PHYSICAL & THERMODYNAMIC PROPERTIES

23

Correlation constants for liquids

Procedures to speed calculations for:

- Surface tensions
- Liquid densities
- Heat capacities
- Thermal conductivities

*Carl L. Yaws, Lamar University, and others**

The correlation constants for liquids presented in this article are based on extensive, available, experimental data. These constants are easy to use in a tabular format for rapid engineering calculations by means of a hand calculator or a computer. Such constants may be used in chemical-reaction engineering, thermodynamics, fluid flow, heat transfer, mass transfer and process design. Whereas this part of the series presents correlation data for liquids only, Part 22 contained correlation data for several gases.

SURFACE TENSIONS OF LIQUIDS

Joseph W. Miller, Jr., and Carl L. Yaws

Surface-tension data are important in many chemical-process engineering applications, such as heat, mass and momentum transfer operations that involve process equipment such as heat exchangers, distillation columns, absorption, and fluid-flow piping.

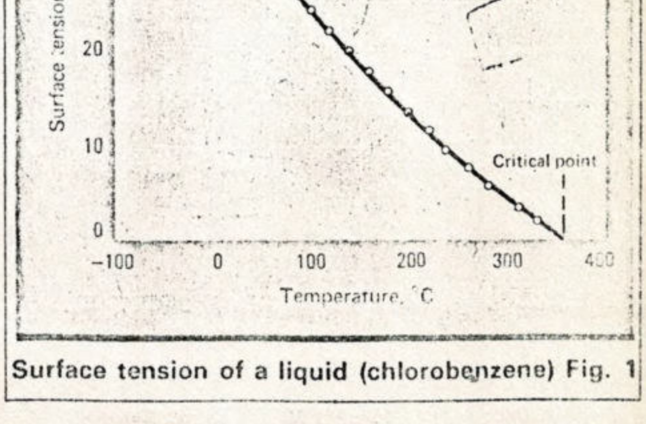
Correlation constants—Table 23—I

Correlation constants for surface tension are based on the Othmer relation:

$$\sigma = \sigma_1 \left[\frac{T_c - T}{T_c - T_1} \right]^n \qquad (23\text{—}1)$$

where σ_1 = surface tension at T_1, dynes/cm; T_c = critical temperature, K; T = temperature, K; and n = correlation parameter.

Tabulated values for the correlation constants are given in Table 23—I, where the temperature range of application is also presented. Deviations between data and calculated values were minimized by using a generalized least-squares computer program to ascertain



Surface tension of a liquid (chlorobenzene) Fig. 1

*For author biographies, see p. 135

Correlation constants: surface tensions

Table 23-1

$$\sigma = \sigma_1 \left[\frac{T_c - T}{T_c - T_1}\right]^n, \text{ dynes/cm}$$

Compound	σ_1, dynes/cm	T_1, °C	T_c, °C	n	Range, °C	References
Halogens						
Fluorine, F_2	16.82	−200.0	−129.0	0.8811	−219.6 to −129.0	31,69,79,637,646
Chlorine, Cl_2	18.4	20.0	144.0	1.0508	−101.0 to 144.0	2,69,33,43,61,79,416
Bromine, Br_2	41.5	20.0	315.0	1.1715	−7.2 to 315.0	2,6,9,43,63,79,416
Iodine, I_2	36.8	125.0	546.0	1.1145	113.6 to 546.0	50
Sulfur oxides						
Sulfur dioxide, SO_2	20.6	30.0	157.6	1.1768	−72.7 to 157.6	79,92,637
Sulfur trioxide, SO_3	30.3	35.3	218.3	1.1854	16.8 to 218.3	6
Nitrogen oxides						
Nitrous oxide, N_2O	1.75	20.0	36.5	1.3115	−89.5 to 36.5	6,9,10,12,79,416,574
Nitric oxide, NO	23.83	−156.0	−93.1	1.5473	−163.8 to −93.1	79
Nitrogen dioxide, NO_2	26.5	25.0	158.0	0.7627	−11.2 to 158.0	6,10,12
Carbon oxides						
Carbon monoxide, CO	9.8	−193.0	−140.1	1.1441	−191.5 to −140.1	2,6,79,416
Carbon dioxide, CO_2	1.16	20.0	31.1	1.3015	−56.5 to 31.1	2,6,9,79,415,416
Hydrogen halides						
Hydorgen fluoride, HF	9.62	10.0	188.0	1.3675	−83.5 to 188.0	4,10,12,70,169
Hydrogen chloride, HCl	24.7	−93.0	51.5	1.0972	−114.2 to 51.5	4,10,12,168
Hydrogen bromide, HBr	27.65	−70.0	90.0	1.2153	−86.9 to 90.0	10,12,79,168
Hydrogen iodide, HI	27.1	−36.0	151.0	1.2824	−50.8 to 151.0	10,12,158
Nitrogen hydrides						
Ammonia, NH_3	36.67	−45.0	132.4	1.1548	−77.74 to 132.4	2,6,12,53,79,416,637
Hydrazine, N_2H_4	66.39	25.0	380.0	1.7652	2.0 to 380.0	4,53,79,189,190,214,416,637
Hydrogen oxides						
Water, H_2O	71.97	25.0	374.2	0.8105	0.0 to 100.0	4,6,9,12,79,238,246,249,250, 416,574,637,646
	58.91	100.0	374.2	1.1690	100.0 to 374.2	
Hydrogen peroxide, H_2O_2	76.1	18.2	455.0	0.9141	−0.43 to 455.0	4,79,249,250,256,257,416
Diatomic gases						
Hydrogen, H_2	2.41	−256.0	−240.2	1.1012	−259.4 to −240.2	9,47,79,265,280,293,307,333,335,416,574,646
Nitrogen, N_2	10.5	−203.0	−146.8	1.2123	−203.9 to −146.8	9,47,79,310,332,416,574,646
Oxygen, O_2	18.01	−202.0	−118.5	1.1933	−218.4 to −118.5	9,79,303,334,416,574,637
Inert gases						
Helium, He	0.2390	−270.0	−268.0	0.5428	−272.66 to −270.0	9,47,79,345,416,574
	0.2390	−270.0	−268.0	1.0638	−270.0 to −268.0	
Neon, Ne	5.5	−248.16	−228.7	1.2393	−248.7 to −228.7	9,47,345,416,574,646
Argon, Ar	12.84	−187.16	−122.4	1.2834	−189.3 to −122.4	9,47,79,310,342,345,382
Olefins						
Ethylene, C_2H_4	19.52	−120.0	9.9	1.2760	−169.2 to 9.9	4,79,246,646
Propylene, C_3H_6	19.98	−70.0	91.9	1.1797	−185.3 to 91.9	10,79,246
1-Butene, C_4H_8	17.84	−20.0	146.2	1.2337	−185.4 to 146.2	10,79,246
Alkanes						
Methane, CH_4	15.026	−168.16	−82.6	1.3941	−182.6 to −82.6	10,47,79,417,646
Ethane, C_2H_6	21.16	−120.0	32.3	1.2060	−183.2 to 32.3	10,79,417,546
Propane, C_3H_8	22.0	−90.0	96.7	1.1982	−187.7 to 96.7	10,79,417
Xylenes						
o-Xylene, $C_6H_4(CH_3)_2$	30.1	20	357.8	1.2111	−25.2 to 357.8	3,6,79,415,416,417,646
m-Xylene, $C_6H_4(CH_3)_2$	28.9	20.0	343.8	1.2629	−47.9 to 343.8	3,6,9,79,415,416,417,574,646
p-Xylene, $C_6H_4(CH_3)_2$	28.31	20.0	344.0	1.2182	13.3 to 344.0	3,6,9,79,415,416,417,574,646
Aromatics						
Benzene, C_6H_6	28.88	20.0	288.94	1.2243	5.53 to 288.94	3,4,79,416,417,495,637,646
Naphthalene, $C_{10}H_8$	28.8	127.0	475.02	1.3511	80.55 to 475.02	3,6,79,574,637
Alkyl aromatics						
Toluene, $C_6H_5CH_3$	28.52	20.0	318.8	1.2364	−95.0 to 318.8	3,9,79,415,417,520,574,637,646
Ethylbenzene, $C_6H_5C_2H_5$	29.29	20.0	344.0	1.2461	−95.0 to 344.0	3,9,79,415,417,520,637
Cumene, $C_6H_5CH(CH_3)_2$	28.21	20.0	360.0	1.2807	−96.0 to 360.0	3,9,79,415,417,520,637,646
Benzene derivatives						
Chlorobenzene, C_6H_5Cl	33.5	20.0	359.2	1.2276	−45.2 to 359.2	3,4,6,79,415,546,569,637,646
Aniline, $C_6H_5NH_2$	42.9	20.0	426.0	1.1022	−6.15 to 426.0	3,6,79,415,546,549,637,646
Phenol, C_6H_5OH	37.13	60.0	420.0	1.0725	40.75 to 420.0	3,6,79,415,569,570,574
Cycloalkanes						
Cyclopropane, C_3H_6	13.25	10.0	124.9	1.3201	−127.42 to 124.9	14
Cyclobutane, C_4H_8	19.13	10.0	190.4	1.3209	−90.73 to 190.4	14
Cyclopentane, C_5H_{10}	22.61	20.0	238.5	1.3323	−93.88 to 238.5	3,4,14,79,415,417,637,646
Cyclohexane, C_6H_{12}	25.24	20.0	280.3	1.4246	6.55 to 280.3	3,4,14,79,415,417,574,637,646
Olefin monomers						
Isobutylene, C_4H_8	12.42	20.0	144.7	1.2095	−140.35 to 144.7	3,4,79,417,620
Styrene, $C_6H_5CHCH_2$	23.01	60.0	369.0	0.4828	−30.6 to 369.0	3,4,79,416,620,621,628

