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PHYSICAL PROPERTIES OF CHEMICAL COMPOUNDS

A systematic tabular presentation of accurate data on the physical properties of 511 organic cyclic compounds compiled by R. R. Dreisbach of the Dow Chemical Co. These comprehensive and basic data were determined for specially prepared, high purity compounds. In addition to the precisely measured properties the author has calculated new values for many constants based upon his new experimental values.



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Introduction

THERE IS A CONTINUING NEED for reliable physical properties of pure chemical compounds by scientists and engineers. Many properties are already available in the literature but the reader often finds himself in doubt as to what extent they should be relied upon. Some of the data are obviously inconsistent, while in some cases it is apparent that precise determinations have been made on compounds of doubtful purity.

Some years ago, Mr. Dreisbach began a systematic compilation of reliable physical properties of pure compounds for his own use and for the use of his associates. As this work progressed, he became intrigued with the possibilities of correlating apparently unrelated properties through the use of well-known equations and others developed by himself. In this way he was able to cross-check calculated values with those carefully determined for this purpose and for the hydrocarbons in the well-known API Project 44. These relationships are now well enough understood so that it is possible to predict a large number of physical properties of a compound quite accurately from a few accurately determined properties.

This compilation of physical properties of organic compounds contains considerable data not hitherto published. It also includes parameters which can be used for interpolating and extrapolating the determined data for practically all the compounds listed.

It is in keeping with the long-established publishing program of The Dow Chemical Co. that these data are now made generally available to scientists and engineers everywhere.

H. S. NUTTING, Director
Central Research Index
The Dow Chemical Co.

Physical Properties Of Chemical Compounds

R. R. Dreisbach

The Dow Chemical Co., Midland, Mich.

Definition of the Symbols and Parameters Used, with the Methods of Calculating the Parameters

Mol. % Pur.: Mole % purity by weight.

F.P.: Freezing point, ° C.

F.P. 100%: Freezing point curve, extrapolated to 100% purity.

B.P. 760 mm., 100 mm., etc.: Boiling points at these pressures, ° C.

P₂₅: Pressures at 25° C., in mm.

P_s: Pressure corresponding to temperature t_s in mm.

d₂₀, etc.: Density at 20° C., etc., g./ml.

a, b: Constants of Law of Rectilinear Diameters, $d_v + d_L = a + bt$

d_v = density of the vapor, g./ml.; d_L = density of the liquid, g./ml.

n_D²⁰, etc.: Refractive index for the sodium line at 20° C., etc.

"C": Constant of the Eykman equation, $(n_D^2 - 1)/(n_D + 0.4) \times 1/d = "C"$

MR (obs.): Molal refraction (obs.) = $(n_D^2 - 1)/(n_D^2 + 2) \times M/d = \text{MR at } 20^\circ \text{ C.}$
(M = mol. wt.)

MR (calc.): Molal refraction calculated from atomic refractive indices. See page 9.

($n_D - d/2$): Refractivity intercept equals refractive index minus one half the density, both at the same temperature, 20° C.

D: Dielectric constant run at a frequency of 10^5 (cycles/sec.) and at 25° C. unless otherwise noted. When reported as data of The Dow Chemical Co., error about ± 0.005 . Where Reference 5 is noted it was obtained by squaring the refractive index at 20° C.

A, B, C: Constants of the Antoine vapor pressure equation for the liquid state, giving P (pressure) in mm. and t (temperature) in ° C. This is in the range between the temperatures as indicated. These temperatures in general are the boiling point at 30 mm. to a T_R of 0.75 to 0.80. See method of obtaining A, B, C on page 6.
Antoine equation: $\log P = A - B/(t + C)$

A*, B*, K, c, t_k , t_x : Constants of the saturated vapor density equation
 $\log d_v(\text{g./ml.}) = A^* - B^*/(t + C)$ to the temperature t_k
 $\log d_v(\text{g./ml.}) = A^* - B^*/(t + C) + K/(1.1 T_c - 273.2 - t) + c$
 from temperature t_k to a reduced temperature, T_R , of 0.92
 t_k = Temperature at which it is necessary to change from the simple vapor density equation to the corrected vapor density equation in the higher ranges, ° C.
 $t_k = t_x + K/c$ and $t_x = (1.1 T_c - 273.2)^\circ \text{C.}$

A* and B* where the latent heat at the atmospheric boiling point is available.

$$V_g - V_L = (31381.7 \times \Delta H_v \times dt/dp)/T$$

Where the latent heat is not available use

$$M(\Delta H_v)/T_B = 21.0 \text{ and from this } \Delta H_v = (T_B \times 21.0)/M$$

The value 21.0 (or any other value as 21.4 say) is obtained from the nearest related compound which has a latent heat available. Then proceed as in case where latent heat is available for V_g value at B.P.

