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CHEMICAL PROPERTIES Handbook

化合物性质手册

Carl L. Yaws

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CHEMICAL PROPERTIES HANDBOOK

PHYSICAL, THERMODYNAMIC, ENVIRONMENTAL, TRANSPORT, SAFETY,
AND HEALTH RELATED PROPERTIES FOR ORGANIC AND INORGANIC CHEMICALS

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Chapter 1

CRITICAL PROPERTIES AND ACENTRIC FACTOR

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ABSTRACT

Results for critical properties and acentric factor are presented for major organic and inorganic compounds. The critical properties include critical temperature, pressure, volume, density, and compressibility factor. The chemical formula, molecular weight, freezing point, and boiling point are also given. The results are displayed in easy-to-use tabulations which are especially applicable for rapid engineering usage with the personal computer or hand calculator. The chemicals encompass hydrocarbon, oxygen, nitrogen, halogen, silicon, sulfur, and other compound types.

INTRODUCTION

Physical and thermodynamic property data for organic and inorganic chemicals are of special value to engineers in the chemical processing and petroleum refining industries. The engineering design of process equipment often requires knowledge of such properties as heat capacity, enthalpy, density, viscosity, thermal conductivity, and others.

In this article, results are presented for critical properties and acentric factor, which are usable in corresponding states correlations to determine properties such as heat capacity, enthalpy, density, viscosity, and thermal conductivity. The results are intended for initial engineering studies and are presented in an easy-to-use tabular format which is especially applicable for rapid engineering usage with the personal computer or hand calculator.

CRITICAL PROPERTIES AND ACENTRIC FACTOR

The results for critical properties and acentric factor are shown in Tables 1-1 and 1-2 for organic and inorganic compounds. The tabulations are based on both experimental data and estimated values.

In the data collection, a literature search was conducted to identify data source publications for organics (1-44) and inorganics (1-59). Both experimental values for the property under consideration and parameter values for estimation of the property are included in the source publications. The publications were screened and copies of appropriate data were made. These data were then keyed into the computer to provide a database of critical properties for compounds for which experimental data are available. The database also served as a basis to check the accuracy of the estimation method.

Upon completion of data collection, estimation of the critical properties and acentric factor for the remaining compounds was performed. For organic compounds, the group contribution method of Joback as given by Reid, Prausnitz, and Poling (29) was primarily used for the estimation of critical temperature (T_c), pressure (P_c), and volume (V_c).

For inorganic compounds, estimates of critical temperature were based on modifications of the Guldberg-Guye rule (11), Gates-Thodos method (11) and Grosse equation (11). Estimates of other critical constants and acentric factor were primarily based on extension of the vapor pressure curve and modifications of the Benson relation (11) and Herzog proposal (11). Very limited experimental data for critical constants and acentric factor are available for inorganic compounds and elements that are solids at room temperature. Thus, the estimates for these substances should be considered rough approximations in the absence of experimental data.

Critical density (ρ_c) was determined from dividing molecular weight by critical volume:

$$\rho_c = MW / V_c \qquad (1\text{-}1)$$

where ρ_c = critical density, g/cm^3
MW = molecular weight, g/mol
V_c = critical volume, cm^3/mol

Critical compressibility factor (Z_c) was ascertained from applying the gas law at the critical point:

$$Z_c = P_c V_c / R T_c \qquad (1\text{-}2)$$

For many of the compounds, the acentric factor (ω) was estimated by the following equation which is given in Reid, Prausnitz, and Poling (29):

$$\omega = \frac{3}{7} \frac{T_B / T_C}{1 - T_B / T_C} (\log P_C) - 1 \qquad (1\text{-}3)$$

where ω = acentric factor
T_B = boiling point temperature, K
T_C = critical temperature, K
P_C = critical pressure, atm

This equation for acentric factor is based on extending the vapor pressure by the Antoine type relation.

Comparisons of estimates and data for critical temperature are shown in Figs. 1-1 and 1-2 for normal alkanes and elements. Both graphs disclose favorable agreement of estimates and data.

A comparison of the estimates with experimental data was favorable for the group contribution method of Joback for organic compounds. Average absolute errors of 0.9%, 6.3%, 4.4%, and 4.6% were experienced for critical temperature (465 compounds), pressure (453 compounds), volume (345 compounds), and compressibility factor (348 compounds). Average absolute error for acentric factor (277 compounds) was about 6%.

