CONTENTS

Introduction

This is a continuation of Mr. Dreisbach's compilation of physical properties of organic compounds. Data on 511 cyclic compounds were published in 1955 as Number 15 of the ADVANCES IN CHEMISTRY SERIES under the title of "Physical Properties of Chemical Compounds." The present volume includes 476 acyclic compounds.

As in the earlier volume, this compilation contains many data not hitherto published. It also includes parameters which can be used for interpolating and extrapolating the determined data for practically all of the compounds listed.

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Physical Properties of Chemical Compounds

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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.

P_{25}: Pressures at 25°C., in mm.

P_t: Pressure corresponding to temperature t, in mm.

d^{20}, 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_D^{20}, 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 (obsd.): Molal refraction (obsd.) = $(n_D^2 - 1)/(n_D^2 + 2) \times M/d$ = MR at 20°C. (M = mol. wt.)

MR (calcd.): Molal refraction calculated from atomic refractive indices. See page 8.

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

D: Dielectric constant determined 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_z: Constants of the saturated vapor density equation
$\log d_v(g./ml.) = A^* - B^*/(t + C)$ to the temperature t_k.
$\log d_v(g./ml.) = A^* - B^*/(t + C) + K/(1.1\ T_c - 273.2 - t) + c$
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.
$t_k = t_z + K/c$ and $t_z = (1.1\ T_c - 273.2)$°C.

A^* and B^* where the latent heat at the atmospheric boiling point is available.
$V_g - V_L = (31381.7 \times \Delta Hv \times dt/dp)/T$

Where the latent heat is not available use
$M(\Delta Hv)/T_B = 21.0$ and from this $\Delta Hv = (T_B \times 21.0)/M$
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 Vg value at B.P.

Since $d_v = 1/Vg$
$\log d_{v760} = A^* - B^*/(t_B + C)$ at 760 mm.
$\log d_{v30} = A^* - B^*/(t_{30} + C)$ 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 Vg at 25°C. $= RT/MP = 62,361 \times (25 + 273.2)/MP$.
Then $dv = 1/Vg$. 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.

$$te = \frac{B^*}{(A^* - \log \mathrm{dv}_e)} - C$$

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. Also $dt/dp = (t + C)^2/2.3\ PB$

ΔHm: Latent heat of fusion in cal./g.

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

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

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

$d, e;\ d', e'$: These are parameters of the latent heat of vaporization equation. ΔHv(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 temperature t_e. Above and below this the latent heat is not linear with temperature except for short intervals.

d_e: Critical density, g./ml.

v_e: Critical volume, ml./g.

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

P_e 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 ±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.

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

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

ΔFf: 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; ΔHv; 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 capacity 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 capacity 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:
$(y_3 - y_2)/(y_2 - y_1)\cdot(t_2 - t_1)/(t_3 - t_2) = 1 - (t_3 - t_1)/(t_3 + C)$
$B = (y_3 - y_1)/(t_3 - t_1)\cdot(t_1 + C)(t_3 + C)$
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., $M\Delta Hv_2$ is given by
$M\Delta Hv_2 = 2.3026\ RB'\ [(t_2 + 273.2)/(t_2 + C')]^2$
where $t_2 = 25$°C. To solve for A', B', C' let
$g_2 = M\Delta Hv_2/2.3026\ R(t_2 + 273.2)^2 = M\Delta Hv_2/406883$ if $t_2 = 25$°C.

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:
$[B'/(t_2 + C')^2][(t_1 + C')^2B'] = g_2(t_1 + C')^2/B' =$ say, h^2
Then $C' = (t_1 - ht_2)/(h - 1)$ and $B' = g_2(t_2 + C')^2$
Also $B' = B[(t_1 + C')/(t_1 + C)]^2$
$A' = \log 30 + B'/(t_1 + C')$ since $P_1 = 30$ 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.
In the case of the alkenes and alkynes the A', B', C' and A'^*, B'^* were not calculated by the above method, since the data for these compounds is much less reliable than in the case of the alkanes.

