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