The normal boiling (T_B) and freezing (T_F) point temperatures are also given in the table. For most compounds, data are available. For the compounds without data, the group contribution method of Joback (29) was used to estimate the boiling and freezing point temperatures for organic compounds. As discussed by Reid, Prausnitz, and Poling (29), no reliable methods are available for precise estimation of freezing point temperature. Thus, the estimates for freezing point temperature should be considered as rough approximations.

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Figure 1-1 Critical Temperature of Normal Alkanes

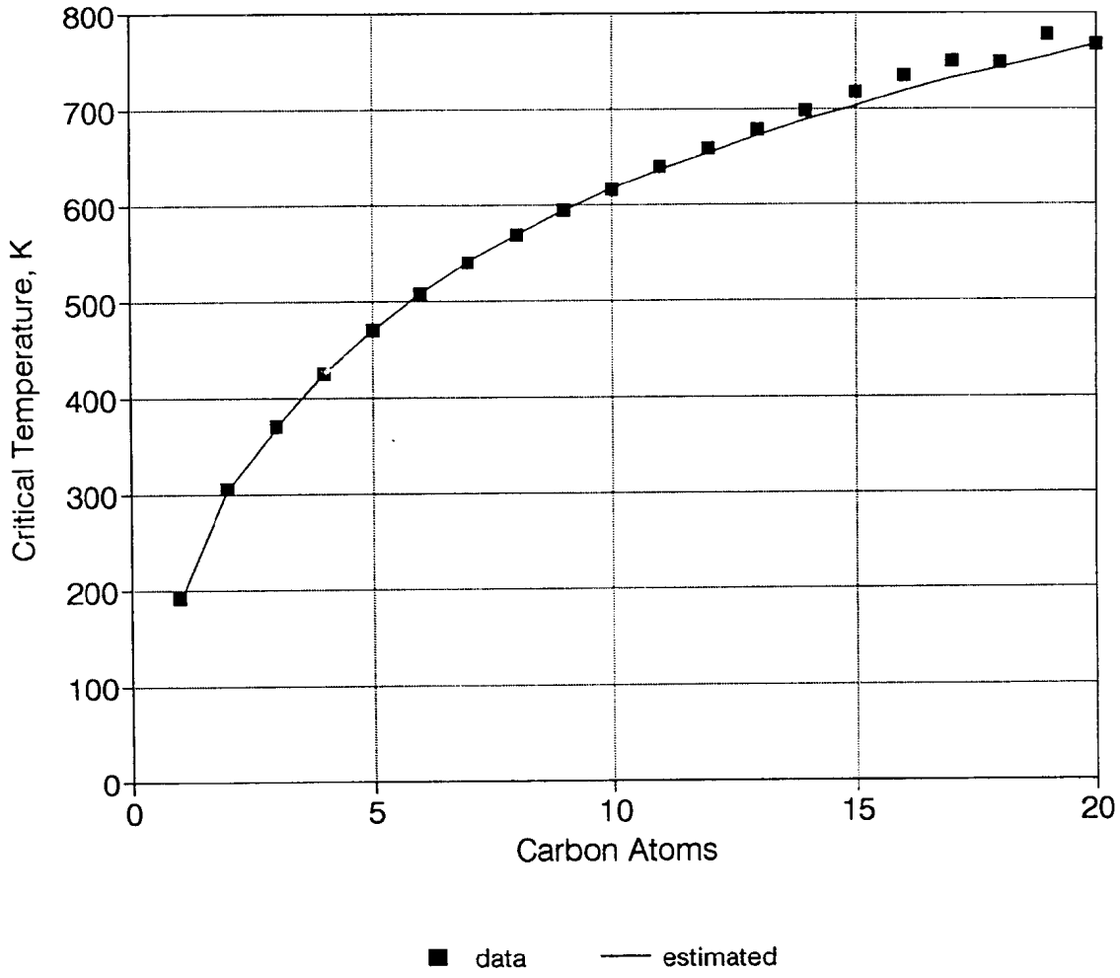

Figure 1-2 Critical Temperature of Elements

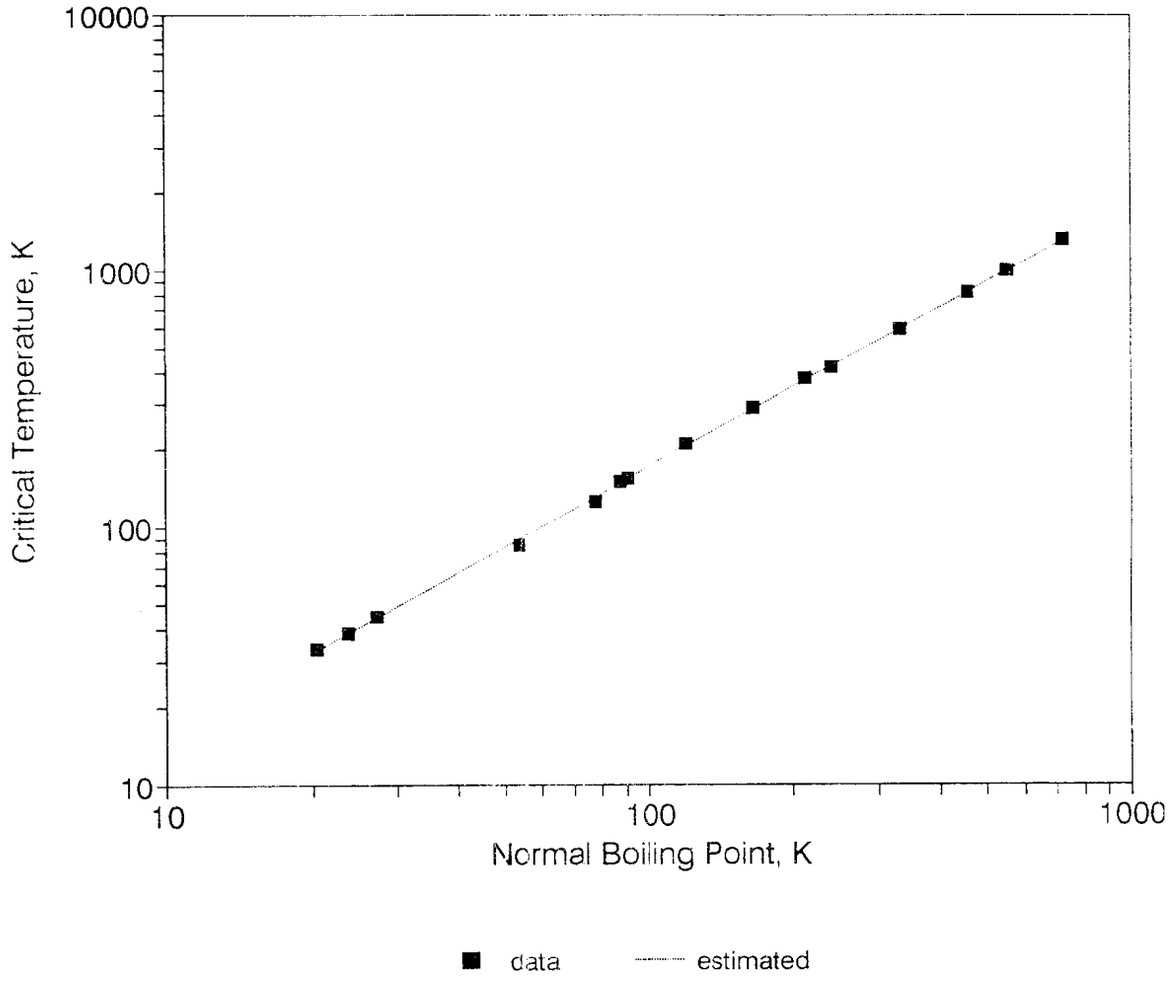

Table 1-1 CRITICAL PROPERTIES AND ACENTRIC FACTOR - ORGANIC COMPOUNDS

NO	FORMULA	NAME	MW	T_F	T_B	T_C	P_C	V_C	RHO_C		
			g/mol	K	K	K	bar	cm3/mol	g/cm3	Z_C	OMEGA
1	CBrClF2	BROMOCHLORODIFLUOROMETHANE	165.365	113.65	269.14	426.15	42.54	246.0	0.6722	0.295	0.187
2	CBrCl3	BROMOTRICHLOROMETHANE	198.273	252.15	378.05	606.00	49.70	264.0	0.6981	0.280	0.192
3	CBrF3	BROMOTRIFLUOROMETHANE	148.910	105.15	215.26	340.15	39.72	200.0	0.7446	0.281	0.173
4	CBr2F2	DIBROMODIFLUOROMETHANE	209.816	163.05	295.94	478.00	53.30	249.0	0.8426	0.334	0.200
5	CClF3	CHLOROTRIFLUOROMETHANE	104.459	92.15	191.74	301.96	39.46	180.3	0.5794	0.283	0.180
6	CClN	CYANOGEN CHLORIDE	61.470	266.65	286.00	449.00	59.90	163.0	0.3771	0.262	0.320
7	CCl2F2	DICHLORODIFLUOROMETHANE	120.913	115.15	243.36	384.95	41.25	217.0	0.5572	0.280	0.180
8	CCl2O	PHOSGENE	98.916	145.37	280.71	455.00	56.74	190.2	0.5200	0.285	0.201
9	CCl3F	TRICHLOROFLUOROMETHANE	137.368	162.04	296.97	471.20	44.08	248.0	0.5539	0.279	0.184
10	CCl4	CARBON TETRACHLORIDE	153.822	250.33	349.79	556.35	45.60	276.0	0.5573	0.272	0.193
11	CF2O	CARBONYL FLUORIDE	66.007	161.89	188.58	297.00	57.60	141.0	0.4681	0.329	0.283
12	CF4	CARBON TETRAFLUORIDE	88.005	89.56	145.09	227.50	37.39	140.0	0.6286	0.277	0.186