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 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.
$B/(t_1 + C)^2 \times (t_c - t_1)/(y_c - y_1) = 1 + (t_c - t_1)/(t_1 + Cc)$
and $Bc = (y_c - y_1)/(t_c - t_1) \times (t_1 + Cc)(t_c + Cc)(t_c + C_c)$; $Ac = B/t_c + C_c + y_c$
where t_1 °C. = T_R 0.75, t_c °C. = critical temperature
$y_1 = \log P$ 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° 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:
$T_c/T_o = 0.283\ (M/d_o)^{0.18}$
where d_o = 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. Alkanes
2. Haloalkanes
3. Alkenes
4. Haloalkenes
5. Diolefins
6. Alkynes

Atomic Refractive Indices Used for Computing Molecular Refractive Index

All values are for the sodium line.

Carbon singly bound and alone	2.592
Carbon singly bound	2.418
Carbon double bond	1.733
Carbon triple bond	2.398
Carbon conjugated	1.27
Hydrogen	1.100
Oxygen—hydroxyl	1.525
Oxygen—ethereal	1.643
Oxygen—ketonic	2.211
Oxygen—as ester	1.64
Sulfur—as SH	7.69
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
NO as nitrites	5.91
NO as nitrosoamine	5.37
NO_2 as alkyl nitrite	7.44
NO_2 as alkyl nitrate	7.59
NO_2 as nitroparaffin	6.72
NO_2 as nitro aromatic	7.30
NO_2 as nitramine	7.51
Fluorine	0.95*
Chlorine	5.967
Bromine	8.865
Iodine	13.900

* 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 C. ALKANES

No. 1

NAME	Methane	STRUCTURAL FORMULA
		CH_4

Mole % Pur.	Ref.	Molecular Formula CH_4	Molecular Weight 16.042

		Ref.
F. P. °C	-182.48	2
F. P. 100%		
B. P. °C		
760 mm	-161.49	2
100	-181.45	2
30	-190.	4
10	-195.51≠	2
1	-207.0	5
Pressure mm -140°C	3289.7	5
t_e	272.1	5
Density g/ml -160°C	0.4222	3
d_4^t -150	0.4075	3
-140	0.3916	3
a -160°C	0.4242	3
b	-0.00126	4
Ref. Index n_D 20°C		
25		
30		
"C"		
MR (Obs.)		
MR (Calc.) (nD-d/2)	6.818	5
Dielectric		
A -180 to	6.61184	2
B __ °C	389.93	2
C	266.00	2
A* -165 to	0.74077	4
B* -130 °C	362.78	4
K	7.79	4
c	-0.15125	4
t_k -130 to		
t_x -100 °C	-63.0	5
A' to		
B' __ °C		
C'		
A'* to		
B'* °C		
Ac to		
Bc t_c °C		
Cc		
Cryos. A°	0.0138	2
consts. B°	0.0057	2
t_e °C	-172.65	4

		Ref.
dt/dP °C/mm		
-140°C	0.00537	5
BP	0.0160	2
t_e	0.3567	5
30 mm	0.2141	4
ΔHm cal/g	14.025	2
ΔHv cal/g		
-140°C	115.67	3
30 mm	133.34	5
BP	121.87	2
t_e	125.30	5
t_e (d, e)	126.36	5
$\Delta Hv/T_e$	19.99	5
d -190 to	56.90	5
e -160 °C	0.4023	5
d' to		
e' °C		
d_c g/ml	0.162	2
v_c ml/g	6.17	2
t_c °C	-82.5	2
P_c mm	34808.	2
PV/RT		
-140°C	0.9208	4
30 mm	1.0000	5
BP	0.9628	4
t_e	0.9726	5
t_c	0.290	2
ΔHc kcal/m	191.76	2
ΔHf		
ΔFf		
Viscosity centistokes		
η -180 °C	0.418	2
-175	0.364	2
-170	0.325	2
-165	0.295	2
B^v -180 to	101.76	4
A^v -160 °C	Z.52937	4
(B^v) to		
(A^v) °C		
c_p liq. 300 °K	0.53310	2
400	0.60691	2
c_p vap. °K		
c_v vap.		