Correlation constants: surface tensions (continued) Table 23—I

$$\sigma = \sigma_1 \left[\frac{T_c - T}{T_c - T_1}\right]^n \text{, dynes/cm}$$

Compound	σ_1, dynes/cm	T_1, °C	T_c, °C	n	Range, °C	References
Diolefins						
1,3 Butadiene, C_4H_6	11.1	40.0	152.0	1.2055	−4.41 to 152.0	3,14
Isoprene, C_5H_8	13.6	50.0	210.2	1.2262	−146.0 to 210.2	14
Chloroprene, C_4H_5Cl	18.4	50.0	261.7	1.2227	−130.0 to 261.7	14,79
Organic oxides						
Ethylene oxide, C_2H_4O	24.33	20.0	195.8	1.1509	−112.5 to 195.8	2,4,10,79,416,574,659
Propylene oxide, C_3H_7O	24.8	0.0	209.1	1.2186	−112.0 to 209.1	14
Butylene oxide, C_4H_9O	26.3	0.0	252.6	1.2201	−150.0 to 252.6	14
Primary alcohols						
Methanol, CH_3OH	22.6	20.0	239.4	0.8115	−97.6 to 239.4	4,6,9,79,415,416,574,637,642,646
Ethanol, C_2H_5OH	22.8	20.0	243.1	0.8760	−114.1 to 243.1	4,6,9,79,415,456,574,637,646
n-Propanol, C_3H_7OH	23.71	20.0	263.6	0.7859	−126.2 to 263.6	4,6,9,79,415,416,574,637
n-Butanol, C_4H_9OH	24.7	20.0	289.8	0.8395	−89.3 to 289.8	6,9,79,415,416,495,574,637
Chloromethanes						
Methyl chloride, CH_3Cl	16.2	20.0	143.1	1.2234	−97.7 to 143.1	4,6,9,79,416,574
Methylene chloride, CH_2Cl_2	28.0	20.0	241.0	1.2057	−96.7 to 241.0	4,6,415,416,637,708,717,721
Chloroform, $CHCl_3$	26.67	25.0	263.4	1.1824	−63.2 to263.4	4,6,9,79,415,416,574,637,708,717,721
Carbon tetrachloride, CCl_4	25.7	30.0	283.2	1.2278	−22.9 to 283.2	4,6,9,79,415,574,637,646,708,717,721

the correlation constants. Average deviations are less than 1–2% in most cases. A comparison of calculated and data values is presented in Fig. 23—1 for a representative chemical.

Example 23-1—Estimate the surface tension of benzene (C_6H_6) at 80°C. The solution to this problem is made by substituting the correlation constants ($\sigma_1 = 28.88$; $T_1 = 20°C = 293.16$ K; $T_c = 288.94°C = 562.1$ K; $T = 80°C = 353.16$ K; and $n = 1.2243$) from Table 23—I into Eq. 23—1:

$$\sigma = \sigma_1\left[\frac{T_c - T}{T_c - T_1}\right]^n$$

$$= 28.88\left[\frac{562.1 - 353.16}{562.1 - 293.16}\right]^{1.2243}$$

$$= 21.2 \text{ dyne/cm}$$

The calculated and data values compare favorably (21.2 versus 21.2).

HEAT CAPACITIES OF LIQUIDS

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Liquid heat-capacity data are important in many process engineering applications. For example, specific heat values are required in liquid-phase chemical reactions (energy requirements for heating liquid reactants up to reaction temperature); in distillation (energy requirements for cooling products to lower temperature for shipment to customer); and in general design of heat exchangers.

Correlation constants—Table 23—II

Correlation constants for liquid heat capacity are based on a series expansion in temperature:

$$C_p = A + BT + CT^2 + DT^3 \qquad (23\text{—}2)$$

where C_p = heat capacity of saturated liquid, cal/(g)(K); A, B, C, D = correlation constants for a chemical compound; and T = temperature, K.