13	CHBr3	TRIBROMOMETHANE	252.731	281.20	422.35	696.00	60.90	286.0	0.8837	0.301	0.156
14	CHClF2	CHLORODIFLUOROMETHANE	86.468	115.73	232.32	369.30	49.71	166.0	0.5209	0.269	0.219
15	CHCl2F	DICHLOROFLUOROMETHANE	102.923	138.15	282.05	451.58	51.84	196.0	0.5251	0.271	0.207
16	CHCl3	CHLOROFORM	119.377	209.63	334.33	536.40	54.72	239.0	0.4995	0.293	0.213
17	CHF3	TRIFLUOROMETHANE	70.014	117.97	190.99	298.89	48.36	133.3	0.5252	0.259	0.267
18	CHI3	TRIIODOMETHANE	393.732	396.16	491.16	794.55	53.12	349.5	1.1266	0.281	0.193
19	CHN	HYDROGEN CYANIDE	27.026	259.91	298.85	456.65	53.91	138.6	0.1950	0.197	0.410
20	CHNS	ISOTHIOCYANIC-ACID	59.086	-------	-------	-------	-------	-------	-------	-------	-------
21	CH2BrCl	BROMOCHLOROMETHANE	129.384	185.20	341.20	557.00	68.10	188.0	0.6882	0.276	0.220
22	CH2Br2	DIBROMOMETHANE	173.835	220.60	370.10	611.00	71.70	223.0	0.7795	0.315	0.210
23	CH2ClF	CHLOROFLUOROMETHANE	68.478	140.16	264.06	424.91	51.31	158.5	0.4320	0.230	0.199
24	CH2Cl2	DICHLOROMETHANE	84.932	178.01	312.90	510.00	60.80	185.0	0.4591	0.265	0.192
25	CH2F2	DIFLUOROMETHANE	52.024	137.00	221.50	351.60	58.30	121.0	0.4300	0.241	0.276
26	CH2I2	DIIODOMETHANE	267.836	279.25	455.15	747.00	54.70	272.0	0.9847	0.240	0.141
27	CH2O	FORMALDEHYDE	30.026	181.15	254.05	408.00	65.86	105.0	0.2860	0.204	0.282
28	CH2O2	FORMIC ACID	46.026	281.55	373.71	580.00	73.90	125.0	0.3682	0.192	0.473
29	CH3Br	METHYL BROMIDE	94.939	179.55	276.71	467.00	80.00	156.0	0.6086	0.321	0.192
30	CH3Cl	METHYL CHLORIDE	50.488	175.45	248.93	416.25	66.79	139.0	0.3632	0.268	0.153
31	CH3Cl3Si	METHYL TRICHLOROSILANE	149.478	195.35	339.55	517.00	35.30	340.0	0.4396	0.279	0.263
32	CH3F	METHYL FLUORIDE	34.033	131.35	194.82	317.70	58.77	113.0	0.3012	0.251	0.204
33	CH3I	METHYL IODIDE	141.939	206.70	315.58	528.00	73.70	185.0	0.7672	0.311	0.193
34	CH3NO	FORMAMIDE	45.041	275.70	493.00	771.00	78.00	163.0	0.2763	0.198	0.453