Since $d_v = 1/V_g$

$$\log d_{v760} = A^* - B^*/(t_B + C) \text{ at 760 mm.}$$

$$\log d_{v30} = A^* - B^*/(t_{30} + C) \text{ at 30 mm.}$$

Solve for A*, B*, since t and d_v at 760 mm. and 30 mm. and C are known.

A', B', C': Constants of the Antoine vapor pressure equation below 30 mm. pressure, covering the temperature range as indicated. See method of obtaining the constants on page 6.

A'', B'': Constants of the vapor density equation below 30 mm. These two values are obtained by using the boiling point at 30 mm. and the pressure at 25° C. (obtained from the values A', B', C') and assuming that at 25° C. the relationship $PV/RT = 1$. Then we have V_g at 25° C. = $RT/MP = 62,361 \times (25 + 273.2)/MP$.

Then $d_v = 1/V_g$. Inserting these values of vapor density we then solve the two equations for the values of A'' and B'' as in the case of A* and B*.

Ac, Bc, Cc: Constants of the Antoine vapor pressure equation for the liquid state from $T_R = 0.75$ (or a higher T_R as indicated) to the critical temperature. See method of obtaining the constants on page 7.

Cryoscopic Constants, A°, B°: Cryoscopic constants for calculating mole % purity. See *J. Research Natl. Bur. Standards*, 35 (1945); RP 1676.

t_e , °C.: Temperature at which a mole of the vapor occupies 22.414 liters and the vapor is in equilibrium with the liquid, in °C.

$$t_e = \frac{B^*}{(A^* - \log dv_e)} - C$$

dt/dp: Rate of change of boiling point with pressure, given by equation $dt/dp = B/[2.3026 \times P \times (A - \log P)^2]$ °C./mm.

ΔH_m : Latent heat of fusion in cal./g.

ΔH_v : Latent heat of vaporization at the temperature designated, cal./g.

$t_e(d, e)$: The latent heat of vaporization at the temperature t_e as given by the equation $\Delta H_v = d - et$, and indicates the accuracy of this equation at the temperature t_e .

$\Delta H_v/T_e$: Molal latent heat of vaporization at t_e divided by T_e . (Equal to the molal entropy of vaporization at t_e .)

$d, e; d', e'$: These are parameters of the latent heat of vaporization equation, ΔH_v (cal./g.) = $d - et$. This is valid between the temperatures indicated. It has been found that the latent heat between the boiling point at 30 mm. and the boiling point at 760 mm. is almost a linear function of the temperature. As seen in most cases this equation holds almost to the temperature t_e . Above and below this the latent heat is not linear with temperature except for short intervals.

d_c : Critical density, g./ml.

v_c : Critical volume, ml./g.

t_c : Critical temperature, °C. See also page 7.

P_c mm.: Critical pressure in mm. Where this was not obtained from the literature it is calculated as follows (The Thomson method, private communication from George W. Thomson): The critical temperature is inserted in the Antoine equation, using the A, B, and C values to calculate the critical pressure.

This value is too low. This is then multiplied by 1.07 and is assumed to be the critical pressure. In the great majority of cases, this will agree with determined values to within $\pm 3\%$. For high boiling compounds this value must be decreased, since in most cases there is somewhat irregular drift with increasing temperature, so this should be continually lowered as the boiling point becomes increasingly higher.

PV/RT: Compressibility at the temperature designated.

$$z = PV/RT$$

where P = pressure in mm., V = volume in ml./mole, and $R = 62361$.

ΔH_c : Heat of combustion, kcal./mole, gas at constant pressure, 298.16° K. or 25° C.

ΔH_f : Heat of formation, kcal./mole, liquid at 298.16° K. or 25° C.

ΔF_f : Free energy of formation, kcal./mole, liquid at 298.16° K. or 25° C.

η : Kinematic viscosity in centistokes, at temperature designated. The kinematic viscosity is given by the equation

$$\log \eta = A^* + B^*/T$$

between the temperatures indicated to an accuracy of 1% or better.

