****
47	aC-OOC	2.0491	23.6563	0.0191	131.0658	3.6401	****	****	7.4161	-0.1516	****	****
48	COO except as above	1.5802	11.7013	0.0112	79.8771	1.3861	-277.0311	-307.1933	9.6822	-0.4116	57.9918	16.8425
49	CH_3O	1.5840	5.6587	0.0133	82.8275	1.5577	-112.7938	-195.3675	4.4580	-0.3882	53.2444	7.4551
50	CH_2O	0.9750	6.2951	0.0152	74.9171	0.6741	-101.6373	-147.7286	4.4603	-0.1205	32.8187	8.8207
51	CH-O	0.3272	5.4851	0.0263	64.3910	-0.0101	-83.3148	-98.9938	5.8192	0.1109	-19.6811	10.2962
52	C-O	-0.3387	7.4881	0.0199	52.4424	-0.2989	-37.5498	-29.5771	2.9553	1.3491	****	9.3276
53	aC-O	1.1476	13.0925	0.0074	31.4549	1.3231	-70.0222	-65.8355	1.2779	0.0450	2.3310	14.0271
54	CH_2NH_2	2.2640	12.9218	0.0068	116.9153	3.3490	47.0463	-49.1973	12.4026	-1.4619	58.6201	14.0998
55	$CHNH_2$	1.4372	11.2221	0.0125	71.5443	36.2974	65.0300	2.6744	5.0882	-1.4109	18.2867	14.5706
56	CNH_2	0.8863	11.0779	0.0142	80.9394	11.5011	85.8747	52.4495	****	-1.2313	****	12.8669
57	CH_3NH	1.9860	10.6020	0.0155	94.4478	2.7394	84.7404	-16.0110	3.2187	-0.8050	54.9961	13.4073
58	CH_2NH	1.2690	9.7528	0.0196	97.5215	2.0378	93.0289	28.5766	7.7184	-0.8698	23.2187	12.3547
59	CHNH	0.5940	8.7773	0.0109	96.3910	1.3226	99.3852	70.2062	1.2992	-0.3477	1.4689	12.4088
60	CH_3N	0.9990	8.1016	0.0192	90.6647	0.8482	121.9323	55.8439	5.6069	-0.3652	48.5699	13.2920
61	CH_2N	0.3324	7.5215	0.0311	82.2100	-0.4084	141.4133	103.5737	2.2815	-0.4084	-13.9652	8.4003
62	aC-NH_2	2.8636	27.9595	0.0020	68.4499	4.3384	58.2977	3.6661	6.0523	-0.3486	118.238	21.6806
63	aC-NH	1.8969	27.0488	-0.0026	73.5060	2.0755	110.7461	102.2474	2.4701	0.2971	54.6446	15.7481
64	aC-N	1.0680	18.8249	0.0086	96.0454	1.4958	179.8623	170.1188	3.2332	0.3297	25.8875	18.6549
65	NH_2 except as above	1.9867	9.4904	-0.0109	56.7075	3.8058	23.7639	5.1575	6.3670	-1.0653	79.3176	18.4004
66	CH=N	1.1099	****	****	****	9.2631	****	****	****	0.1306	****	****
67	C=N	0.7839	****	****	****	1.3710	****	****	****	0.7815	****	****
68	CH_2CN	3.5608	26.0349	0.0260	147.4795	2.6918	112.9462	53.6676	6.7706	-0.5195	98.3123	21.9015
69	CHCN	2.7070	21.2132	0.0267	128.5271	1.7476	137.1556	112.3365	8.1993	-0.0542	****	23.6917
70	CCN	1.7225	18.0005	0.0291	117.4941	2.8220	150.5683	127.2755	4.1660	-0.0882	43.3055	20.5769
71	aC-CN	3.0904	29.1952	0.0157	98.0862	5.1611	152.9964	151.8327	4.9390	-0.1215	****	****
72	CN except as above	2.7378	14.6309	0.0045	56.4647	3.3709	110.1491	128.0467	5.0569	0.0015	95.8883	21.1206
73	CH_2NCO	2.8854	****	****	****	****	****	****	****	****	****	****
74	CHNCO	2.2381	****	****	****	****	****	****	****	****	****	****
75	CNCO	****	****	****	****	9.8915	****	****	****	****	****	****
76	aC-NCO	2.3798	17.1127	0.0191	134.8280	2.5987	8.1264	-29.1997	****	****	****	****
77	$CH2NO_2$	3.7227	24.3223	0.0146	154.9994	2.7999	****	-102.5905	10.0398	-0.3330	116.331	29.5463
78	$CHNO_2$	2.8721	24.1207	0.0140	138.5443	0.8539	20.5327	-46.2192	****	-0.0986	80.9275	27.9017
79	CNO_2	2.1309	****	****	****	6.4251	****	-4.2455	-3.7756	0.1837	****	-39.1161
80	aC-NO_2	3.4712	33.7131	0.0123	121.4476	4.5278	43.7819	-31.2082	8.3930	0.0748	120.364	24.0833
81	NO_2 except as above	2.8709	24.3559	****	****	3.4847	****	-60.9454	5.4098	-0.4689	125.036	26.2064
82	ONO	1.7330	****	****	****	****	****	****	****	****	****	****
83	ONO_2	2.7558	****	****	****	2.5511	****	-133.8964	8.4812	-0.0640	****	****
84	$HCON(CH_2)_2$	4.4591	****	****	****	****	****	****	****	****	****	36.6521
85	$HCONHCH_2$	5.9314	****	****	****	****	****	****	****	-1.6324	****	46.3963
86	$CONH_2$	5.2882	64.8568	-0.0024	136.4310	11.8818	-147.2546	-236.6971	15.8998	-1.4315	****	****
87	$CONHCH_3$	4.2196	50.9572	0.0160	188.4310	6.5932	-122.6546	-239.9268	16.4898	-0.7471	****	47.9897

88	$CONHCH_2$	5.0238	****	****	****	4.8098	****	-179.2666	****	-0.8403	****	51.4156
89	$CON(CH_3)_2$	4.7548	36.3175	0.0316	242.4310	3.7173	-76.1546	-224.9268	10.5998	-0.5938	153.036	38.1963
90	$CONCH_3CH_2$	****	****	****	****	1.7487	****	****	****	-0.7131	****	****
91	$CON(CH_2)_2$	3.3830	****	****	****	2.1882	****	****	****	-0.0733	****	38.8180