			Ref.
f to			
g __ °K			
h			
f' to			
g' __ °K			
h'			
m 300 to		0.1259	4
n 600 °K		0.0015	4
o		0.0_666	4
m' 700 to		0.1408	4
n' 1000 °K		0.0013	4
o'		-0.0_634	4
Surface tension dynes/cm. -180°C		18.0	2
γ -170		15.8	2
-160		13.7#	2
Parachor [P] 20°C			
30			
40			
Sugd.		73.2	5
Exp. L. 1. %/wt. u.			
Dispersion			
Flash Point °C			
Fire Point			
M. Spec.			
Ultra V.			
X-Ray Dif.			
Infrared		Yes	2
Solubility in +			
Acetone			
Carbon tet.			
Benzene			
Ether			
n-Heptane			
Ethanol			
Water			
Water in			

≠ solid # at saturation pressure + 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 Young

No. 2

NAME	Ethane	STRUCTURAL FORMULA
		CH_3CH_3

Mole % Pur.	Ref.	Molecular Formula C_2H_6	Molecular Weight 30.068

		Ref.
F.P. °C	-183.27	2
F.P. 100%		
B.P. °C		
760 mm	-88.63	2
100	-119.33	2
30	-132.74	4
10	-142.88	5
1	-159.51	5
Pressure mm 25°C	29290.	5
t_e	480.9	5
Density g/ml-60°C	0.509	3
d_4^t 20	0.363	3
30	0.30	3
a	0.364	4
b	-0.0363	4
Ref. Index n_D 20°C		
25		
30		
"C"		
MR (Obs.)		
MR (Calc.)		
(nD-d/2)		
Dielectric		
A -132 to	6.80266	2
B -44 °C	656.40	2
C	256.00	2
A* -132 to	0.98156	5
B* -90 °C	613.9	5
K		
c		
t_k to		
t_x °C		
A' to		
B' °C		
C'		
A'* to		
B'* °C		
Ac -44 to	7.67290	5
Bc t_c °C	1096.9	5
Cc	320.54	5
Cryos. A*	0.04256	2
consts. B*	0.0095	2
t_e °C	-96.7	5

		Ref.
dt/dP °C/mm		
25°C	0.00213	5
BP	0.0244	2
t_e	0.0351	5
30 mm	0.3350	5
ΔHm cal/g	22.728	2
ΔHv cal/g		
25°C	76.86	5
30 mm	129.71	5
BP	116.97	2
t_e	119.45	5
t_e (d, e)	119.33	5
$\Delta Hv/T_e$	20.36	5
d -132 to	91.37	5
e -90 °C	0.2888	5
d' to		
e' °C		
d_c g/ml	0.203	2
v_c ml/g	4.92	2
t_c °C	32.27	2
P_c mm	36632.	2
PV/RT		
25°C	1.0000	5
30 mm	1.0000	5
BP	0.9622	5
t_e	0.9735	5
t_c	0.288	2
ΔHc kcal/m	341.26	2
ΔHf		
ΔFf		
Viscosity centistokes		
η -120 °C	0.438	2
-110	0.387	2
-100	0.348	2
-90	0.314	2
B^V -130 to	135.71	4
A^V -80 °C	2.75615	4
(B^V) to		
(A^V) °C		
c_p liq. °K		
c_p vap. 300 °K	0.41225	2
400	0.52148	2
c_v vap.		