A generalized least-squares computer program for minimizing deviation between collected data and calculated results was used to determine the correlation constants. Average deviations are less than 1–3%.

Tabulated values are given in Table 23—II, where the temperature range is also provided. In most instances, the usable range covers the saturated liquid from its boiling point to temperatures above the boiling point, and in the general region (about 80–90% of T_c) of the critical point. The results are not recommended for use in the immediate vicinity of the critical point (90–100% of T_c). A comparison of calculated and collected data values is presented in Fig. 2 for a representative chemical, which in this case is ethanol.

Example 23-2—Estimate the heat capacity of benzene (C_6H_6) at 20°C. To solve this problem, substitute the correlation constants from Table 23—II: $A = -1.481$; $B = 15.46 \times 10^{-3}$; $C = -43.70 \times 10^{-6}$; and $D = 44.09 \times 10^{-9}$; and the temperature ($T = 20°C = 293.16$ K) into Eq. 23—2:

$$C_p = -1.481 + 15.46 \times 10^{-3}(293.16) - 43.70 \times 10^{-6}(293.16)^2 + 44.09 \times 10^{-9}(293.16)^3$$

$$= 0.406 \text{ cal/(g)(K)}$$

Correlation constants: heat capacity of liquid

Table 23-11

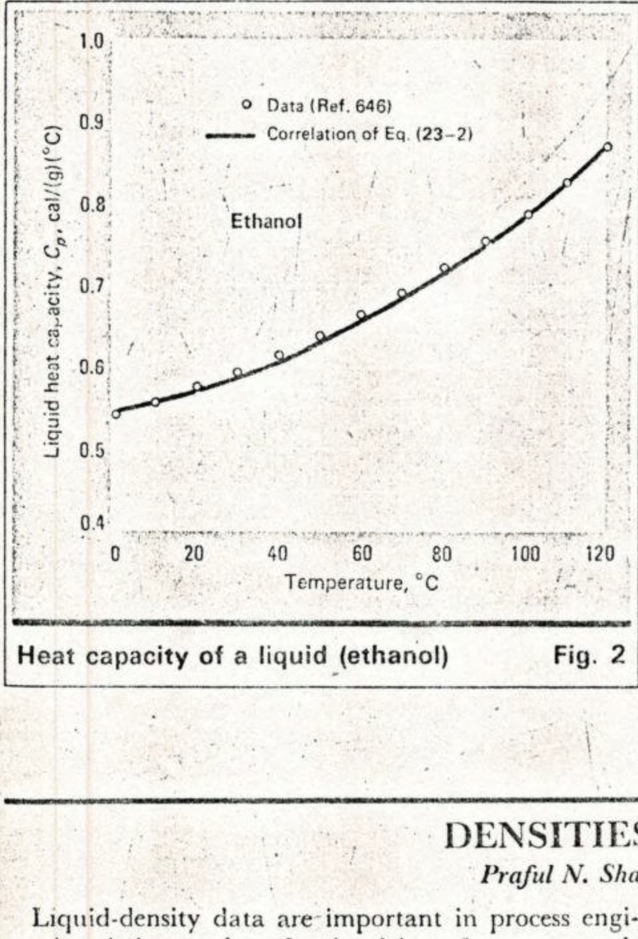
$$C_p = A + BT + CT^2 + DT^3$$

Compound	A	$B \times 10^3$	$C \times 10^6$	$D \times 10^9$	C_p at 25°C cal/(g)(°C)	Range, °C	References
Halogens							
Fluorine, F_2	−0.268	252.8	−331.0	1,464	0.35 @ −183.1	−219 to −140.0	19,42,55,56
Chlorine, Cl_2	−0.1322	4.720	−20.37	28.94	0.226 @ −34.06	−101 to 80	19,32,44,61,71
Bromine, Br_2	−0.3986	4.452	−13.36	13.22	0.09	−7.2 to 280	4,19,43
Iodine, I_2	−0.06263	51.87	−105.4	0.1247	0.075	113.6 to 500	4,19,43
Sulfur oxides							
Sulfur dioxide, SO_2	−0.5737	10.34	−40.28	52.85	0.32 @ −10	−72.7 to 150	4,10,19,92
Sulfur trioxide, SO_3	−3.978	40.16	−116.5	118.0	0.79	16.8 to 200	4,85,91
Nitrogen oxides							
Nitrous oxide, N_2O	−2.915	44.24	−197.5	301.3	0.42 @ −89.5	−90.8 to 30	19,100
Nitric oxide, NO	−19.06	523.6	−4,704.5	14,217	0.61 @ −151.8	−163.8 to −135	19,106,116,134
Nitrogen dioxide, NO_2	−1.625	16.99	−61.72	68.77	0.37 @ 21.2	−11.2 to 140	4,19,107,120
Carbon oxides							
Carbon monoxide, CO	0.5645	4.798	−143.7	911.95	0.515 @ −191.5	−205 to −150	12,14,19
Carbon dioxide, CO_2	−19.30	254.6	−1,095.5	1,573.3	0.46 @ −30	−56.5 to 20	19,147,157
Hydrogen halides							
Hydorgen fluoride, HF	−1.414	20.41	−69.21	83.59	0.73 @ 19.5	−83.5 to 175	4,10,12,169,184
Hydrogen chloride, HCl	−0.1121	7.048	−35.31	66.21	0.405 @ −85.03	−114.2 to 20	12,18
Hydrogen bromide, HBr	−0.6353	10.02	−41.47	58.95	0.18 @ −66.8	−86.9 to 80	4,12
Hydrogen iodide, HI	−0.6418	7.739	−26.55	30.95	0.112 @ −35.5	−50.8 to 140	4,164
Nitrogen hydrides							
Ammonia, NH_3	−1.923	31.1	−110.9	137.6	1.05 @ −33.43	−77.4 to 100	6,12,13,19,194
Hydrazine, N_2H_4	−4.634	49.00	−150.1	156.3	0.75	2 to 200	6,14,20,215,218
Hydrogen oxides							
Water, H_2O	0.6741	2.825	−8.371	8.601	1.0	0 to 350	9,12,238,246
Hydrogen peroxide, H_2O_2	0.444	1.199	−2.738	2.615	0.63	−0.43 to 425	4,240,242,244,256,257,260
Diatomic gases							
Hydrogen, H_2	3.79	−329.8	12,170.9	−2,434.8	2.1 @ −252.8	−253.4 to −245	19,47,284,293,302,306,307,311,321,333,335
Nitrogen, N_2	−1.064	59.47	−768.7	3,257.3	0.49 @ −195.8	−209.9 to −160	19,43,47,300,306,321,325,331,332
Oxygen, O_2	−0.4587	32.34	−395.1	1,575.7	0.405 @ −183.0	−218.4 to −130	19,47,300,303,306,321,334
Inert gases							
Helium, He	−1.733	1,386.0	−293,133.	27,280,000	0.96 @ −268.9	−270 to −268.5	10,47,345
Neon, Ne	−1.726	210.97	−6,982.4	79,375.0	0.44 @ −246	−248.7 to −230	10,43,47
Argon, Ar	−0.4778	23.17	−254.5	972.7	0.25 @ −185.9	−189.3 to −130	19,43,47
Olefins							