92	CONHCO	5.7621	****	****	****	9.2737	****	****	****	-1.8911	****	****
93	CONCO	4.0044	****	****	****	3.3303	****	****	****	-0.8259	****	33.8599
94	aC-$CONH_2$	6.3135	****	****	****	14.8384	****	-176.9197	17.8290	-1.0998	****	****
95	aC-NH(CO)H	5.6658	57.2696	0.0176	141.0862	6.6017	-53.7736	-135.7997	9.6690	-0.5095	****	****
96	aC-N(CO)H	3.7475	****	****	****	3.5580	****	****	****	-0.4768	****	****
97	aC-CONH	5.4326	****	****	****	8.0247	****	****	16.1644	-0.5282	****	****
98	aC-NHCO	5.3177	****	****	****	9.4041	****	****	4.7040	-0.2305	91.5792	****
99	aC-(N)CO	****	****	****	****	6.6280	****	****	****	-0.8181	****	****
100	NHCONH	****	****	****	****	9.7180	****	****	9.4056	-1.3506	****	****
101	NH_2CONH	****	****	****	****	14.2361	****	****	13.6695	-1.3177	****	****
102	NH_2CON	****	****	****	****	11.6648	****	****	10.5200	-0.7922	****	****
103	NHCON	5.1251	****	****	****	7.9386	****	****	12.2240	-0.3600	****	****
104	NCON	2.5898	****	****	****	3.5801	****	46.6202	10.2211	-0.9818	****	****
105	aC-$NHCONH_2$	4.4036	****	****	****	18.8093	****	****	17.7190	-0.7682	****	****
106	aC-NHCONH	0.7496	****	****	****	20.9688	****	****	21.1744	-0.0756	****	****
107	NHCO except as above	****	****	****	****	4.0641	****	****	****	-0.9979	****	45.5635
108	CH_2Cl	2.2537	11.9698	0.0136	108.2855	1.9463	-45.1420	-110.0475	4.0297	0.4860	61.4828	12.4608
109	CHCl	1.4829	11.5923	0.0138	100.7734	1.1265	-28.7904	-59.5835	****	0.8969	31.7411	10.8717
110	CCl	0.8215	9.0686	0.0130	87.9394	1.3438	-7.1753	-12.4505	-0.9337	0.9630	****	8.1451
111	$CHCl_2$	2.7459	16.9228	0.0191	156.5512	2.4934	-49.6445	-120.2947	6.2575	0.8117	88.8318	17.2831
112	CCl_2	2.1307	****	****	****	3.2470	****	****	1.3969	0.9687	****	18.9721
113	CCl_3	3.1057	18.9929	0.0267	202.4310	4.2883	-63.8646	-142.2268	2.5398	1.5932	****	17.9505
114	CH_2F	1.5154	6.6904	0.0121	85.4310	1.6657	-199.9546	-264.3268	6.1898	-0.1018	****	8.7998
115	CHF	****	5.2651	-0.0269	****	-0.2090	****	****	****	-0.1733	****	****
116	CF	****	****	****	****	****	****	****	****	****	****	****
117	CHF_2	1.6440	6.2516	0.0201	88.5150	1.9149	-430.9546	-500.7268	6.0598	1.0622	****	9.4149
118	CF_2	0.3991	2.3528	0.0096	94.3249	0.3514	****	****	****	0.7829	****	4.0020
119	CF_3	1.1119	1.1505	0.0388	104.5703	1.1548	-630.5845	-708.6621	2.7118	0.7518	****	1.8678
120	CCl_2F	2.1787	9.2817	0.0213	167.3950	3.3365	-272.1993	-341.0621	2.5541	1.5051	****	7.6163
121	HCClF	1.8171	****	****	****	1.2161	****	****	****	0.4974	****	10.8681
122	$CClF_2$	1.5077	5.3324	0.0337	143.0217	1.8010	-416.6797	-502.1936	1.2142	0.9896	****	10.0948
123	aC-Cl	1.6649	16.8708	0.0106	76.7178	1.9911	-8.7977	-27.4387	5.4034	0.8081	65.1890	10.1842
124	aC-F	0.6830	2.8682	0.0099	52.7142	0.9216	-176.9036	-173.3276	1.8430	0.3064	****	4.3095
125	aC-I	2.9439	34.1338	0.0105	110.0862	2.6445	82.3264	84.3003	3.8090	0.8562	****	****
126	aC-Br	2.2390	17.4668	0.0064	76.8793	2.6398	33.9317	28.1830	6.6370	0.9233	80.6631	13.6133
127	-I except as above	2.6522	17.5551	0.0015	100.6734	2.3998	33.5620	19.9974	5.3497	0.5399	****	14.3642
128	-Br except as above	2.0281	11.7182	-0.0045	74.1998	2.0416	-16.2205	-41.4766	3.1165	0.2971	72.8523	9.8075
129	-F except as above	0.7179	-0.3199	0.0132	23.0339	0.8649	-206.2543	-289.2168	3.8168	-0.0005	****	-3.3490
130	-Cl except as above	1.3561	5.2618	0.0038	56.6942	1.4163	-54.4633	-88.5982	4.5154	0.0896	33.3408	6.0183
131	CHNOH	3.7479	****	****	****	4.0756	****	****	****	-0.2921	****	****
132	CNOH	3.1107	****	****	****	4.0968	****	****	****	-0.6688	****	****
133	aC-CHNOH	****	****	****	****	9.4614	****	****	****	-0.1853	****	****

134	OCH_2CH_2OH	3.8181	19.6026	0.0183	155.8593	2.4297	-256.7970	-385.5345	6.8430	-1.1960	131.271	31.2064
135	$OCHCH_2OH$	3.1220	****	****	****	10.9421	****	****	****	-0.6443	****	****
136	OCH_2CHOH	2.9869	17.9260	0.0185	146.6521	1.7527	-219.5128	-314.0364	11.9899	-0.7404	****	****
137	-O-OH	2.9996	10.9856	-0.0037	52.9544	4.1968	****	-166.8624	****	****	21.8059	****
138	CH_2SH	2.5879	16.1803	0.0115	106.0166	2.1851	6.9435	-46.5497	8.3721	0.3193	66.4735	15.1089