B.P. °C., 30 mm.; dt/dp; ΔH_v ; PV/RT: These values at 30 mm. are calculated from the Antoine equation using A, B, and C. It has been found that at 30 mm. in almost all Cox Chart Families the ratio PV/RT is negligibly different from one. This, then, has been taken as one point (the other point being the B.P. at 760 mm.) from which to calculate A^* and B^* , always assuming the compressibility as 1.0000 at 30 mm.

c_p : Specific heat at constant pressure at temperature designated, cal./g. ° K.

c_v : Specific heat at constant volume at temperature designated, cal./g. ° K.

f, g, h, f', g', h' : Parameters of the heat content equation for the liquid for the temperature ranges designated, ° K.

$$c_p (\text{liquid}) = f + gT + hT^2$$

m, n, o, m', n', o' : Parameters of the heat content equation for the vapor for the temperature ranges designated, ° K.

$$c_p (\text{vapor}) = m + nT + oT^2$$

γ : Surface tension in dynes/cm., at temperature designated.

[P]: Parachor at the temperature designated:

$$M(\gamma)^{1/4}/(d_L - d_v) = [P]$$

[P] Sugd.: Parachor from atomic and structural values as given by Sugden. See Table. The parachor value for oxygen as hydroxyl (alcohols) in these tables is taken as 15. Sugden gives the values of 20 for oxygen and 30 for oxygen in esters, which does not seem to work for alcohols and phenols.

Exp. L.L.; Exp. L.U.: Explosion limits lower and upper range, % by wt.

Dispersion: Specific dispersion, $10^4(n_F - n_C)/d$, ml./g. at 25° C.

n_F, n_C = refractive index for F and C lines.

d = density, g./ml.

Flash and Fire Points, ° C.: Cleveland open cup (ASTM D 92-46) if not otherwise designated. Closed cup (ASTM D 56-36) will be designated as such.

M Spec.: Mass Spectrograph.

Ultra V.: Ultraviolet.

X-Ray Dif.: X-Ray Diffraction.

Infrared: Infrared Spectrograph.

Solubility at 25° C., in solvents as designated.

Explanation of the methods used for calculating the various parameters in the foregoing:

A, B, C: The A, B, and C constants, except where given by the API reports, are calculated by means of the Thomson method [*Chem. Revs.*, **38**, 1-39 (1946)] using the determined boiling points at three different pressures. The three formulas for this are as follows:

$$(y_3 - y_2)/(y_2 - y_1) \cdot (t_2 - t_1)/(t_3 - t_2) = 1 - (t_3 - t_1)/(t_3 + C)$$

$$B = (y_3 - y_1)/(t_3 - t_1) \cdot (t_1 + C)(t_3 + C) \text{ and}$$

$$A = y_1 + B/(t_1 + C)$$

where y_1, y_2 , and y_3 are equal to $\log P_1, \log P_2$, and $\log P_3$ at temperatures t_1, t_2 , and t_3 .

Unless the data for the three points are *very* accurate the C value can be considerably in error. As a check on this method an empirical formula developed by Thomson (private communication from George W. Thomson) will give a much better value of C if the data are much in error. This formula is $C = 239 - 0.19t_B$. The A and B values can then be readily determined from the two points given, since they are much less critical.

A', B', C' (for pressures below 30 mm.): Applicable when molar heats of vaporization are available at 25° C. and the Antoine equation can be used to obtain the boiling point at 30 mm. Let A, B, C be the constants of the usual Antoine equation valid above 30 mm. and let A', B', C' be the constants of the Antoine equation sought for below 30 mm. These two equations are taken to give the same value of the pressure-temperature slope at 30 mm.

$$\log 30 = A - B/(t_1 + C) = A' - B'/(t_1 + C')$$

$$B'/(t_1 + C')^2 = B/(t_1 + C)^2$$

Since PV/RT may be assumed to be 1.0000 at t_1 , the temperature corresponding to 30 mm., and is also 1.0000 at 25°C ., the molar heat of vaporization at 25°C ., $M\Delta H_{v_2}$, is given by

$$M\Delta H_{v_2} = 2.3026 RB' [(t_2 + 273.2)/(t_2 + C')]^2$$

where $t_2 = 25^\circ \text{C}$. To solve for A' , B' , C' let

$$g_2 = M\Delta H_{v_2}/2.3026 R(t_2 + 273.2)^2 = M\Delta H_{v_2}/406883 \text{ if } t_2 = 25^\circ \text{C}.$$