		Ref.
f	to	
g	°K	
h		
f'	to	
g'	°K	
h'		
m	to	
n	°K	
o		
m'	to	
n'	°K	
o'		
Surface tension dynes/cm. 110°C	19.57	2
100	17.93	2
-90	16.31	2
Parachor [P] 20°C		
30		
40		
Sugd.	112.2	5
Exp. L. t. %/wt.		
u.		
Dispersion		
Flash Point °C		
Fire Point		
M Spec.		
Ultra V.		
X-Ray Dif.		
Infrared		
Solubility in +		
Acetone		
Carbon tet.		
Benzene		
Ether		
n-Heptane		
Ethanol		
Water		
Water in		

T_R = 0.75 T_c ≠ at saturation pressure + 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 Young

TABLE C. ALKANES

No. 3

NAME	Propane	STRUCTURAL FORMULA
		$CH_3-CH_2-CH_3$

Mole % Pur. | Ref. | Molecular Formula C_3H_8 | Molecular Weight 44.094

		Ref.
F. P. °C	-187.69	2
F\P. 100%		
B. P. °C 760 mm	-42.07	2
100	-79.63	2
30	-96.07	4
10	-108.5	4
1	-129.	5
Pressure mm 25°C	7095.	4
t_e	608.5	4
Density g/ml 20°C	0.5005≠	2
d_4^t 25	0.4928≠	2
30	0.4861	4
a	0.5375	4
b	-0.0399	4
Ref. Index n_D 20°C	1.2898	5
25		
30		
"C"	0.766	5
MR (Obs.)		
MR (Calc.)	16.054	5
(nD-d/2)	1.04	5
Dielectric	1.66	5
A -130 to	6.82973	2
B -5 °C	813.200	2
C	248.00	2
A* -100 to	1.05579	5
B* -40 °C	756.21	5
K	17.62	4
c	-0.13012	4
t_k -40 to		
t_x 65 °C	134.0	5
A' to		
B' °C		
C'		
A'* to		
B'* °C		
Ac 5 to	7.33829	4
Bc t_c °C	1090.0	4
Cc	287.8	4
Cryos. A*	0.05802	2
consts. B*	0.0073	2
t_e °C	-46.98	5

		Ref.
dt/dP °C/mm		
25°C	0.00561	4
BP	0.0298	2
t_e	0.0355	5
30 mm	0.4109	4
ΔHm cal/g	19.10	2
ΔHv cal/g		
25°C	81.76	4
30 mm	114.70	5
BP	101.76	2
t_e	102.98	5
t_e (d, e)	102.94	5
ΔHv/T_e	20.07	5
d -100 to	91.68	5
e -45 °C	0.2396	5
d' to		
e' °C		
d_c g/ml	0.220	2
v_c ml/g	4.358	2
t_c °C	96.8	2
P_c mm	31928.	2
PV/RT		
25°C	0.8461	4
30 mm	1.0000	5
BP	0.9612	4
t_e	0.9669	5
t_c	0.278	2
ΔHc kcal/m	488.53	2
ΔHf	-28.643	2
ΔFf		
Viscosity centistokes		
η -80 °C	0.524	2
-70	0.470	2
-60	0.425	2
-50	0.387	2
B^v -85 to	190.47	4
A^v -30 °C	Σ.73347	4
(B^v) -140 to	184.09	4
(A^v) -85 °C	Σ.76598	4
c_p liq. °K		
c_p vap 300°K	0.40051	2
400	0.51118	2
c_v vap.		

			Ref.
f	to		
g	°K		
h			
f'	to		
g'	°K		
h'			
m	300 to	0.0169	4
n	600 °K	0.0014	4
o		$-0.0_6 43$	4
m'	700 to	0.0960	4
n'	1000 °K	0.0012	4
o'		$-0.0_6 40$	4
Surface tension dynes/cm. -70°C		19.2	2
σ -60		17.85	2
-50		16.49	2
Parachor [P] 20°C			
30			
40			
Sugd.		151.2	5
Exp. L. l. %/wt.			
u,			
Dispersion			
Flash Point °C			
Fire Point			
M. Spec.			
Ultra V.			
X-Ray Dif.			
Infrared		Yes	2
Solubility in +			
Acetone			
Carbon tet.			
Benzene			
Ether			
n-Heptane			
Ethanol			
Water			
Water in			
Viscosity centistokes			
η -130°C		1.126	2
-90		0.590	2
-40		0.355	2