35	CH3NO2	NITROMETHANE	61.040	244.60	374.35	588.15	63.13	173.4	0.3520	0.224	0.348
36	CH3NO2	METHYL-NITRITE	61.040	256.16	261.16	-------	-------	-------	-------	-------	-------
37	CH3NO3	METHYL-NITRATE	77.040	190.86	339.16	-------	-------	-------	-------	-------	-------
38	CH4	METHANE	16.043	90.67	111.66	190.58	46.04	99.3	0.1616	0.288	0.011
39	CH4Cl2Si	METHYL DICHLOROSILANE	115.034	182.55	314.70	483.00	39.50	289.0	0.3980	0.284	0.276
40	CH4O	METHANOL	32.042	175.47	337.85	512.58	80.96	117.8	0.2720	0.224	0.566
41	CH4O3S	METHANESULFONIC ACID	96.107	292.81	561.00	-------	-------	220.0	0.4369	-------	-------
42	CH4S	METHYL MERCAPTAN	48.109	150.18	279.11	469.95	72.35	145.0	0.3318	0.268	0.146
43	CH5ClSi	METHYL CHLOROSILANE	80.589	139.05	281.85	442.00	41.70	246.0	0.3276	0.279	0.225
44	CH5N	METHYLAMINE	31.057	179.69	266.82	430.05	74.58	154.0	0.2017	0.321	0.281
45	CH6Si	METHYL SILANE	46.144	116.34	216.25	352.50	48.40	205.0	0.2251	0.339	0.139
46	CN4O8	TETRANITROMETHANE	196.033	287.05	398.85	540.00	17.40	468.0	0.4189	0.181	0.516
47	CO	CARBON MONOXIDE	28.010	68.15	81.70	132.92	34.99	93.1	0.3009	0.295	0.066
48	COS	CARBONYL SULFIDE	60.076	134.35	223.00	378.80	63.49	135.1	0.4447	0.272	0.097
49	CO2	CARBON DIOXIDE	44.010	216.58	194.67	304.19	73.82	94.0	0.4682	0.274	0.228
50	CS2	CARBON DISULFIDE	76.143	161.58	319.37	552.00	79.03	160.0	0.4759	0.276	0.108
51	C2BrF3	BROMOTRIFLUOROETHYLENE	160.921	------	270.65	432.00	44.80	239.0	0.6733	0.298	0.175
52	C2Br2F4	1,2-DIBROMOTETRAFLUOROETHANE	259.824	162.65	320.41	487.80	33.93	341.0	0.7619	0.285	0.250
53	C2ClF3	CHLOROTRIFLUOROETHYLENE	116.470	115.00	245.30	379.15	40.53	212.0	0.5494	0.273	0.264
54	C2ClF5	CHLOROPENTAFLUOROETHANE	154.467	173.71	234.04	353.15	31.57	252.0	0.6130	0.271	0.251
55	C2Cl2F4	1,2-DICHLOROTETRAFLUOROETHANE	170.921	179.15	276.92	418.85	32.63	293.7	0.5820	0.275	0.252
56	C2Cl3F3	1,1,2-TRICHLOROTRIFLUOROETHANE	187.375	238.15	320.75	487.25	34.15	325.3	0.5760	0.274	0.255
57	C2Cl4	TETRACHLOROETHYLENE	165.833	250.80	394.40	620.00	44.90	248.0	0.6687	0.216	0.214