$$\text{Also } g_2 = B'/(t_2 + C')^2$$

Since t_1 , t_2 and all values on left hand side of equations above are known then B' and C' are readily obtained as follows:

$$[B'/(t_2 + C')^2][(t_1 + C')^2/B'] = g_2 (t_1 + C')^2/B' = \text{say, } h^2$$

$$\text{Then } C' = (t_1 - ht_2)/(h - 1) \text{ and } B' = g_2(t_2 + C')^2$$

$$\text{Also } B' = B[(t_1 + C')/(t_1 + C)]^2$$

$$A' = \log 30 + B'/(t_1 + C') \text{ since } P_1 = 30 \text{ mm.}$$

These formulas were developed with the aid of George Thomson.

When heats of vaporization at 25°C . are not known:

In this case the C' value is estimated and A' and B' are calculated from known data. It was noticed that C' has a value approximately 18 higher than C when latent heats at 25°C . are known. By adding this increment to C we have C' , then B' from the relation for the first case

$$B' = B[(t_{30} + C')/(t_{30} + C)]^2$$

and then A' as in first case.

Ac, Bc, Cc: This method was developed by George Thomson [*Chem. Revs.*, **38**, No. 1, 23 (1946)] and is similar to the one for obtaining A' , B' , C' . It is assumed that the parameters A , B , C of the Antoine equation are good to a T_R 0.75 or a higher reduced temperature, and this temperature corresponds to the 25°C . in the case of A' , B' , C' , and the critical point corresponds to the 30 mm. point.

$$B/(t_1 + C)^2 \cdot (t_c - t_1)/(y_c - y_1) = 1 + (t_c - t_1)/(t_1 + Cc)$$

$$\text{and } Bc = (y_c - y_1)/(t_c - t_1) \cdot (t_1 + Cc)(t_c + Cc); \text{ Ac} = B/(t_c + Cc) + y_c$$

where $t_1^\circ \text{C} = T_R$ 0.75, $t_c^\circ \text{C} =$ critical temperature

$$y_1 = \log P \text{ at } t_1, y_c = \log P_c$$

The first equation is used to evaluate Cc , the second, Bc , and the third, Ac .

Association: The association in the vapor phase of organic acids seems to vary inversely as the temperature for some acids, at least for part of the range. In part of the range, and also apparently for some acids over the whole range, the association is fairly constant. The association is given in these sheets by the formula $M_x = p - rt$. For instance, for acetic acid this formula would be $M_x = 2.225 - 0.004085 t$ from 0°C . to 100°C . From 100°C . to a T_R of 0.92, $M_x = 1.85$. That is to say, the vapor density as calculated by the A^* , B^* formula would have to be multiplied by this correction factor to take care of the association. Further, if the reciprocal of the density is used as calculated to give vapor volume, it would be necessary to divide by 1.85 to get the actual vapor volume.

t_c : Where the critical temperature has not been determined, it is calculated by Watson's equation:

$$T_c/T_c = 0.283(M/d.)^{0.18}$$

where $d.$ = liquid density, g./ml. at the boiling point, and M = molecular weight.

This is used for all hydrocarbons and halohydrocarbons.

f, g, h, m, n, o, etc.: For a short temperature range the equation $C_p = f + gT + hT^2$ reproduces almost exactly determined data. The parameters were set up on the IBM machines using eight determined values where that many or more were available.

The IBM machines were used to set up the Antoine constants from determined data. A preliminary C value was obtained from the equation $C = 239. - 0.19t_B$. A and B were then obtained and new C values either side of the first C used and new A and B values found. In each case above, the boiling points at the experimental pressures were calculated and compared with the determined boiling points.

Actually the value of C was generally obtained from $C = 239. - 0.19t_B$, since the determined values must be *very very* accurate to give better values of C.

Cox Chart Families

- | | |
|----------------------------|---|
| 1. Alkyl and halo benzenes | 12. Aromatic alcohols (Phenyl ethyl alcohols) |
| 2. Styrenes | 13. Aromatic ketones |
| 3. Thiaalkyl benzenes | 14. Aromatic esters |
| 4. Thiophenes | 15. Cyclopentanes |
| 5. Alkyl naphthalenes | 16. Cyclopentenes |
| 6. Tetrahydronaphthalenes | 17. Thiacyclopentanes |
| 7. Decahydronaphthalenes | 18. Thiacyclopropanes |
| 8. Aromatic phenols | 19. Cyclohexanes |
| 9. Thiophenols | 20. Cyclohexenes |
| 10. Aromatic amines | 21. Thiacyclohexanes |
| 11. Nitrobenzenes | 22. Miscellaneous |

Atomic Refractive Indices Used for Computing Molecular Refractive Index

All values are for the sodium line.