T_R = 0.75 T_c ≠ at saturation pressure + 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:

No. 4

NAME	n-Butane	STRUCTURAL FORMULA
		$CH_3CH_2CH_2CH_3$

Mole % Pur.	Ref.	Molecular Formula C_4H_{10}	Molecular Weight 58.120

		Ref.
F.P. °C	-138.350	2
F.P. 100%		
B.P. °C		
760 mm	-0.50	2
100	-44.17	2
30	-63.30	4
10	-77.76	4
1	-101.5	5
Pressure mm 25°C	1823.	4
t_e	724.6	5
Density g/ml 20°C	0.5788≠	2
d_4^t 25	0.5730≠	2
30	0.5671	4
a	0.6039	4
b	-0.0_399	4
Ref. Index n_D 20°C	1.3326≠	2
25	1.3292≠	2
30	1.3252	5
"C"	0.7730	4
MR (Obs.)	20.63≠	2
MR (Calc.)	20.772	5
(nD-d/2)	1.0432≠	2
Dielectric	1.776	5
A | -60 to	6.83029	2
B | 45 °C	945.9	2
C	240.0	2
A* | -60 to	1.11497	5
B* | 30 °C	881.81	5
K		
c		
t_x | to		
t_x | °C		
A' | to		
B' | °C		
C'		
A'* to		
B'* °C		
Ac | 45 to	7.39949	4
Bc | t_c °C	1299.	4
Cc	289.1	4
Cryos. A°	0.03085	2
consts. B°	0.0048	2
t_e °C	-1.75	5

		Ref.
dt/dP °C/mm		
25°C	0.01768	4
BP	0.03465	2
t_e	0.03597	5
30 mm	0.4778	4
ΔHm cal/g	19.167	2
ΔHv cal/g		
25°C	86.63	2
30 mm	105.08	5
BP	92.09	2
t_e	92.35	5
t_e (d, e)	92.35	5
$\Delta Hv/T_e$	19.77	5
d | -60 to	91.99	5
e | 0 °C	0.2069	5
d' | 0 to	91.98	4
e' | 30 °C	0.2228	4
d_c g/ml	0.228	2
v_c ml/g	4.387	2
t_c °C	152.01	2
P_c mm	28477.	2
PV/RT		
25°C	0.9286	4
30 mm	1.0000	5
BP	0.9582	4
t_e	0.9595	5
t_c	0.274	2
ΔHc kcal/m	635.05	2
ΔHf	-35.29	2
ΔFf		
Viscosity centistokes		
η -40 °C	0.491	2
-30	0.446	2
-20	0.407	2
-10	0.375	2
B^V | -40 to	234.16	4
A^V | 10 °C	2.68698	4
(B^V) | -100 to	227.42	4
(A^V) | -40 °C	2.71750	4
c_p liq. °K		
c_p vap. 300 °K	0.40261	2
400	0.50929	2
c_v vap.		

			Ref.
f |	to		
g |	°K		
h'			
f' |	to		
g' |	°K		
h'			
m |	300 to	0.0351	4
n |	600 °K	0.0013	4
c		-0.0_640	4
m' |	700 to	0.0974	4
n' |	1000 °K	0.0012	4
o'		-0.0_640	4
Surface tension dynes/cm.	-30°C	18.43	2
γ	-20	17.22	2
	-10	16.02	2
Parachor [P]	20°C		
	30		
	40		
	Sugd.	190.2	4
Exp. L.1.%/wt. u.			
Dispersion			
Flash Point °C		-60.	3
Fire Point			
M Spec.			
Ultra V.			
X-Ray Dif.			
Infrared		Yes	2
Solubility in +			
Acetone			
Carbon tet.			
Benzene			
Ether			
n-Heptane			
Ethanol			
Water			
Water in			
Viscosity centistokes			
η	-90°C	0.91	2
	-50	0.545	2
	0	0.350	2