58	C2Cl4F2	1,1,2,2-TETRACHLORODIFLUOROETHANE	203.830	299.15	366.00	551.00	33.40	351.0	0.5807	0.264	0.291
59	C2Cl4O	TRICHLOROACETYL CHLORIDE	181.832	------	391.15	590.00	41.00	332.0	0.5477	0.277	0.348
60	C2Cl6	HEXACHLOROETHANE	236.738	459.95	460.00	698.00	33.40	412.0	0.5746	0.237	0.221
61	C2F4	TETRAFLUOROETHYLENE	100.016	142.00	197.51	306.45	39.44	172.0	0.5815	0.266	0.226
62	C2F6	HEXAFLUOROETHANE	138.012	172.45	194.95	292.80	29.79	224.0	0.6161	0.274	0.245
63	C2HBrClF3	HALOTHANE	197.382	------	323.35	521.00	39.20	296.0	0.6668	0.268	0.091
64	C2HClF2	2-CHLORO-1,1-DIFLUOROETHYLENE	98.479	134.65	254.55	400.55	44.58	197.0	0.4999	0.264	0.219
65	C2HCl3	TRICHLOROETHYLENE	131.388	188.40	360.10	571.00	49.10	256.0	0.5132	0.265	0.217
66	C2HCl3O	DICHLOROACETYL CHLORIDE	147.387	------	382.15	579.00	46.10	288.0	0.5118	0.276	0.371
67	C2HCl3O	TRICHLOROACETALDEHYDE	147.387	216.00	370.85	565.00	44.10	288.0	0.5118	0.270	0.332
68	C2HCl5	PENTACHLOROETHANE	202.293	244.15	433.03	665.00	36.80	369.0	0.5482	0.246	0.246
69	C2HF3	TRIFLUOROETHENE	82.025	94.53	221.01	347.22	45.16	182.5	0.4495	0.286	0.238
70	C2HF3O2	TRIFLUOROACETIC ACID	114.024	257.90	344.95	491.25	32.58	204.0	0.5589	0.163	0.524
71	C2HF5	PENTAFLUOROETHANE	120.022	170.15	225.15	342.00	34.40	216.0	0.5557	0.261	0.259
72	C2H2	ACETYLENE	26.038	192.40	189.15	308.32	61.39	113.0	0.2305	0.271	0.187
73	C2H2Br4	1,1,2,2-TETRABROMOETHANE	345.654	273.15	516.65	824.00	46.00	401.0	0.8620	0.269	0.177
74	C2H2Cl2	1,1-DICHLOROETHYLENE	96.943	150.65	304.71	482.00	51.90	224.0	0.4328	0.290	0.272
75	C2H2Cl2	cis-1,2-DICHLOROETHYLENE	96.943	193.15	333.65	527.00	51.90	224.0	0.4328	0.265	0.264
76	C2H2Cl2	trans-1,2-DICHLOROETHYLENE	96.943	223.35	320.85	508.00	51.90	224.0	0.4328	0.275	0.264
77	C2H2Cl2O	CHLOROACETYL CHLORIDE	112.943	251.15	379.15	581.00	51.10	245.0	0.4610	0.259	0.358
78	C2H2Cl2O	DICHLOROACETALDEHYDE	112.943	223.00	362.00	555.00	49.50	245.0	0.4610	0.263	0.344