Carbon singly bound and alone	2.592	NO as nitrites	5.91
Carbon singly bound	2.418	NO as nitrosoamine	5.37
Carbon double bond	1.733	NO ₂ as alkyl nitrite	7.44
Carbon triple bond	2.398	NO ₂ as alkyl nitrate	7.59
Carbon conjugated	1.27	NO ₂ as nitro paraffin	6.72
Hydrogen	1.100	NO ₂ as nitro aromatic	7.30
Oxygen—hydroxyl	1.525	NO ₂ as nitramine	7.51
Oxygen—ethereal	1.643	Fluorine	0.95*
Oxygen—ketonic	2.211	Chlorine	5.967
Oxygen—as ester	1.64	Bromine	8.865
Sulfur—as SH	7.69	Iodine	13.900
Sulfur—as RSR	7.97		
Sulfur—as RCNS	7.91		
Sulfur—as RSSR	8.11		
Nitrogen			
as aliphatic primary amine	2.45		
as aromatic primary amine	3.21		
as aliphatic secondary amine	2.65		
as aromatic secondary amine	3.59		
as aliphatic tertiary amine	3.00		
as aromatic tertiary amine	4.36		
as hydroxylamine	2.48		
as hydrazine	2.47		
as aliphatic cyanide	3.05		
as aromatic cyanide	3.79		
as aliphatic oxime	3.93		
as primary amide	2.65		
as secondary amide	2.27		
as tertiary amide	2.71		


* This value for one fluorine atom attached to carbon. The value 1.1 is to be used for each fluorine atom in polyfluorides.

Atomic and Structural Constants for Calculation of Parachor


	Sugden		Sugden
CH ₂	39.0	Br.....	68.0
C.....	4.8	I.....	91.0
H.....	17.1	Single bond.....	..
O.....	20.0	Double bond.....	23.2
O (Alcohol).....	15.0	Triple bond.....	46.6
O ₂ (Ester).....	60.0	3-Membered ring.....	16.7
N.....	12.5	4-Membered ring.....	11.6
N (Nitrile).....	14.4	5-Membered ring.....	8.5
S.....	48.2	6-Membered ring.....	6.1
F.....	25.7	7-Membered ring.....	..
Cl.....	54.3	Aliphatic alcohol...subtract	6.0

TABLE I. ALKYL AND HALO BENZENES


No. 1

NAME		Benzene		STRUCTURAL FORMULA	
					
Mole % Pur.	99.996	Ref. 2	Molecular Formula C ₆ H ₆	Molecular Weight 78.108	
		Ref.		Ref.	
F.P. °C	5.533	2	dt/dP °C/mm		
F.P. 100%			25°C	0.2276	5
B.P. °C			BP	0.04272	2
760 mm	80.100	2	t _e	0.0355	5
100	26.075	2	30 mm	0.5949	4
30	2.30	4	ΔHm cal/g	30.09	2
10	-15.7	5	ΔHv cal/g		
1	-45.	5	25°C	103.57	2
Pressure			30 mm	108.19	4
mm 25°C	95.18	5	BP	94.14	2
t _e	964.4	5	t _e	92.65	5
Density			t _e (d, e)	92.71	5
g/ml 20°C	0.87901	2	ΔHv/T _e	20.03	5
d _t 25	0.87370	2	d 25 to	107.85	5
d ₄ 30	0.86837	4	e 90 °C	0.1711	5
a	0.90025	4	d' 0 to	108.79	5
b	-0.00105	4	e' 25 °C	0.2088	5
Ref. Index			d _e g/ml	0.300	2
n _D 20°C	1.50112	2	v _c ml/g	3.333	2
25	1.49792	2	t _c °C	289.45	2
30	1.49468	4	P _c mm	36936.	2
"C"	0.7500	4	PV/RT		
MR (Obs.)	26.1835	2	25°C	0.9922	4
MR (Calc.)			30 mm	1.0000	5
(n _D -d/2)	1.06162	2	BP	0.9658	4
Dielectric	2.283	1	t _e	0.9596	5
A 0 to	6.90565	2	t _c	0.274	2
B 160 °C	1211.033	2	ΔHc kcal/m	757.52	2
C 220.79		2	ΔHf	11.718	2
A* 15 to	1.19411	4	ΔHf	29.756	2
B* 150 °C	1127.9	4	Viscosity		
K	25.0	4	centistokes		
c	-0.13147	4	η 20 °C	0.7427	1
t _k 150 to	155.	4	30	0.6592	1
t _x 245 °C	345.8	5	50	0.5156	1
A' to			70	0.4148	1
B' °C			B _v 25 to	523.4	4
C' °C			A _v 80 °C	2.09290	4
A* to			{B _v } to		
B* °C			{A _v } °C		
Ac 160 to	7.42912	5	c liq. 300°K	0.4178	3 ²
Bc 1628.32		5	320	0.4315	3 ²
Cc 279.56		5	c _p vap. 300°K	0.2516	2
Cryos. A°	0.01523	2	400	0.3424	2
consts. B°	0.0032	2	c _v vap.		
t _e °C	88.04	5			
TR = 0.77 T _c		# closed cup		+ grams/100 grams solvent	
REFERENCES: 1-Dow 2-API 3-Lit. 4-Calc. from det. data 5-Calc. by formula					
SOURCE: API					
PURIFICATION: API					
LITERATURE REFERENCES: 3 J.A.C.S. 73, 1573 (1951); 3 ¹ Chem. Met. Eng. 44-12, 733 (1947); 3 ² Timmermans					