Ethylene, C_2H_4	−0.3402	6.218	−50.12	126.3	0.572 @ −103.7	−169 to −40	19,246,415,425,439,440
Propylene, C_3H_6	0.4706	1.683	−16.82	44.07	0.51 @ −47.7	−185.3 to 40	10,246,415,425,439,440
1-Butene, C_4H_8	0.5422	−1.179	3.409	2.195	0.515 @ −6.3	−185.4 to 80	10,246,415,425,441
Alkanes							
Methane, CH_4	1.23	−10.33	72.0	−107.3	0.824 @ −161.5	−182.6 to −110	10,19,47,415,425,464
Ethane, C_2H_6	0.1388	8.481	−56.54	126.1	0.583 @ −88.2	−183.2 to 20	10,19,246,415,425,453
Propane, C_3H_8	0.3326	2.332	−13.36	30.16	0.532 @ −42.1	−187.7 to 80	10,19,246,415,425,463
Xylenes							
o-Xylene, $C_6H_4(CH_3)_2$	−0.4498	6.892	−18.60	17.86	0.415	−25.2 to 325	9,413,488
m-Xylene, $C_6H_4(CH_3)_2$	−0.08753	3.829	−10.71	11.46	0.40	−47.9 to300	9,413,488
p-Xylene, $C_6H_4(CH_3)_2$	−0.8429	8.961	−21.46	18.45	0.41	13.3 to 325	9,413,415,416,487,488
Aromatics							
Benzene, C_6H_6	−1.481	15.46	−43.70	44.09	0.41	5.53 to 250	3,19,415,481,503
Naphthalene, $C_{10}H_8$	−1.412	11.61	−25.26	19.63	0.42 @ 100	80.55 to 410	415,501,510
Alkyl aromatics							
Toluene, $C_6H_5CH_3$	−0.1461	4.584	−13.46	14.25	0.395	−95 to 310	9,19,415,518
Ethylbenzene, $C_6H_5C_2H_5$	0.04941	2.711	−7.210	7.649	0.418	−95 to 320	9,415
Cumene, $C_6H_5CH(CH_3)_2$	0.1201	2.457	−6.92	7.646	0.43	−96 to 340	15,343
Benzene derivatives							
Chlorobenzene, C_6H_5Cl	−0.1467	3.826	−10.66	10.41	0.31	−45.2 to 340	3,4,6,415,416,571,574
Aniline, $C_6H_5NH_2$	0.1407	2.467	−6.085	5.927	0.49	−6.15 to 360	4,415,416,556,574
Phenol, C_6H_5OH	−0.6896	8.218	−18.42	14.47	0.535 @ 60	40.75 to 400	415,558,563,570,574
Cycloalkanes							
Cyclopropane, C_3H_6	−0.02618	6.913	−34.77	59.9	0.46 @ −32.8	−127.42 to 100	455,589,595
Cyclobutane, C_4H_8	−0.346	7.745	−27.0	33.42	0.445 @ 12.51	−90.73 to 180	594
Cyclopentane, C_5H_{10}	−0.02117	4.146	−13.16	15.95	0.41	−93.88 to 220	415,416,546,597
Cyclohexane, C_6H_{12}	−1.284	13.39	−35.1	32.27	0.43	6.55 to 260	415,416,503,546,577,601,603
Olefin monomers							
Isobutylene, C_4H_8	−0.1905	3.653	−16.79	28.92	0.525 @ −6.9	−140.35 to 125	10,415,534,607,613,619,627
Styrene, $C_6H_5CHCH_2$	−0.3154	5.465	−14.30	−14.34	0.41	−30.60 to 325	4,620,622,626
Diolefins							
1,3 Butadiene, C_4H_6	0.3735	1.049	−5.761	13.74	0.512 @ −4.41	−108.9 to 120	10,415,416,640,646
Isoprene, C_5H_8	0.1457	2.317	−5.033	13.66	0.405	−146 to 200	416,620,633,645
Chloroprene, C_4H_5Cl	0.0140	2.540	−8.839	11.20	0.315	−130 to 260	4,620

Correlation constants: heat capacity of liquid (continued) — **Table 23—II**

$$C_p = A + BT + CT^2 + DT^3$$

Compound	A	$B\times10^3$	$C\times10^6$	$D\times10^9$	C_p at 25°C, cal/(g)(°C)	Range, °C	References
Organic oxides							
Ethylene oxide, C_2H_4O	0.2839	2.347	−11.66	20.04	0.47 @ 10.55	−112.5 to 180	4,659
Propylene oxide, C_3H_7O	0.1610	3.670	−15.48	22.94	0.495	−112 to 200	4,654,659
Butylene oxide, C_4H_9O	0.3182	2.037	−9.306	14.62	0.49	−150 to 240	14
Primary alcohols							
Methanol, CH_3OH	0.8382	−3.231	8.296	−0.1689	0.608	−97.6 to 220	4,6,9,415,416,646,689,697,699 700,701
Ethanol, C_2H_5OH	−0.3499	9.559	−37.86	54.59	0.58	−114.1 to 180	4,6,19,415,416,646,692,693,700
n-Propanol, C_3H_7OH	−0.2761	8.573	−34.2	49.85	0.57	−126.2 to 200	4,6,415,416,692,698
n-Butanol, C_4H_9OH	−0.7587	12.97	−46.12	58.59	0.56	−89.3 to 200	4,6,415,692,697,700
Chloromethanes							
Methyl chloride, CH_3Cl	0.04123	4.188	−19.11	29.73	0.358 @ −23.8	−97.5 to 120	4,19,646,208,717
Methylene chloride, CH_2Cl_2	0.01117	3.009	−11.43	14.97	0.285	−96.7 to 230	4,6,415,708,717,721
Chloroform, $CHCl_3$	−0.09154	3.149	−10.64	12.4	0.225	−63.2 to 250	4,6,19,415,416,417,208,717,721
Carbon tetrachloride, CCl_4	−0.01228	2.058	−7.04	8.610	0.20	−22.9 to 260	4,6,19,415,416,646,708,717,721



Heat capacity of a liquid (ethanol) — **Fig. 2**

The calculated and data values compare favorably (0.406 versus 0.405).