Table 1-1 CRITICAL PROPERTIES AND ACENTRIC FACTOR - ORGANIC COMPOUNDS (continued)

NO	FORMULA	NAME	MW	T_F	T_B	T_C	P_C	V_C	RHO_C		
			g/mol	K	K	K	bar	cm3/mol	g/cm3	Z_C	OMEGA
79	C2H2Cl2O2	DICHLOROACETIC ACID	128.942	286.55	467.15	686.00	51.70	265.0	0.4866	0.240	0.555
80	C2H2Cl3F	1,1,1-TRICHLOROFLUOROETHANE	151.394	------	366.00	565.00	39.90	294.0	0.5149	0.250	0.250
81	C2H2Cl4	1,1,1,2-TETRACHLOROETHANE	167.849	202.94	403.65	624.00	40.20	325.0	0.5165	0.252	0.242
82	C2H2Cl4	1,1,2,2-TETRACHLOROETHANE	167.849	229.35	418.25	645.00	40.90	325.0	0.5165	0.248	0.259
83	C2H2F2	1,1-DIFLUOROETHYLENE	64.035	129.15	187.50	302.80	44.58	154.0	0.4158	0.273	0.139
84	C2H2F2	cis-1,2-DIFLUOROETHENE	64.035	107.90	247.86	394.67	47.69	163.5	0.3917	0.238	0.210
85	C2H2F2	trans-1,2-DIFLUOROETHENE	64.035	107.90	247.86	394.67	47.69	163.5	0.3917	0.238	0.210
86	C2H2F4	1,1,1,2-TETRAFLUOROETHANE	102.031	172.15	247.15	380.00	36.90	203.0	0.5026	0.237	0.239
87	C2H2O	KETENE	42.037	122.00	223.34	370.00	58.10	144.0	0.2919	0.272	0.126
88	C2H2O4	OXALIC ACID	90.036	462.65	569.00	804.00	70.20	205.0	0.4392	0.215	0.918
89	C2H3Br	VINYL BROMIDE	106.950	135.35	288.95	473.00	71.80	200.0	0.5348	0.355	0.282
90	C2H3Cl	VINYL CHLORIDE	62.499	119.36	259.78	432.00	56.70	179.0	0.3492	0.283	0.101
91	C2H3ClF2	1-CHLORO-1,1-DIFLUOROETHANE	100.495	142.35	263.14	410.20	41.24	231.0	0.4350	0.279	0.237
92	C2H3ClO	ACETYL CHLORIDE	78.498	160.30	323.90	508.00	57.40	196.0	0.4005	0.266	0.334
93	C2H3ClO	CHLOROACETALDEHYDE	78.498	------	358.00	555.00	53.70	201.0	0.3905	0.234	0.330
94	C2H3ClO2	CHLOROACETIC ACID	94.497	333.15	462.50	686.00	57.80	221.0	0.4276	0.224	0.551
95	C2H3ClO2	METHYL CHLOROFORMATE	94.497	------	344.00	525.00	53.60	221.0	0.4276	0.271	0.393
96	C2H3Cl3	1,1,1-TRICHLOROETHANE	133.404	242.75	347.23	545.00	42.96	281.0	0.4747	0.266	0.216
97	C2H3Cl3	1,1,2-TRICHLOROETHANE	133.404	236.50	387.00	602.00	44.80	281.0	0.4747	0.252	0.260
98	C2H3F	VINYL FLUORIDE	46.044	112.65	200.95	327.80	52.39	144.0	0.3198	0.277	0.189
99	C2H3F3	1,1,1-TRIFLUOROETHANE	84.041	161.85	225.75	346.25	37.58	194.0	0.4332	0.253	0.253
100	C2H3N	ACETONITRILE	41.053	229.32	354.75	545.50	48.33	173.0	0.2373	0.184	0.338
101	C2H3NO	METHYL ISOCYANATE	57.052	256.15	312.00	505.00	51.90	190.0	0.3003	0.235	0.175
102	C2H4	ETHYLENE	28.054	104.01	169.47	282.36	50.32	129.1	0.2174	0.277	0.085