139	CHSH	1.8393	15.0348	0.0092	104.5443	0.5814	31.1527	11.0465	3.0682	-0.0226	****	15.7706
140	CSH	1.1874	15.2220	0.0097	94.9394	4.7552	58.0047	63.0195	-0.5437	0.6687	****	14.8015
141	aC-SH	2.5228	25.5444	0.0070	94.1050	3.0328	39.7264	30.9003	5.5190	0.3323	****	16.6333
142	-SH except as above	2.0774	13.1905	-0.0079	68.4257	2.6727	-3.1011	-19.2417	5.8759	0.1163	****	11.0794
143	CH_3S	2.5029	14.4849	0.0126	117.9143	1.8635	12.2115	-40.4012	6.6582	0.3952	55.8869	14.2894
144	CH_2S	1.9548	16.7752	0.0138	108.2180	0.8881	34.4285	12.9621	3.8234	0.5640	****	15.7534
145	CHS	1.2626	****	****	****	0.5935	****	****	****	0.9271	****	16.6865
146	CS	0.6391	****	****	****	1.5882	****	****	****	1.7367	****	15.2424
147	aC-S-	1.7834	28.7804	0.0093	****	0.9894	****	****	****	0.6474	****	****
148	SO	4.7622	53.1166	-0.0023	84.4107	5.3103	-49.0917	-66.3478	12.9969	-1.1205	144.796	****
149	SO_2	5.0639	48.1596	0.0032	89.2717	6.4215	-255.0761	-301.6848	17.3369	-0.5708	****	****
150	SO_3 (sulfite)	2.8972	21.9226	0.0072	116.7550	****	****	-426.4866	****	0.1555	****	****
151	SO_3 (Sulfonate)	5.0139	****	****	****	5.9382	****	****	****	-1.2153	****	****
152	SO_4 (Sulfate)	4.1394	50.7355	-0.0207	146.0830	3.7901	-516.8267	-616.8872	****	-0.7612	139.035	****
153	aC-SO	4.3678	****	****	****	4.9397	****	****	****	-0.5474	****	****
154	aC-SO_2	****	****	****	119.9644	4.3705	-306.4516	-345.7812	3.2803	-0.7439	****	****
155	PH (phosphine)	****	****	****	****	****	****	****	****	****	****	****
156	P (Phospine)	0.7096	****	****	****	0.0729	****	****	****	****	****	****
157	PO_3 (Phospite)	1.7858	****	****	****	****	****	****	****	-1.5939	****	****
158	PHO_3 (Phosponate)	4.2814	****	****	****	-0.9347	****	****	****	-2.1734	****	****
159	PO_3 (Phosponate)	2.8787	****	****	****	0.4993	****	****	****	-0.8413	****	****
160	PHO_4 (Phospate)	****	****	****	****	2.3569	****	****	****	-1.9393	****	****
161	PO_4 (Phospate)	2.5427	49.3085	****	91.1666	1.9244	****	-1014.5970	****	-1.5680	88.4741	****
162	aC-PO_4	****	****	****	****	-2.2355	****	-930.1374	8.6616	-0.6473	7.2252	****
163	aC-P	****	158.1177	****	-186.3333	0.1950	****	147.3626	-1.2584	1.0544	****	****
164	CO_3 (Carbonate)	2.2078	16.9427	0.0145	104.0830	2.7606	-434.3517	-513.6866	11.0669	-0.9028	****	20.3300
165	C_2H_3O	2.7140	13.5385	0.0118	122.4399	1.5194	-17.0936	-167.9292	****	-0.6951	74.9195	15.5756
166	C_2H_2O	1.7850	15.4180	0.0077	192.5740	-2.0258	-0.5394	****	****	****	43.4273	****
167	C_2HO	****	****	****	****	-0.3680	****	****	****	0.1716	****	****
168	CH_2 (cyclic)	0.7147	3.6308	0.0068	48.7395	0.5313	8.7292	-29.2709	0.9905	0.1646	17.9616	3.6900
169	CH (cyclic)	0.4137	4.7661	0.0065	38.8249	-0.1298	0.9855	-72.8957	0.8855	0.4600	7.5875	4.8950
170	C (cyclic)	-0.3809	3.6886	0.0081	39.2170	0.1322	24.3604	116.3572	2.1359	0.6366	-24.2854	3.4363
171	CH=CH (cyclic)	1.3771	6.4667	0.0091	83.8235	1.2254	75.1097	37.0718	1.0124	0.2761	26.9856	7.4405
172	CH=C (cyclic)	0.9247	9.1574	0.0087	74.9435	0.8270	63.4709	41.6830	3.7399	0.6105	33.0981	5.9475
173	C=C (cyclic)	0.6624	****	****	****	1.0683	****	****	****	0.8714	****	****
174	CH_2=C (cyclic)	1.2533	10.0641	0.0120	85.4343	0.8039	****	****	4.1053	-0.1397	28.9457	3.9756
175	NH (cyclic)	1.7013	9.1560	-0.0051	48.0002	4.0385	67.3973	24.7863	6.9466	-0.6511	65.6901	16.1331
176	N (cyclic)	1.1003	7.2820	-0.0042	31.1881	0.5618	86.2105	87.1284	-1.2058	-0.4759	49.4879	****
177	CH=N (cyclic)	5.5397	24.3788	0.0353	****	4.9854	****	42.0845	4.1633	-0.2166	****	12.1611
178	C=N (cyclic)	4.9400	****	****	****	5.7227	****	27.9418	****	0.3032	****	****
179	O (cyclic)	0.8846	6.3360	-0.0021	16.3127	1.3472	-123.3599	-147.1515	3.1984	-0.5295	31.0579	6.5706

180	CO (cyclic)	2.2024	33.8819	-0.0025	54.3917	3.3615	-169.6483	-208.3909	4.9552	-0.3100	83.2582	18.2291
181	S (cyclic)	1.8863	11.8977	-0.0024	39.1695	1.7124	-16.8568	-4.2069	4.5015	0.2996	****	13.1644
182	SO_2 (cyclic)	****	68.0095	-0.0014	91.1026	5.7787	-264.2897	-318.0956	8.7491	-0.9653	****	****
183	>NH	****	****	****	****	1.7669	****	****	****	-0.4627	****	****
184	-O-	1.1379	10.6443	0.0011	24.7209	0.6836	-112.0890	****	0.2581	-0.1556	-8.8090	****