No. 2

NAME		Toluene		STRUCTURAL FORMULA		
		Methylbenzene				
Mole % Pur.	99.999	Ref. 2	Molecular Formula C ₇ H ₈	Molecular Weight 92.134		
		Ref.		Ref.	Ref.	
F.P. °C	-94.991	2	dt/dP °C/mm		f 5 to 0.3971 4	
F.P. 100%			25°C	0.6803 4	g 110 °K -0.0359 4	
B.P. °C			BP	0.0463 2	h 0.0521 4	
760 mm	110.625	2	t _e	0.0360 5	f' to	
100	51.944	4	30 mm	0.6487 4	g' °K	
30	26.04	4	ΔHm cal/g	17.17 2	h'	
10	6.37	5	ΔHv cal/g		m 300 to -0.0654 4	
1	-26.1 ?	5	25°C	98.55 2	n 1700 °K -0.0013 4	
Pressure mm 25°C	28.437	4	30 mm	97.9 5	o -0.0655 4	
t _e	1048.2	4	BP	86.80 2	m' 700 to 0.0471 4	
Density g/ml 20°C	0.86694	2	t _e (d,e)	84.73 5	n' 1100 °K 0.0398 4	
d ₄ 25	0.86230	2	ΔHv/T _e	85.17 5	o' -0.0635 4	
d ₄ 30	0.85757	4	d 25 to 101.98 5	Surface tension dynes/cm. 20°C		
a	0.88547	4	e 130. °C 0.1372 5	30	28.53 2	
b	-0.03924	4	e' to °C	40	27.32 2	
Ref. Index					26.15 2	
n _D 20°C	1.49693	2	d _c g/ml	0.288 2	Parachor [P]	
25	1.49414	2	v _c ml/g	3.473 2	20°C	245.63 4
30	1.49129	4	t _c °C	320.8 2	30	245.68 4
"C"	0.7545	4	P _c mm	30400. 2	40	245.71 4
MR (Obs.)	31.095	2	PV/RT		Sugd.	246.1 5
MR (Calc.) (nD-d/2)	30.925	5	25°C	0.9968 4	Exp. L.I. %/wt.	1.24 3'
	1.06346	2	30 mm	0.9966 4	u.	19.3 3'
Dielectric	2.379	3	BP	0.9613 4	Dispersion	184.7 2
A 20 to	6.95334	2	t _e	0.9522 5	Flash Point °C	4.44* 3'
B 200 °C	1343.943	2	t _c	0.263 4	Fire Point	
C	219.377	2	ΔHc kcal/m	901.50 2	M Spec.	Yes 1
A* 20 to	1.27923	4	ΔHf	2.867 2	Ultra V.	Yes 1
B* 175 °C	1252.3	4	ΔFf	27.282 2	X-Ray Dif.	
K	23.	5	Viscosity centistokes		Infrared	865. 1
c	-0.11760	5	η		Solubility in +	
t _k 175 to	175.	5	20 °C	0.67778 1	Acetone	∞
t _x 270 °C	380.0	5	40	0.56457 1	Carbon tet.	∞
A' to			60	0.45825 1	Benzene	∞
B' °C			80	0.39119 1	Ether	∞
C' °C			B ^v 40 to	440.66 4	n-Heptane	∞
A'* to			A ^v 90 °C	2.34476 4	Ethanol	∞
B'* °C			(B ^v) to		Water	7.3 1
Ac 200 to	7.45657	4	(A ^v) °C		Water in	0.055 1
Bc t _c °C	1796.9	4	c _p liq. °K			
Cc °C	284.62	4	c _p vap. 300°K	0.2708 2		
Cryos. A°	0.02508	2	400	0.3609 2		
consts. B°	0.0019	2	c _v vap.			
t _e °C	122.34	5				
* closed cup						
+ grams/100 grams solvent						
REFERENCES: 1-Dow 2-API 3-Lit. 4-Calc. from det. data 5-Calc. by formula						
SOURCE: API						
PURIFICATION: API						
LITERATURE REFERENCES: 3 NBS 514; 3' Nat. Fire Prot. Assoc. 325 (1949)						