Example 23-3—Estimate the energy required to heat toluene from 20°C to 100°C under saturation conditions. Recall from thermodynamics these conditions:

$$Q = \Delta H \simeq \int C_p dT = \int_{T_1}^{T_2} (A + BT + CT^2 + DT^3) dT$$

$$= AT + \frac{BT^2}{2} + \frac{C}{3}(T^3) + \frac{D}{4}(T^4)\Big]_{T_1}^{T_2}$$

Substituting correlation constants A, B, C and D from Table 23—II, and temperatures T_1 and T_2 into the above equation yields:

$$\Delta H = -(0.1461)(373.16 - 293.16) +$$
$$(4.584/2)(10^{-3})(373.16^2 - 293.16^2) -$$
$$(13.46/3)(10^{-6})(373.16^3 - 293.16^3) +$$
$$(14.25/4)(10^{-9})(373.16^4 - 293.16^4)$$
$$= 33.04 \text{ cal/g}$$

DENSITIES OF LIQUIDS

Praful N. Shah and Carl L. Yaws

Liquid-density data are important in process engineering design, such as for the sizing of storage vessels that contain basic raw materials for a plant. In distillation, engineering design of condensers and reboilers requires knowledge of saturated liquid-density values for the column's overhead and bottom products. Additional usage is encountered in various heat, mass and momentum-transfer operations involving liquids.

Correlation constants—Table 23—III

Saturated liquid densities, at any temperature, were based on the following correlation:

$$\rho_L = AB^{-(1-T_r)^{2/7}} \qquad (23\text{—}3)$$

where ρ_L = saturated liquid density, g/cm^3; A,B = correlation constants for a chemical compound; and T_r = reduced temperature, T/T_c.

Tabulated values for the correlation constants A and B are given in Table 23—3. The temperature range over which the correlation constants are valid covers the entire saturated liquid state, from the melting point to the critical point. A generalized least-squares computer

Correlation constants: liquid densities

Table 23—II

$$\rho_L = AB^{-(1-T_r)^{2/7}},\ \text{g/cm}^3$$

Compound	A	B	T_c, °C	ρ at 25°C, g/cm³	Range, °C	No. of data points	Average deviation, %	References
Halogens								
Fluorine, F_2	0.5649	0.2828	−129.00	1.51 @ −188.14	−219.6 to −129.0	100	0.26	31,69,646,720
Chlorine, Cl_2	0.5615	0.2770	144.0	1.39	−101.0 to 144.0	94	0.27	9,43,71,74,637,646
Bromine, Br_2	1.2267	0.3225	315.0	3.10	−7.2 to 315.0	31	0.47	6,12,28,43
Iodine, I_2	1.6059	0.3400	546.0	3.70 @ 184.35	113.6 to 546.0	36	0.71	6,12,28,43
Sulfur oxides								
Sulfur dioxide, SO_2	0.5164	0.2554	157.6	1.37	−72.7 to 157.6	106	0.49	4,10,12,81,637
Sulfur trioxide, SO_3	0.5956	0.2274	218.3	1.90	16.8 to 218.3	42	2.22	9,12
Nitrogen oxides								
Nitrous oxide, N_2O	0.4413	0.2645	36.5	0.75	−90.8 to 36.5	86	0.92	9,10,12,103,118,133
Nitric oxide, NO	0.5201	0.2353	−93.1	1.27 @ −151.74	−163.8 to −93.1	8	1.01	637
Nitrogen dioxide, NO_2	0.5859	0.2830	158.0	1.43	−11.2 to 158.00	58	1.28	4,10,12,128,637
Carbon oxides								
Carbon monoxide, CO	0.2931	0.2706	−140.1	0.79 @ −191.52	−205.0 to −140.1	56	0.56	9,12,637,646
Carbon dioxide, CO_2	0.4576	0.2590	31.1	0.71	−56.5 to 31.1	125	0.20	9,12,141,153,637,646
Hydrogen halides								
Hydorgen fluoride, HF	0.2865	0.1950	188.0	0.96	−83.5 to 188.0	44	0.85	4,10,12,183
Hydrogen chloride, HCl	0.4183	0.2619	51.5	0.80	−114.2 to 51.5	85	0.61	4,6,9,10,12,167,171,174,637
Hydrogen bromide, HBr	0.7358	0.2560	90.0	2.16 @ −66.8	−86.9 to 90.0	17	0.10	6,10,12,637
Hydrogen iodide, HI	0.9475	0.2545	151.0	2.80 @ −35.5	−50.8 to 151.0	18	0.08	4,10,12,174,637
Nitrogen hydrides								
Ammonia, NH_3	0.2312	0.2471	132.4	0.60	−77.74 to 132.4	87	0.29	4,9,194,646
Hydrazine, N_2H_4	0.3171	0.2538	380.0	1.00	2.0 to 380.0	18	0.11	4,189
Hydrogen oxides								
Water, H_2O	0.3471	0.2740	374.2	1.00	0.0 to 374.2	148	2.27	4,246,257,637
Hydrogen peroxide, H_2O_2	0.4375	0.2505	455.0	1.44	−0.43 to 455.0	25	0.27	4,239,249,257,261
Diatomic gases								
Hydrogen, H_2	0.0315	0.3473	−240.2	0.07 at −252.78	−259.4 to −240.2	85	0.70	4,10,304,321,333,335
Nitrogen, N_2	0.3026	0.2763	−146.8	0.81 @ −195.81	−209.9 to −146.8	110	0.25	4,10,315,321,331,332
Oxygen, O_2	0.4227	0.2797	−118.5	1.14 @ −183.16	−218.4 to −118.5	56	0.30	4,43,321,324,331
Inert gases								
Helium, He	0.0747	0.4406	−268.0	0.12 @ −268.9	−271 to −268.0	28	1.44	9,646
Neon, Ne	0.4843	0.3035	−228.7	−1.21 @ −246.16	−248.7 to −228.7	17	0.05	646
Argon, Ar	0.5082	0.2735	−122.4	1.39 @ −185.88	−189.3 to −122.4	90	0.46	9,10,43,149,358,365,737
Olefins								
Ethylene, C_2H_4	0.2118	0.2784	9.9	0.57 @ −103.8	−169.2 to 9.9	63	0.56	9,10,415,436,637,646
Propylene, C_3H_6	0.2252	0.2696	91.9	0.61 @ −47.7	−185.3 to 91.9	61	0.41	10,637,646
1-Butene, C_4H_8	0.2333	0.2620	146.2	0.59	−185.4 to 146.2	47	0.31	10,415,637,646
Alkanes								
Methane, CH_4	0.1611	0.2877	−82.6	0.42 @ −161.5	−182.6 to −82.6	285	0.67	9,10,47,454,455,637,735,736,737,739,741,742
Ethane, C_2H_6	0.2202	0.3041	32.3	0.33	−183.2 to 32.3	84	0.73	9,10,448,637,646
Propane, C_3H_8	0.2204	0.2753	96.7	0.49	−187.7 to 96.7	65	0.32	10,637,646
Xylenes								
o-Xylene, $C_6H_4(CH_3)_2$	0.2870	0.2619	357.8	0.88	−25.2 to 357.8	123	0.16	415,473,474,637,646
m-Xylene, $C_6H_4(CH_3)_2$	0.2809	0.2587	343.8	0.86	−47.9 to 343.8	111	0.21	415,473,637,646
p-Xylene, $C_6H_4(CH_3)_2$	0.2812	0.2603	344.0	0.86	13.3 to 344.0	119	0.13	415,473,474
Aromatics								
Benzene, C_6H_6	0.3051	0.2714	288.94	0.87	5.53 to 288.94	200	0.22	9,473,474,481,484,497,637
Naphthalene, $C_{10}H_8$	0.3241	0.2653	475.02	0.86 @ 217.0	80.55 to 475.02	44	0.59	4,473,474,637
Alkyl aromatics								
Toluene, $C_6H_5CH_3$	0.2883	0.2624	318.8	0.86	−95.0 to 318.8	150	0.22	4,415,473,524,637
Ethylbenzene, $C_6H_5C_2H_5$	0.2835	0.2606	344.0	0.86	−95.0 to 344.0	84	0.14	415,473,524
Cumene, $C_6H_5CH(CH_3)_2$	0.2770	0.2576	360.0	0.86	−96.0 to 360.0	44	0.07	4,415,473,524
Benzene derivatives								
Chlorobenzene, C_6H_5Cl	0.3706	0.2708	359.2	1.10	−45.2 to 359.2	47	0.16	415,550,560
Aniline, $C_6H_5NH_2$	0.3392	0.2761	426.0	1.01	−6.15 to 426.0	72	0.19	4,415,484,550,561,646
Phenol, C_6H_5OH	0.4094	0.3246	420.0	1.04 @ 60.0	40.75 to 420.0	29	0.17	4,415,418,563
Cycloalkanes								
Cyclopropane, C_3H_6	0.2614	0.2826	124.9	0.62	−127.42 to 124.9	57	0.88	473,588,589,600
Cyclobutane, C_4H_8	0.2575	0.2711	190.4	0.72 @ −5.0	−90.73 to 190.4	3	0.44	473
Cyclopentane, C_5H_{10}	0.2701	0.2737	238.5	0.74	−93.88 to 238.5	40	0.20	415,473,580,585
Cyclohexane, C_6H_{12}	0.2729	0.2727	280.3	0.77	6.55 to 280.3	97	0.16	415,473
Olefin monomers								
Isobutylene, C_4H_8	0.2323	0.2651	144.7	0.59	−140.35 to 144.7	107	0.24	4,10,607,613,619,620
Styrene, $C_6H_5CHCH_2$	0.2823	0.2493	369.0	0.90	−30.6 to 369.0	34	0.27	4,611,620
Diolefins								
1,3 Butadiene, C_4H_6	0.2444	0.2710	152.0	0.61	−108.9 to 152.0	200	0.15	10,639,640
Isoprene, C_5H_8	0.2562	0.2812	210.2	0.68	−146.0 to 210.2	21	0.59	4,473,620,645
Chloroprene, C_4H_5Cl	0.3400	0.2764	261.7	0.95 @ 70.0	−130.0 to 261.7	3	0.64	4