185	-S-	1.1954	****	****	****	2.1318	****	****	****	0.7433	****	****
186	>CO	1.0955	****	****	****	1.6089	****	****	****	-0.1157	****	12.4620
187	PO_2	1.3468	****	****	****	****	****	****	****	****	****	****
188	CH-N	0.0212	****	****	****	-0.1632	****	****	****	-0.3074	****	****
189	SiHO	0.0296	****	****	****	-0.8740	****	****	****	****	****	****
190	SiO	-0.3420	****	****	****	-1.4431	****	****	****	0.4349	-43.1666	****
191	SiH_2	0.9301	****	****	****	0.3230	****	****	****	****	****	****
192	SiH	0.2832	****	****	****	0.1946	****	****	****	1.1489	-6.8441	****
193	Si	-0.4468	7.8493	0.0268	****	0.6939	****	****	****	1.9372	-34.2494	****
194	$(CH_3)_3N$	****	****	****	****	****	****	****	****	****	****	****
195	N=N	****	****	****	****	-1.6010	****	181.9486	****	-0.4715	****	15.7447
196	C_{cyclic}=N-	1.2598	****	****	****	0.7097	****	203.4075	****	0.2718	****	****
197	C_{cyclic}=CH-	0.9120	****	****	****	0.1177	****	****	****	0.2950	****	10.7613
198	C_{cyclic}=NH	****	****	****	****	****	****	****	****	-0.4757	****	****
199	N=O	3.0538	****	****	****	1.6530	****	****	****	-0.3601	****	15.2480
200	C_{cyclic}=C	0.4266	17.0856	0.0171	****	0.1965	****	****	****	0.7928	****	****
201	P=O	****	****	****	****	4.2169	****	****	****	-0.5399	****	****
202	N=N	****	****	****	****	0.2488	****	253.6044	****	0.8576	****	7.3987
203	C=NH	****	****	****	****	3.8635	****	****	****	-0.0351	****	****
204	>C=S	****	****	****	****	2.7979	****	99.3628	****	0.5259	****	****
205	aC-CON	****	****	****	****	8.9197	****	****	****	-1.1599	****	****
206	aC=O	****	****	****	****	4.6063	****	****	0.6430	-0.4841	****	****
207	aN-	****	****	****	****	1.7679	****	226.6172	****	-1.7973	****	****
208	-Na	****	****	****	****	****	****	****	****	****	****	****
209	-K	****	****	****	****	****	****	****	****	****	****	****
210	HCONH	****	****	****	****	9.8261	****	****	****	-0.9709	****	44.1463
211	CHOCH	****	****	****	****	0.8353	****	****	****	****	****	****
212	C_2O	****	****	****	****	****	****	****	****	****	****	****
213	SiH_3	****	****	****	****	****	****	****	****	****	****	****
214	SiH_2O	****	****	****	****	****	****	****	****	****	****	****
215	CH=C=CH	****	****	****	****	****	****	****	****	****	****	****
216	CH=C=C	****	****	****	****	****	****	****	****	****	****	****
217	OP(=S)O	****	****	****	****	****	****	****	****	****	****	****
218	R	****	****	****	****	****	****	****	****	****	****	****
219	$CF_{2cyclic}$	0.5117	****	0.0106	****	0.8727	****	****	****	0.5911	****	4.6026
220	CF_{cyclic}	0.4264	****	****	****	-0.8641	****	****	****	0.2909	****	-0.8287

[a] The symbols T_{b1i}, T_{c1i}, P_{c1i}, V_{c1i}, T_{m1i}, G_{f1i}, H_{f1i}, H_{fus1i}, $LogK_{ow1i}$, F_{p1i}, and H_{v1i}, represent the contributions (C_i) of the first-order groups for the corresponding properties

Table S5 (Continued). MG method based property models analysed using simultaneous regression method: First-order groups and their contributions [a] for the properties÷ H_{vb}, S_{vb}, δ_D, δ_P, δ_H, δ, AiT, ω and V_m

	Group	H_{vb1i}	S_{vb1i}	δ_{D1i}	δ_{P1i}	δ_{H1i}	δ_{1i}	$AiT1_{1i}$	$AiT2_{1i}$	ω_{1i}	V_{m1i}
1	CH_3	2.3797	-0.4840	7.5983	2.3037	2.2105	-1.8029	-0.3516	-57.8605	0.0017	0.0238
2	CH_2	2.3004	0.6423	-0.0023	-0.1664	-0.2150	-0.1323	0.1009	2.6047	0.0019	0.0166
3	CH	1.6577	0.6894	-7.5390	-3.3851	-2.6826	1.0139	0.5829	79.2115	0.0029	0.0084
4	C	0.6634	-0.1297	-15.6455	-5.1979	-6.4821	1.2449	0.6668	95.9781	0.0008	-0.0015
5	CH_2=CH	3.6704	0.3739	7.7504	3.6752	2.7673	-2.1839	-0.2295	-72.0187	0.0027	0.0333
6	CH=CH	3.6489	0.1313	0.4284	3.0492	0.8631	-0.3708	0.0768	-116.5855	0.0046	0.0244
7	CH_2=C	3.2053	0.5815	0.1956	2.3059	1.0623	-0.8300	0.0794	-44.1695	0.0020	0.0230
8	CH=C	4.7812	1.9897	-7.0086	1.2790	-0.1204	1.6192	0.5499	-66.0852	0.0036	0.0108
9	C=C	5.0939	3.0012	-14.6160	-1.4590	-2.9995	2.7550	0.8132	11.7928	0.0007	-0.0021
10	CH_2=C=CH	6.5451	1.2959	7.7662	2.2910	3.6733	-2.7895	****	****	0.0037	0.0431
11	CH_2=C=C	****	****	-0.0965	-2.1075	0.0791	-1.3229	****	****	0.0020	0.0365