No. 4

NAME		o-Xylene		STRUCTURAL FORMULA	
		1,2-Dimethylbenzene			
Mole % Pur. 99.999	Ref. 2	Molecular Formula C ₈ H ₁₀	Molecular Weight 106.160		
		Ref.		Ref.	
F.P. °C	-25.182	2	dt/dP °C/mm	2.545	5
F.P. 100%			25°C	0.0497	2
B.P. °C			BP	0.0359	5
760 mm	144.411	2	t _e	0.7002	4
100	81.31	2	30 mm		
30	53.38	4	ΔHm cal/g	30.61	2
10	32.0	5	ΔHv cal/g		
1	-3.7	5	25°C	97.79	2
Pressure mm 25°C	6.688	5	30 mm	95.05	4
t _e	1149.	5	BP	82.90	2
Density g/ml 20°C	0.88020	2	t _e	80.75	5
d ₄ 25	0.87596	2	t _e (d, e)	80.72	5
d ₄ 30	0.87172	4	ΔHv/T _e	19.75	5
a	0.89715	4	d 50 to °C	102.17	4
b	-0.03846	4	e 160 to °C	0.1334	4
Ref. Index n _D 20°C	1.50545	2	d' 10 to °C	100.21	4
25	1.50295	2	e' 50 °C	0.0967	4
30	1.50025	4	d _v g/ml	0.28	2
"C"	0.7550	4	v _c ml/g	3.58	2
MR (Obs.)	35.800	2	t _c °C	359.0	2
MR (Calc.)	35.543	5	P _c mm	27360.	2
(nD-d/2)	1.06535	2	PV/RT 25°C	1.0000	5
Dielectric	2.266	5	30 mm	1.0000	5
A 50 to	6.99891	2	BP	0.9630	4
B 200 °C	1474.679	2	t _e	0.9518	5
C	213.686	2	t _c	0.26	2
A* 50 to	1.36031	5	ΔHc kcal/m	1045.94	2
B* 170 °C	1380.0	5	ΔHf	-5.841	2
K			ΔFf	26.370	2
c			Viscosity centistokes		
t _k to °C			η 20 °C	0.919	2
t _x to °C			40	0.724	2
A' 25 to	7.35638	5	60	0.592	2
B' 55 °C	1671.8	5	80	0.497	2
C'	231.0	5	B ^v 25 to	449.07	4
A* 25 to	1.71752	5	A ^v 90 °C	2.42593	4
B* 55 °C	1570.59	5	(B ^v) 90 to	436.36	4
Ac 200 to	7.4175	5	(A ^v) 150 °C	2.45900	4
Bc t _c °C	1842.1	5	c _p liq. °K		
Cc	262.4	5	c _p vap. 300°K	0.30162	2
Cryos. A*	0.02659	2	400	0.38649	2
consts. B*	0.0030	2	c _v vap.		
t _e °C	160.74	5			

T_R = 0.75 T_c + grams/100 grams solvent

REFERENCES: 1-Dow 2-API 3-Lit. 4-Calc. from det. data 5-Calc. by formula

SOURCE: API

PURIFICATION: API

LITERATURE REFERENCES: 3 Nat. Fire Prot. Assoc. 325 (1949)