Correlation constants: liquid densities (continued) — **Table 23—III**

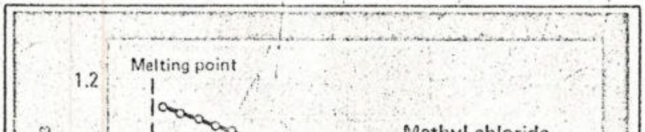
$$\rho_L = AB^{-(1-T_r)^{2/7}},\ \text{g/cm}^3$$

Compound	A	B	T_c, °C	ρ at 25°C, g/cm³	Range, °C	No. of data points	Average deviation, %	References
Organic oxides								
Ethylene oxide, C_2H_4O	0.3172	0.2608	195.8	0.86	−112.5 to 195.8	43	0.83	4,10,637
Propylene oxide, C_3H_7O	0.3123	0.2739	209.1	0.82	−112.0 to 209.1	6	0.04	4
Butylene oxide, C_4H_8O	0.2902	0.2649	252.6	0.83 @ 20.0	−150.0 to 252.6	2	0.01	4
Primary alcohols								
Methanol, CH_3OH	0.2928	0.2760	239.4	0.79	−97.6 to 239.4	71	1.14	4,415,484,637,646
Ethanol, C_2H_5OH	0.2903	0.2765	243.1	0.79	−114.1 to 243.1	108	1.35	4,415,484,637
n-Propanol, C_3H_7OH	0.2915	0.2758	263.6	0.80	−126.2 to 263.6	63	1.05	4,415,484,646
n-Butanol, C_4H_9OH	0.2633	0.2477	289.8	0.80	−89.3 to 289.8	25	1.60	4,415,484,646
Chloromethanes								
Methyl chloride, CH_3Cl	0.3542	0.2573	143.1	0.91	−97.7 to 143.1	87	0.85	9,637,708,712,718,733
Methylene chloride, CH_2Cl_2	0.3333	0.2141	241.0	1.32	−96.7 to 241.0	80	0.93	637,708,721,729,732,733
Chloroform, $CHCl_3$	0.5165	0.2666	263.4	1.48	−63.2 to 263.4	47	1.06	637,708,721,733,734
Carbon tetrachloride, CCl_4	0.5591	0.2736	283.2	1.59	−22.9 to 283.2	91	0.26	9,637,646,708,710,718,719,721

program (for minimizing deviations between calculated and data values) was effectively used to process the several thousand data points. The average deviation for all compounds tested is 0.55%.

If correlation constants are not available, one may make reasonable estimates of saturated liquid densities by letting $A = \rho_c$, and $B = Z_c$ (critical compressibility factor). This method reduces the above correlation to the Rackett equation [*489**]. Application of this method to all compounds tested produced much greater deviations (average of 5%). Calculated and data values are compared in Fig. 23—3 for a representative chemical compound.

*Part 12 of this series, July 21, 1975, p. 122.



Liquid density of a liquid (methyl chloride) — Fig. 3

Example 23-4—Estimate the saturated liquid density of chlorobenzene (C_6H_5Cl) at 50°C. To solve this problem, substitute the correlation constants ($A = 0.3706$; $B = 0.2708$; $T_c = 359.2°C = 632.4$ K) from Table 23—3, and the temperature ($T = 50°C = 323.2$ K) into Eq. 23-3:

$$\rho_L = AB^{-(1-T_r)^{2/7}}$$
$$= (0.3706)(0.2708)^{-[1-(323.2/632.4)]^{2/7}}$$
$$= 1.075 \text{ g/cm}^3$$

The calculated and data values compare favorably (1.075 versus 1.074).