12	C=C=C	****	****	****	****	****	****	****	****	****	****
13	CH≡C	5.8019	3.2387	7.7801	3.0384	3.7484	-1.3175	-0.8833	-	0.0034	0.0263
14	C≡C	7.6846	4.8196	-0.0503	-0.5528	1.9582	1.0184	****	****	0.0034	0.0159
15	aCH	2.5866	0.1971	3.1133	0.9190	0.7694	-0.0782	-0.1131	-5.1387	0.0013	0.0120
16	aC fused with aromatic ring	4.7372	2.2507	-3.0510	-1.1299	-2.7569	-0.1111	-34.8062	-54.7826	-0.0014	0.0046
17	aC fused with non-aromatic ring	3.4588	1.5553	-4.4881	-0.3554	-2.6898	-1.2301	23.2758	-2.4889	-0.0004	0.0035
18	aC except as above	****	****	-6.6777	-3.0946	-1.4992	-1.2037	-1.9551	-5.7471	0.0016	0.0071
19	aN in aromatic ring	8.0608	9.8797	3.4095	5.9010	3.9266	-0.8197	-0.0832	-62.5438	0.0008	0.0052
20	aC-CH_3	4.1963	-0.8843	3.0811	-1.1846	0.1713	-0.5759	-0.3481	-214.5329	0.0031	0.0302
21	aC-CH_2	4.5211	1.0856	-5.0406	-4.1990	-3.1805	-0.0100	0.1472	-51.0665	0.0042	0.0229
22	aC-CH	****	****	-13.6223	-5.2318	-7.0890	-0.3146	0.5689	19.7360	0.0020	0.0162
23	aC-C	5.6746	3.4909	-21.2544	-8.0888	-7.8370	1.2302	0.6880	-28.5784	0.0015	0.0095
24	aC-CH=CH_2	10.6661	7.6835	3.0147	-2.4385	1.0566	-1.0365	-0.9888	-	0.0044	0.0409
25	aC-CH=CH	****	****	-4.6886	-2.0934	-3.6608	0.1657	9.8720	364.5115	0.0056	0.0287
26	aC-C=CH_2	****	****	****	****	****	-0.1801	0.1098	-43.9833	0.0040	0.0297
27	aC-C≡CH	****	****	3.2337	-1.7949	0.1531	-1.5935	-0.0661	-42.2879	0.0009	0.0347
28	aC-C≡C	****	****	-4.3549	****	-2.9946	-0.6637	****	****	0.0007	0.0413
29	OH	17.3709	21.1170	8.0503	5.2379	11.8005	3.0524	-0.1516	32.3056	0.0180	0.0042
30	aC-OH	15.8230	12.8929	3.3399	1.3244	7.7635	1.9054	-0.3393	-153.1902	0.0119	0.0170
31	COOH	****	****	8.4172	3.1400	7.5917	3.6819	0.0375	120.0741	0.0206	0.0207
32	aC-COOH	****	****	3.0852	0.9871	4.5546	2.1528	-0.3866	-293.2920	0.0218	0.0478
33	CH_3CO	8.9922	2.8550	8.1107	6.3823	3.4394	0.4030	0.1335	119.8078	0.0077	0.0347
34	CH_2CO	9.9376	4.9255	0.5371	1.2706	-0.0788	0.7468	0.1214	94.5070	0.0080	0.0283
35	CHCO	9.1129	4.9603	****	****	****	2.5361	****	****	0.0091	0.0199
36	CCO	2.0596	-7.9027	-15.7596	****	****	0.6865	****	****	0.0012	0.0281
37	aC-CO	****	****	-3.8648	0.0858	-0.8306	1.3457	8.4848	260.6371	0.0089	0.0208
38	CHO	8.7662	4.9348	7.8411	7.8726	5.3761	1.4631	0.4254	-30.4259	0.0079	0.0167
39	aC-CHO	****	****	3.7273	3.7488	2.3964	1.2651	6.0646	-33.3858	0.0102	0.0187
40	CH_3COO	13.5533	8.9566	8.1606	2.0405	5.0132	-0.3355	-0.1427	76.0028	0.0111	0.0423
41	CH_2COO	13.1456	9.5467	0.5148	0.2595	2.7824	1.1235	0.1089	110.1176	0.0109	0.0364

42	CHCOO	10.0655	6.4184	-7.2639	-2.8697	-1.1517	2.1116	0.5128	162.2212	0.0087	0.0284
43	CCOO	8.7002	5.7309	-13.1897	-13.7021	-10.5735	****	****	****	0.0092	0.0224
44	HCOO	10.9176	8.7201	7.9230	4.8158	6.8448	-0.1553	-0.3396	-62.1878	0.0086	0.0256
45	aC-COO	15.3658	16.3010	-5.0497	-0.3862	-0.5041	1.3267	0.2576	76.3038	0.0075	0.0312
46	aC-OOCH	****	****	****	****	****	****	****	****	****	****
47	aC-OOC	****	****	-3.6494	-2.0901	-0.0219	1.6265	****	****	0.0091	0.0249
48	COO except as above	10.4710	7.4628	0.4220	2.2043	2.6377	2.4779	0.3262	213.8562	0.0152	0.0196
49	CH_3O	5.8379	1.7348	7.6317	3.2154	3.3464	-1.3922	-0.1637	-64.8653	0.0055	0.0281
50	CH_2O	4.9874	2.8233	0.1706	0.5137	0.8246	0.0991	0.3876	15.7001	0.0064	0.0228
51	CH-O	4.0605	3.6325	-7.6174	-2.7093	-2.1543	0.5968	0.3381	82.8063	0.0030	0.0205
52	C-O	2.8917	1.8475	****	****	****	2.1448	****	****	0.0037	0.0049
53	aC-O	8.5679	6.9671	-4.4171	-1.2975	0.0149	1.8991	1.3612	-25.1637	0.0068	0.0084
54	CH_2NH_2	9.6773	5.7817	8.1995	5.2101	6.7984	0.3355	0.0522	36.9000	0.0104	0.0262
55	$CHNH_2$	8.1069	7.0637	-0.3812	0.5616	2.8953	1.8389	50.4249	235.1768	0.0101	0.0214
56	CNH_2	8.1526	10.6406	****	****	****	0.2906	****	****	0.0053	0.0144
57	CH_3NH	9.4451	7.0907	7.7307	2.5065	7.2551	-0.2982	34.8042	220.7430	0.0071	0.0279
58	CH_2NH	6.6499	3.3224	0.0223	-0.7159	1.4183	0.2836	0.2006	14.3974	0.0096	0.0246
59	CHNH	5.0623	2.7686	-7.5377	-4.6694	-2.2824	1.1362	0.7001	67.2698	0.0091	0.0182
60	CH_3N	3.2572	1.9902	0.3494	-0.4250	2.4585	-0.4539	13.4754	57.8333	0.0049	0.0265
61	CH_2N	5.2316	5.2118	-6.7232	-0.7354	-7.3014	0.0284	1.2799	120.7779	0.0067	0.0190