103	C2H4Br2	1,1-DIBROMOETHANE	187.862	210.15	381.15	628.00	60.30	276.0	0.6807	0.319	0.125
104	C2H4Br2	1,2-DIBROMOETHANE	187.862	282.94	404.51	650.15	54.77	261.6	0.7182	0.255	0.207
105	C2H4Cl2	1,1-DICHLOROETHANE	98.959	176.19	330.45	523.00	50.66	240.0	0.4123	0.280	0.244
106	C2H4Cl2	1,2-DICHLOROETHANE	98.959	237.49	356.59	561.00	53.70	220.0	0.4498	0.253	0.288
107	C2H4Cl2O	BIS(CHLOROMETHYL)ETHER	114.959	231.65	378.00	579.00	45.80	258.0	0.4456	0.245	0.324
108	C2H4F2	1,1-DIFLUOROETHANE	66.051	156.15	247.35	386.60	44.99	181.0	0.3649	0.253	0.263
109	C2H4F2	1,2-DIFLUOROETHANE	66.051	------	303.65	476.00	43.40	202.0	0.3270	0.222	0.224
110	C2H4I2	1,2-DIIODOETHANE	281.863	356.16	473.16	749.91	47.30	323.5	0.8713	0.245	0.223
111	C2H4O	ACETALDEHYDE	44.053	150.15	293.55	461.00	55.50	157.0	0.2806	0.227	0.317
112	C2H4O	ETHYLENE OXIDE	44.053	161.45	283.85	469.15	71.94	140.3	0.3140	0.259	0.198
113	C2H4OS	THIOACETIC-ACID	76.113	150.16	360.16	577.34	69.21	219.5	0.3468	0.317	0.304
114	C2H4O2	ACETIC ACID	60.053	289.81	391.05	592.71	57.86	171.0	0.3512	0.201	0.462
115	C2H4O2	METHYL FORMATE	60.053	174.15	304.90	487.20	59.98	172.0	0.3491	0.255	0.254
116	C2H4S	THIACYCLOPROPANE	60.114	165.37	328.07	555.00	73.80	151.5	0.3968	0.214	0.154
117	C2H5Br	BROMOETHANE	108.966	154.55	311.50	503.80	62.32	214.9	0.5070	0.320	0.183
118	C2H5Cl	ETHYL CHLORIDE	64.514	136.75	285.42	460.35	52.69	200.0	0.3226	0.275	0.204
119	C2H5ClO	2-CHLOROETHANOL	80.514	205.65	401.75	585.00	59.20	212.0	0.3798	0.258	0.637
120	C2H5F	ETHYL FLUORIDE	48.060	129.95	235.45	375.31	50.28	164.0	0.2930	0.264	0.209
121	C2H5I	ETHYL IODIDE	155.966	162.05	345.45	561.00	59.90	238.0	0.6553	0.306	1.137
122	C2H5N	ETHYLENEIMINE	43.068	195.20	329.00	537.00	68.50	173.0	0.2489	0.265	0.089
123	C2H5NO	ACETAMIDE	59.068	354.15	494.30	761.00	66.00	215.0	0.2747	0.224	0.189
124	C2H5NO	N-METHYLFORMAMIDE	59.068	269.35	472.66	721.00	56.20	215.0	0.2747	0.202	0.192
125	C2H5NO2	NITROETHANE	75.067	183.63	387.22	593.00	51.60	236.0	0.3181	0.247	0.265
126	C2H5NO3	ETHYL-NITRATE	91.066	178.56	360.36	------	------	------	------	------	------
127	C2H6	ETHANE	30.070	90.35	184.55	305.42	48.80	147.9	0.2033	0.284	0.099
128	C2H6AlCl	DIMETHYLALUMINUM CHLORIDE	92.054	252.15	399.15	619.00	36.20	320.0	0.2877	0.225	0.183
129	C2H6O	DIMETHYL ETHER	46.069	131.66	248.31	400.10	53.70	170.0	0.2710	0.274	0.204