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THERMAL CONDUCTIVITIES OF LIQUIDS

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Liquid thermal conductivity data are important in numerous chemical engineering applications that involve heat transfer. Representative examples include partial condensers handling liquids; total condensers for the column-overhead product in a distillation operation; reboilers processing the column bottom in a distillation; liquid-phase reactors requiring heating or cooling; and general heat exchangers handling liquids.

Correlation constants: thermal conductivity of liquids

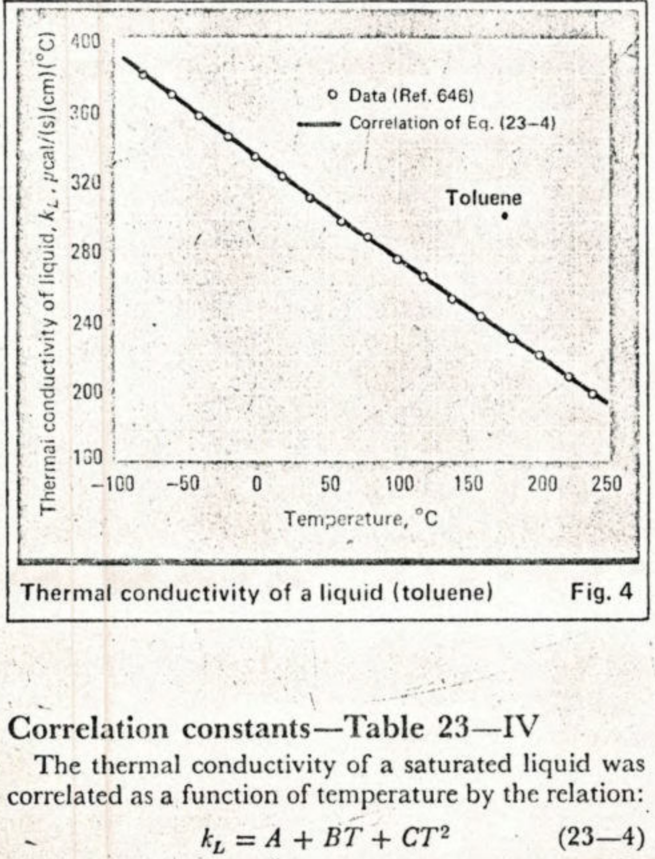
Table 23–IV

$k_L = A + BT + CT^2$

Compound	A	$B \times 10^2$	$C \times 10^4$	k_L at 20°C, (micro-cal)/(s) (cm) (°K)	Range, °C	References
Halogens						
Fluorine, F_2	612.54	−162.29	−118.41	320 at −170.0	−219.0 to −140	14,65
Chlorine, Cl_2	599.01	−48.30	−15.24	327	−101 to 132	14,65
Bromine, Br_2	384.05	−3.07	−8.04	300	−7.2 to 300	14,63,65
Iodine, I_2	320.12	10.26	−4.85	275 at 156	113 to 512	14,65
Sulfur oxides						
Sulfur dioxide, SO_2	2,140.81	−783.66	71.43	458	−50 to 150	93
Sulfur trioxide, SO_3	2271.20	−760.56	66.60	615	10 to 210	743
Nitrogen oxides						
Nitrous oxide, N_2O	846.95	−213.60	−4.29	120	−102 to 20	14,125,126
Nitric oxide, NO	423.34	253.19	−212.35	438 at −160	−163 to −96	14,65
Nitrogen dioxide, NO_2	519.74	6.22	−25.73	317	−11 to 142	14,19
Carbon oxides						
Carbon monoxide, CO	475.48	3.31	−214.26	360 at −200	−205 to −145	14,19,65
Carbon dioxide, CO_2	972.06	−201.53	−22.99	184	−56 to 26	14,19,142,151,152
Hydrogen halides						
Hydorgen fluoride, HF	1,695.67	−205.91	−15.38	950	−83 to 165	13,14,65
Hydrogen chloride, HCl	1,071.70	−18.44	−65.81	453	−114 to 31	14,65,173,175,176
Hydrogen bromide, HBr	579.89	38.34	−41.11	339	−87 to 70	14,65,173
Hydrogen iodide, HI	620.79	−10.27	−21.73	404	−50 to 110	14,65,173
Nitrogen hydrides						
Ammonia, NH_3	2,551.30	−376.62	−29.35	1,196	−77 to 100	13,14,19,207
Hydrazine, N_2H_4	2,859.98	−175.23	−24.16	2,139	2 to 318	13,14
Hydrogen oxides						
Water, H_2O	−916.62	1,254.73	−152.12	1,452	0 to 350	4,13,14,19,238,246,258
Hydrogen peroxide, H_2O_2	−466.56	805.86	−87.58	1,143	0 to 400	13,14,258
Diatomic gases						
Hydrogen, H_2	−20.41	2,473.70	−5,347.26	268 @ −250	−259 to −241	19,47,272,287,290,293,298,304,307,317,333
Nitrogen, N_2	627.99	−368.91	−22.57	275 @ −182.5	−209 to −152	19,47,65,288,290,299,300,303,306,316,317,328,332
Oxygen, O_2	583.79	−210.49	−48.31	355 @ −183	−218 to −135	19,47,65,288,300,317,327,334
Inert gases						
Helium, He	−954.21	$1.55 \cdot 10^5$	$-5.0 \cdot 10^6$	200 @ −271.3	−271.3 to −271.0	19,44,47,290,345,364,374,392,399
	98.35	−4,376.85	$9.05 \cdot 10^4$	50 @ −270.0	−271.0 to −268.3	
Neon, Ne	32.82	2,004.4	−4,121.7	240 @ −239.5	−248.7 to −229.5	19,43,44,290,374,392
Argon, Ar	444.63	−96.43	−85.71	260 @ −173	−189.3 to −128.0	19,43,44,47,288,290,306,316,328,345,374,392,[illegible]
Olefins						
Ethylene, C_2H_4	851.45	−228.94	−4.71	351 @ −63	−169.2 to −4.0	14,19,84,246,421,440
Propylene, C_3H_6	694.04	−144.57	0.30	275	−185 to 70	14,246,422,426,430,440
1 Butene, C_4H_8	609.89	−95.16	−2.71	312	−185 to 120	14,246
Alkanes						
Methane, CH_4	722.72	−144.42	−76.36	325 @ −120	−182.6 to −90.0	19,47,288,459,464
Ethane, C_2H_6	699.31	−165.88	−4.87	170	−183.2 to 20	288,444
Propane, C_3H_8	623.51	−126.79	−2.12	234	−187.7 to 80.0	288,445
Xylenes						
o-Xylene, $C_6H_4(CH_3)_2$	393.83	−17.77	−3.38	313	−25.2 to 332.0	6,9,409,413,481,486
m-Xylene, $C_6H_4(CH_3)_2$	392.29	−3.50	−5.70	333	−47.9 to 330.0	6,9,409,413,470,471,481,482,483,486
p-Xylene, $C_6H_4(CH_3)_2$	355.0	6.49	−6.74	316	13.3 to 336.0	475,481,483
Aromatics						
Benzene, C_6H_6	424.26	1.14	−9.03	350	5.53 to 260	14,19,443,481,484,492,493,494,514
Naphthalene, $C_{10}H_8$	317.24	14.22	−4.04	311 at 120°	80.55 to 460.0	443,496
Alkyl aromatics						
Toluene, $C_6H_5CH_3$	485.10	−53.84	−0.59	322	−95 to 308	9,14,19,288,409,470,471,475,481,482,483,486,[illegible] 516,525,526,527,528,530,531
Ethylbenzene, $C_6H_5C_2H_5$	511.66	−82.15	4.64	311	−95 to 300	14,481,516,535,539
Cumene, $C_6H_5CH(CH_3)_2$	471.26	−57.82	0.49	306	−96 to 305	14,483,486,516,532,546
Benzene derivatives						
Chlorobenzene, C_6H_5Cl	432.04	−38.31	−1.12	310	−45.2 to 330	14,409,413,416,481,484,486,535,539,546,552,[illegible], 559,562,565,566,567,568,572
Aniline, $C_6H_5NH_2$	537.55	−30.42	−1.49	436	−6.15 to 408	4,14,409,413,416,481,484,486,535,539,546,551,[illegible], 559,562,565,566,568,572
Phenol, C_6H_5OH	440.93	86.70	−7.01	400 at 222°C	40.75 to 395	14
Cycloalkanes						
Cyclopropane, C_3H_6	396.82	−42.10	−6.72	216	−127.42 to 117.0	431
Cyclobutane, C_4H_8	346.67	−29.07	−3.62	230	−90.73 to 162.0	431
Cyclopentane, C_5H_{10}	511.73	−61.80	−1.39	319	−93.88 to 215.0	14,481,539,606,
Cyclohexane, C_6H_{12}	388.26	−22.72	−3.30	293	6.55 to 254.0	14,481,486,496,539,566,605,606
Olefin monomers						
Isobutylene, C_4H_8	555.29	−124.28	6.23	245	−140.35 to 100.0	14,481
Styrene, $C_6H_5CHCH_2$	643.97	−60.82	0.40	411	−30.6 to 350	14,481