62	$aC\text{-}NH_2$	13.1059	6.6437	4.3726	1.9767	6.3616	1.9769	-0.1176	9.8937	0.0096	0.0260
63	aC-NH	****	****	-3.9623	-2.6745	3.2590	0.2889	-0.0471	-212.9195	0.0089	0.0118
64	aC-N	****	****	****	****	****	1.4103	1.0105	132.0401	0.0049	0.0190
65	NH_2 except as above	11.6741	9.8812	9.0936	6.3555	9.0778	5.1519	0.2561	-2.1921	0.0066	0.0096
66	CH=N	****	****	****	****	****	****	****	****	****	****
67	C=N	****	****	-8.1282	-3.2229	-3.1673	-5.1194	****	****	****	****
68	CH_2CN	14.2018	2.7796	8.5643	10.8264	3.3144	3.0873	-0.0555	146.0208	0.0123	0.0314
69	CHCN	13.0032	3.1950	1.3130	4.1991	1.7584	4.4365	****	****	0.0116	0.0254
70	CCN	10.6693	2.2812	-7.7575	-0.8832	0.4757	4.0573	0.2795	2.3359	0.0069	0.0211
71	aC-CN	17.8661	14.1320	3.4370	4.8030	0.6067	1.3967	****	****	0.0085	0.0294
72	CN except as above	12.3216	1.1962	8.1538	9.6317	1.9219	1.2762	-0.3003	9.1856	0.0071	0.0158
73	CH_2NCO	****	****	7.8017	9.6963	0.2895	****	****	****	0.0122	0.0402
74	CHNCO	****	****	****	****	****	****	****	****	****	****
75	CNCO	****	****	****	****	****	****	****	****	****	****
76	aC-NCO	****	****	3.4988	1.1837	1.8845	0.0056	****	****	0.0092	0.0325
77	$CH2NO_2$	19.6283	13.0219	8.9178	11.3660	3.1398	0.8521	59.6801	194.5951	0.0131	0.0330
78	$CHNO_2$	17.4132	10.8352	0.8885	6.5226	0.8294	3.5365	0.1970	42.1198	0.0134	0.0249
79	CNO_2	-24.0533	-4.1948	-6.8570	0.3445	-0.5293	-4.4203	****	****	-0.0083	0.0504
80	$aC\text{-}NO_2$	****	****	3.7302	2.8689	1.2032	1.1883	0.5271	173.0964	0.0123	0.0308
81	NO_2 except as above	16.5635	7.4912	7.5368	3.8857	2.9346	0.8944	-0.0279	13.3422	0.0132	0.0180
82	ONO	****	****	****	****	****	****	****	****	****	****
83	ONO_2	****	****	8.0032	7.4830	2.7871	0.1194	2.1376	-22.3503	0.0157	0.0280
84	$HCON(CH_2)_2$	****	****	0.7580	5.8753	1.6091	4.5168	****	****	****	****
85	$HCONHCH_2$	****	****	9.6017	7.6963	11.7895	9.2857	****	****	****	****
86	$CONH_2$	****	****	9.0888	9.0329	10.6398	11.2741	****	****	0.0148	0.0147
87	$CONHCH_3$	****	****	7.4017	1.9963	3.4895	8.0908	****	****	0.0160	0.0380

88	$CONHCH_2$	****	****	****	****	****	8.0168	****	****	****	****
89	$CON(CH_3)_2$	****	****	9.0040	8.9127	6.8046	3.2384	0.0473	15.4733	0.0124	0.0533
90	$CONCH_3CH_2$	****	****	****	****	****	****	****	****	****	****
91	$CON(CH_2)_2$	****	****	-6.3948	4.3888	0.8686	5.0479	****	****	****	****
92	CONHCO	****	****	****	****	****	****	****	****	****	****
93	CONCO	****	****	****	****	****	****	****	****	****	****
94	$aC\text{-}CONH_2$	****	****	5.6337	10.1051	7.3531	****	****	****	0.0175	0.0349
95	aC-NH(CO)H	****	****	****	****	****	4.3137	****	****	0.0168	0.0353
96	aC-N(CO)H	****	****	****	****	****	****	****	****	****	****
97	aC-CONH	****	****	****	****	****	****	****	****	****	****
98	aC-NHCO	****	****	-4.0045	4.0298	3.8028	1.8432	-0.3394	-924.4939	0.0179	0.0326
99	aC-(N)CO	****	****	****	****	****	3.8786	****	****	****	****
100	NHCONH	****	****	****	****	****	****	****	****	****	****
101	NH_2CONH	****	****	10.9112	5.5671	8.1602	****	****	****	****	****
102	NH_2CON	****	****	****	****	****	****	****	****	****	****
103	NHCON	****	****	****	****	****	****	****	****	****	****
104	NCON	****	****	-13.6930	-1.0149	2.1581	8.3790	****	****	****	****
105	$aC\text{-}NHCONH_2$	****	****	****	****	****	****	****	****	****	****
106	aC-NHCONH	****	****	****	****	****	****	****	****	****	****
107	NHCO except as above	****	****	****	****	****	****	****	****	****	****
108	CH_2Cl	9.1122	3.1362	8.8569	4.3288	2.1489	-0.0226	-0.3251	-7.3040	0.0041	0.0317
109	CHCl	6.1613	1.0093	0.6805	2.4897	-0.5733	-0.0418	-1.1691	-	0.0036	0.0267
110	CCl	3.2834	0.4579	-7.3725	0.7705	-6.9931	0.7536	****	****	0.0015	0.0188
111	$CHCl_2$	11.3784	3.5583	9.2349	3.3634	2.5206	-0.4749	23.7818	279.1836	0.0043	0.0448
112	CCl_2	****	****	1.0669	1.0329	-1.4311	0.5181	****	****	****	****
113	CCl_3	12.3064	2.4613	9.9021	2.0681	0.1333	-1.9254	-0.3384	-6.9506	0.0037	0.0621
114	CH_2F	9.1503	10.1686	7.3856	4.3614	-1.2477	-0.7769	****	****	0.0050	0.0251
115	CHF	****	****	-0.0751	-1.0634	-0.2549	****	****	****	-0.0027	0.0193