130	C2H6O	ETHANOL	46.069	159.05	351.44	516.25	63.84	166.9	0.2760	0.248	0.637
131	C2H6OS	DIMETHYL SULFOXIDE	78.135	291.67	462.15	726.00	56.50	227.0	0.3442	0.212	0.209
132	C2H6O2	ETHYLENE GLYCOL	62.068	260.15	470.45	645.00	75.30	191.0	0.3250	0.268	1.137
133	C2H6O4S	DIMETHYL SULFATE	126.133	241.35	461.95	758.00	51.60	293.0	0.4305	0.240	0.089
134	C2H6S	DIMETHYL SULFIDE	62.136	174.88	310.48	503.04	55.30	200.9	0.3093	0.266	0.189
135	C2H6S	ETHYL MERCAPTAN	62.136	125.26	308.15	499.15	54.90	207.0	0.3002	0.274	0.192
136	C2H6S2	DIMETHYL DISULFIDE	94.202	188.44	382.90	606.00	53.60	252.0	0.3738	0.268	0.265
137	C2H7N	DIMETHYLAMINE	45.084	180.96	280.03	437.65	53.09	187.0	0.2411	0.273	0.294
138	C2H7N	ETHYLAMINE	45.084	192.15	289.73	456.15	56.24	182.0	0.2477	0.270	0.285
139	C2H7NO	MONOETHANOLAMINE	61.084	283.65	444.15	638.00	68.70	225.0	0.2715	0.291	0.797
140	C2H8N2	ETHYLENEDIAMINE	60.099	284.29	390.41	593.00	62.90	264.0	0.2276	0.337	0.479
141	C2H8Si	DIMETHYL SILANE	60.171	122.93	253.55	402.00	35.60	258.0	0.2332	0.275	0.132
142	C2N2	CYANOGEN	52.036	245.25	252.00	400.15	59.78	195.0	0.2669	0.350	0.279
143	C3F6	HEXAFLUOROPROPYLENE	150.023	116.65	243.55	368.00	29.00	268.0	0.5598	0.254	0.204
144	C3F6O	HEXAFLUOROACETONE	166.023	151.15	245.88	357.14	28.37	329.0	0.5046	0.314	0.364
145	C3F8	OCTAFLUOROPROPANE	188.020	125.46	236.40	345.05	26.80	299.0	0.6288	0.279	0.326
146	C3H2N2	MALONONITRILE	66.062	304.90	491.50	715.00	40.40	248.0	0.2664	0.169	0.509
147	C3H3Cl	PROPARGYL CHLORIDE	74.510	------	331.00	541.00	53.00	211.0	0.3531	0.249	0.152
148	C3H3N	ACRYLONITRILE	53.064	189.63	350.50	535.00	44.80	212.0	0.2503	0.214	0.350
149	C3H3NO	OXAZOLE	69.063	------	342.65	554.00	63.20	237.0	0.2914	0.325	0.233
150	C3H4	METHYLACETYLENE	40.065	170.45	249.94	402.39	56.28	164.0	0.2443	0.276	0.216
151	C3H4	PROPADIENE	40.065	136.87	238.65	393.15	54.70	162.0	0.2473	0.271	0.160
152	C3H4Cl2	2,3-DICHLOROPROPENE	110.970	191.50	365.75	577.00	43.80	277.0	0.4006	0.253	0.206
153	C3H4O	ACROLEIN	56.064	185.45	325.84	506.00	50.00	197.0	0.2846	0.234	0.320
154	C3H4O	PROPARGYL ALCOHOL	56.064	221.35	386.75	580.00	65.30	176.0	0.3185	0.238	0.555
155	C3H4O2	ACRYLIC ACID	72.064	286.65	414.15	615.00	56.60	208.0	0.3465	0.230	0.518
156	C3H4O2	beta-PROPIOLACTONE	72.064	239.75	435.15	686.00	69.10	195.0	0.3696	0.236	0.345