Correlation constants: thermal conductivity of liquids (continued) Table 23—IV

Compound	$k_L = A + BT + CT^2$					References
	A	$B \times 10^2$	$C \times 10^4$	k_L at 20°C, (micro-cal)/(s) (cm) (°K)	Range, °C	
Diolefins						
1,3 Butadiene, C_4H_6	718.26	−187.18	11.74	268	−108.9 to 120.0	481
Isoprene, C_5H_8	523.95	−75.70	−1.32	290	−146 to 160	445,646
Chloroprene, C_4H_5Cl	459.65	−82.14	3.56	252	−130 to 220	481
Organic oxides						
Ethylene oxide, C_2H_4O	676.62	−79.51	−2.85	369	−112.50 to 180	14,481
Propylene oxide, C_3H_7O	563.51	−53.40	−5.08	363	−112 to 180	14,481
Butylene oxide, C_4H_9O	512.56	−28.56	−7.30	366	−150 to 240	14,481
Primary alcohols						
Methanol, CH_3OH	770.13	−114.23	2.79	459.2	−97.6 to 210.0	6,9,14,19,416,475,486,562,637,646,674,680,684,685, 686,690,694
Ethanol, C_2H_5OH	628.0	−91.88	5.28	404	−114.1 to 190	6,9,14,19,416,475,484,846,537,562,639,646,674,680, 684,685,686,690,694
n-Propanol, C_3H_7OH	442.74	−8.04	−5.29	368	−126.2 to 220	9,14,465,486,562,637,646,663,680,684,685,686,690, 694,704
n-Butanol, C_4H_9OH	546.51	−64.42	0.316	361	−89.3 to 230.0	6,14,416,475,484,486,561,637,646,663,680,684,685, 686,690,694
Chloromethanes						
Methyl chloride, CH_3Cl	902.96	−158.57	−4.21	402	−97.7 to 123.0	19,637,708 717
Methylene chloride, CH_2Cl_2	537.74	−60.47	−2.69	338	−96.7 to 186.0	481,637,708,717
Chloroform, $CHCl_3$	390.25	−20.59	−5.06	287	−63.2 to 237.0	9,19,481,532,637,708,717
Carbon tetrachloride, CCl_4	383.95	−45.45	−0.24	249	−22.9 to 224.0	9,19,475,481,532,540,637,646,707,708,717



Thermal conductivity of a liquid (toluene) **Fig. 4**

Correlation constants—Table 23—IV

The thermal conductivity of a saturated liquid was correlated as a function of temperature by the relation:

$$k_L = A + BT + CT^2 \qquad (23\text{—}4)$$

where k_L = thermal conductivity of saturated liquid, microcal/[(s)(cm)(K)]; A, B, C = correlation constants for a chemical compound; and T = temperature, K.

Deviations between data and calculated results were minimized by using a generalized least-squares computer program to determine the correlation constants. Average deviations in most cases are less than 2.5%.

The correlation constants are presented in Table 23—IV. The usable temperature range covers the saturated liquid-phase from the melting point to temperatures above the boiling point, and in the region 80–90% of T_c of the critical point. The results are not recommended in the immediate vicinity of the critical point (90–100% of T_c). Correlation and data values are compared in Fig. 23—4 for a representative chemical.

Example 23-5—Estimate the thermal conductivity of liquid toluene ($C_6H_5CH_3$) at 150°C. To solve this problem, substitute the correlation constants ($A = 485.1$; $B = -53.8 \times 10^{-2}$; $C = -0.59 \times 10^{-4}$) from Table 23—IV, and the temperature ($T = 150$°C = 423.16 K) into Eq. 23—4:

$$k_L = A + BT + CT^2$$
$$= 485.1 - (53.84)(10^{-2})(423.16) - (0.59)(10^{-4})(423.16)^2$$
$$= 247 \text{ microcal/(s)(cm)(K)}$$

The calculated and data values compare favorably (247 versus 249).

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Biographical sketches for **Joseph W. Miller, Jr., Gordon R. Schorr** and **Carl L. Yaws** appeared in the Aug. 16 issue, p. 87, 1976. **J. W. Miller** was formerly a process engineer with E. I. du Pont de Nemours & Co.