116	CF	****	****	****	****	****	****	****	****	****	****
117	CHF_2	****	****	7.6277	6.0103	1.0771	-2.7521	****	****	0.0050	0.0349
118	CF_2	2.3658	0.7630	-0.7251	****	****	-0.5348	****	****	0.0007	0.0252
119	CF_3	1.0289	-0.6317	7.8128	3.1133	2.0149	-3.7366	****	****	0.0095	0.0412
120	CCl_2F	4.2921	-2.2831	7.0790	-1.0631	****	-3.1637	****	****	0.0040	0.0567
121	HCClF	6.9857	2.3493	7.7475	0.3389	3.8252	-2.6893	-0.2184	32.3070	0.0035	0.0398
122	$CClF_2$	7.4432	2.6054	6.5642	1.2526	****	-3.6482	-0.4535	-18.0351	0.0044	0.0546
123	aC-Cl	5.9998	-0.2357	3.6334	0.5595	0.6238	-0.1939	-0.3539	-188.8730	0.0030	0.0258
124	aC-F	2.7989	0.9716	2.9653	0.4144	0.2767	-0.6712	****	****	0.0026	0.0167
125	aC-I	****	****	3.9337	1.4051	2.2531	0.0471	****	****	0.0019	0.0361
126	aC-Br	****	****	4.0118	1.7621	1.6744	-0.0395	-0.1804	-59.0137	0.0026	0.0300
127	-I except as above	9.7527	-4.1295	9.2913	2.8794	3.7401	0.5685	****	****	0.0018	0.0246
128	-Br except as above	6.5560	0.9157	9.2791	3.3944	2.9788	-0.4249	-0.4514	-94.6302	0.0020	0.0213
129	-F except as above	-0.3582	-0.4755	6.4464	4.7756	5.1354	-1.2592	-0.6446	-173.0902	0.0017	0.0123
130	-Cl except as above	6.2737	2.5943	8.0525	2.7611	1.8748	-0.7342	-0.5500	-151.2099	0.0018	0.0181
131	CHNOH	****	****	8.7017	1.6963	17.9895	****	****	****	0.0262	0.0227
132	CNOH	****	****	0.3046	-0.2243	5.0366	****	****	****	****	****
133	aC-CHNOH	****	****	****	****	****	****	****	****	****	****

134	OCH_2CH_2OH	21.6722	14.5475	8.3027	5.7113	9.9562	2.3257	47.4817	30.5117	0.0213	0.0417
135	$OCHCH_2OH$	****	****	0.3121	-1.5734	5.1167	****	****	****	0.0279	0.0381
136	OCH_2CHOH	****	****	0.0881	0.7182	4.8512	4.2940	****	****	0.0225	0.0392
137	-O-OH	****	****	7.4017	12.6963	27.7895	5.2932	****	****	0.0257	0.0104
138	CH_2SH	9.9537	2.4892	8.5494	3.8374	4.2415	-0.4082	-0.0764	-87.3884	0.0042	0.0341
139	CHSH	8.4819	2.4729	1.3616	1.9228	2.2675	0.0341	****	****	0.0035	0.0289
140	CSH	6.7795	1.2260	****	****	****	0.3420	****	****	0.0021	0.0216
141	aC-SH	11.8961	5.4663	4.4582	0.0702	4.5741	0.7639	****	****	0.0027	0.0269
142	-SH except as above	8.2684	2.2265	8.7339	2.5118	6.0326	0.8350	****	****	0.0022	0.0161
143	CH_3S	9.6582	2.4728	8.8002	3.6190	3.2506	-0.5579	10.4369	11.5754	0.0037	0.0356
144	CH_2S	9.1184	2.8496	0.7294	-0.0130	0.1251	0.8547	****	****	0.0047	0.0294
145	CHS	7.8976	3.7003	****	****	****	****	****	****	****	0.0717
146	CS	4.7265	-0.3659	****	****	****	****	****	****	0.0036	0.0133
147	aC-S-	****	****	-3.5646	-2.0986	-1.3574	****	****	****	0.0053	0.0317
148	SO	****	****	1.7892	7.4639	3.7447	9.5655	6.3266	78.1180	0.0019	0.0143
149	SO_2	****	****	1.6660	8.4335	-0.3325	4.2270	****	****	0.0070	0.0237
150	SO_3 (sulfite)	****	****	****	****	****	2.0409	****	****	0.0141	0.0314
151	SO_3 (Sulfonate)	****	****	0.8540	2.5127	2.8046	****	****	****	-0.0042	0.0552
152	SO_4 (Sulfate)	****	****	1.5058	11.4089	4.1941	4.1431	7.2272	185.8736	0.0074	0.0341
153	aC-SO	****	****	-3.7969	6.4368	-1.0695	****	****	****	****	****
154	aC-SO_2	****	****	-3.2918	9.0285	-0.3191	-11.2009	****	****	****	****
155	PH (phosphine)	****	****	****	****	****	****	****	****	****	****
156	P (Phospine)	****	****	-5.7575	-4.6832	****	****	****	****	0.0024	0.0192
157	PO_3 (Phospite)	****	****	****	****	****	2.5231	****	****	****	****
158	PHO_3 (Phosponate)	****	****	****	****	****	8.4168	****	****	****	****
159	PO_3 (Phosponate)	****	****	-6.0459	5.4504	0.6291	****	****	****	****	****
160	PHO_4 (Phospate)	****	****	****	****	****	****	****	****	****	****
161	PO_4 (Phospate)	****	****	-6.3010	4.3366	2.1176	3.6003	0.1377	74.6000	0.0107	0.0314
162	aC-PO_4	****	****	-13.4419	1.7377	-1.7608	-0.1182	4.8253	66.4905	0.0190	0.0609
163	aC-P	****	****	****	****	****	1.3236	****	****	-0.0039	0.0346
164	CO_3 (Carbonate)	****	****	0.1058	0.6589	2.3941	2.2994	****	****	0.0124	0.0231
165	C_2H_3O	10.5281	6.8989	9.5480	4.6184	7.9801	0.9020	-0.8075	-210.2024	-0.0038	0.0285
166	C_2H_2O	****	****	4.6310	4.0936	2.0651	0.2605	-2.2121	-73.3599	0.0016	0.0290
167	C_2HO	****	****	****	****	****	****	****	****	****	****
168	CH_2 (cyclic)	2.3438	-0.0399	2.6693	0.5104	0.6159	-0.3085	0.0198	-3.1112	0.0009	0.0160
169	CH (cyclic)	2.2834	0.6520	-3.6903	-3.2065	-0.5171	-0.6304	0.0719	15.8622	-0.0078	0.0059
170	C (cyclic)	3.0140	4.0775	-10.2229	-2.6202	-2.6329	1.4521	-0.5077	79.6787	-0.0002	0.1393
171	CH=CH (cyclic)	4.8318	1.2589	7.1860	0.7482	1.9775	-0.7844	-0.4279	-49.4820	0.0024	0.0246
172	CH=C (cyclic)	6.2169	4.4891	-1.1666	3.3074	-1.5025	1.1486	0.2903	33.1340	0.0059	0.0020
173	C=C (cyclic)	****	****	-7.5565	-7.2796	-17.0120	-1.9522	****	****	0.0127	-0.0361
174	CH_2=C (cyclic)	-5.4822	-21.8222	7.2048	4.2872	2.4163	-0.0635	4.6088	-32.6637	0.0040	0.0313
175	NH (cyclic)	10.2414	7.9218	4.9384	2.5434	3.4090	1.8061	-0.3537	-51.9576	0.0047	0.0035
176	N (cyclic)	****	****	-3.1834	-0.6202	-0.6760	0.4942	0.4415	-47.7728	0.0000	0.0017
177	CH=N (cyclic)	8.3067	5.6143	7.5704	10.7679	6.2565	-3.0842	****	****	0.0022	0.0220
178	C=N (cyclic)	****	****	****	****	****	****	****	****	0.0021	****
179	O (cyclic)	4.4546	3.0407	4.1019	3.1910	2.8020	0.9963	-0.3026	-111.5440	0.0040	0.0020

180	CO (cyclic)	20.3720	27.1918	3.7195	6.5431	2.7658	3.1548	12.9173	198.8266	0.0091	0.0120
181	S (cyclic)	9.1865	2.9614	5.4726	3.0043	2.9683	1.6101	****	****	0.0013	0.0101
182	SO_2 (cyclic)	****	****	7.9131	11.9870	4.9204	4.9452	****	****	0.0094	0.0164
183	>NH	****	****	****	****	****	2.3229	****	****	0.0084	0.0061
184	-O-	****	****	-0.7007	-3.1505	0.2654	-3.7715	0.0998	88.3361	-0.0014	0.0104
185	-S-	****	****	0.3194	-0.5306	-0.1864	****	****	****	0.0052	0.0157
186	>CO	****	****	0.1063	1.0367	1.6226	-1.5646	****	****	0.0111	0.0128
187	PO_2	****	****	****	****	****	****	****	****	****	****
188	CH-N	****	****	****	****	****	****	****	****	****	****
189	SiHO	****	****	****	****	****	****	****	****	****	****
190	SiO	****	****	****	****	****	1.8263	0.8070	145.5876	0.0020	0.0283
191	SiH_2	****	****	****	****	****	-3.3919	8.9508	93.3669	****	****
192	SiH	****	****	****	****	****	-1.9389	1.1989	189.5422	****	****
193	Si	****	****	****	****	****	0.3123	0.9090	113.5107	0.0008	0.0221
194	$(CH_3)_3N$	****	****	****	****	****	****	****	****	****	****
195	N=N	****	****	7.7650	8.1102	8.7799	****	****	****	****	****
196	C_{cyclic}=N-	****	****	****	****	****	-2.3272	****	****	-0.0037	0.0369
197	C_{cyclic}=CH-	4.8627	0.6920	****	****	****	****	****	****	0.0053	0.0269
198	C_{cyclic}=NH	****	****	****	****	****	****	****	****	****	****
199	N=O	****	****	11.1114	11.1997	1.6523	8.1503	****	****	0.0033	0.0258
200	C_{cyclic}=C	****	****	-13.7208	-4.6294	-5.0268	3.6338	****	****	0.0036	-0.0006
201	P=O	****	****	-6.8355	2.2530	-5.2535	3.6955	****	****	-0.0051	0.0089
202	N=N	****	****	****	****	****	0.0376	****	****	0.0032	0.0387
203	C=NH	****	****	****	****	****	****	****	****	0.0086	0.0535
204	>C=S	****	****	1.3419	7.7242	2.2395	-5.6389	****	****	0.0014	0.0197
205	aC-CON	****	****	****	****	****	****	****	****	****	****
206	aC=O	****	****	****	****	****	****	****	****	****	****
207	aN-	****	****	****	****	****	****	****	****	****	****
208	-Na	****	****	****	****	****	-9.4455	-0.5718	-91.0759	****	****
209	-K	****	****	****	****	****	****	****	****	****	****
210	HCONH	****	****	9.8017	16.4963	13.6895	11.3879	****	****	0.0141	0.0194
211	CHOCH	****	****	****	****	****	****	****	****	****	****
212	C_2O	****	****	****	****	****	****	****	****	****	****
213	SiH_3	****	****	****	****	****	-5.0540	8.9664	-64.2746	****	****
214	SiH_2O	****	****	****	****	****	****	****	****	****	****
215	CH=C=CH	****	****	****	****	****	-0.7141	****	****	0.0035	0.0352
216	CH=C=C	****	****	****	****	****	****	****	****	****	****
217	OP(=S)O	****	****	****	****	****	****	****	****	****	****
218	R	****	****	****	****	****	****	****	****	****	****
219	$CF_{2cyclic}$	3.3419	1.2815	2.0667	****	****	-1.4072	****	****	0.0029	0.0294
220	CF_{cyclic}	-3.1022	-4.1327	-5.7462	****	****	0.8010	****	****	-0.0016	0.0121

[a] The symbols H_{vb1i}, S_{vb1i}, δ_{D1i}, δ_{P1i}, δ_{H1i}, Ait_{a1i}, Ait_{b1i}, ω_{1i}, and V_{m1i} represent the contributions (C_i) of the first-order groups for the corresponding properties.