≠ at saturation pressure $T_R = 0.75\,T_c$ + grams/100 grams solvent

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

SOURCE: API

PURIFICATION: API

LITERATURE REFERENCES: 3 NFPA 325

TABLE C. ALKANES

No. 5

NAME	2-Methylpropane Isobutane		STRUCTURAL FORMULA $CH_3CH(CH_3)_2$
Mole % Pur.	Ref.	Molecular Formula C_4H_{10}	Molecular Weight 58.120

		Ref.
F. P. °C	-159.600	2
F.P. 100%		
B.P. °C 760 mm	-11.730	2
100	-54.07	2
30	-72.52	4
10	-86.4	4
1	-109.2	5
Pressure mm 25°C	2611.	4
t_e	697.	5
Density g/ml 20°C	0.5572≠	2
d_4^t 25	0.5510≠	2
30	0.5450	4
a	0.5846	4
b	-0.0_398	4
Ref. Index n_D 20°C	1.3169	5
25		
30		
"C"	0.7675	5
MR (Obs.)	20.772	5
MR (Calc.) (nD-d/2)		
Dielectric	1.734	5
A -75 to	6.74808	2
B 30 °C	882.80	2
C	240.00	2
A* -75 to	1.04221	5
B* 0 °C	820.37	5
K		
c		
t_k to		
t_x °C		
A' to		
B' °C		
C'		
A'* to		
B'* °C		
Ac 30 to	7.42067	4
Bc t_c °C	1288.1	4
Cc	296.7	4
Cryos. A°	0.04234	2
consts. B°	0.0057	2
t_e °C	-13.90	5

		Ref.
dt/dP		
°C/mm		
25°C	0.0132	5
BP	0.0337	2
t_e	0.0361	5
30 mm	0.4600	4
ΔHm cal/g	18.668	2
ΔHv cal/g		
25°C	78.63	2
30 mm	99.79	5
BP	87.56	2
t_e	87.99	5
t_e (d, e)	88.00	5
$\Delta Hv/T_e$	19.72	5
d -75 to	85.20	5
e -10 °C	0.2011	5
d' -10 to	84.71	4
e' 25 °C	0.2431	4
d_c g/ml	0.221	2
v_c ml/g	4.525	2
t_c °C	134.98	2
P_c mm	27360.	2
PV/RT		
25°C	0.9083	5
30 mm	1.0000	5
BP	0.9648	4
t_e	0.9668	5
t_c	0.283	2
ΔHc kcal/m	633.05	2
ΔHf	-37.87	2
ΔFf		
Viscosity centistokes		
η -50 °C	0.619	2
-40	0.549	2
-30	0.491	2
-20	0.443	2
B^v -90 to	265.10	4
A^v -55 °C	Z.6035	4
(B^v) -55 to	273.73	4
(A^v) 0 °C,	Z.5653	4
c_p liq. °K		
c_p vap. 300°K	0.40003	2
400	0.51222	2
c_v vap.		

			Ref.
f	to		
g	°K		
h			
f'	to		
g'	°K		
h'			
m	300 to	-0.0058	4
n	600 °K	0.0015	4
o		-0.0_658	4
m'	700 to	0.0920	4
n'	1000 °K	0.0013	4
o'		-0.0_641	4
Surface tension dynes/cm. -40°C		17.68	2
γ -30		16.48	2
-20		15.28	2
Parachor [P] 20°C			
30			
40			
Sugd.		190.2	5
Exp. L.1.%/wt, u.			
Dispersion			
Flash Point °C		-87.	5
Fire Point			
M. Spec.			
Ultra V.			
X-Ray Dif.			
Infrared		Yes	2
Solubility in +			
Acetone			
Carbon tet.			
Benzene			
Ether			
n-Heptane			
Ethanol			
Water			
Water in			
Viscosity centistokes			
η -80°C		0.946	2
-60		0.703	2
-10		0.403	2

≠ at saturation pressure $T_R = 0.75\ T_c$ + 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:

No. 6

NAME	n-Pentane	STRUCTURAL FORMULA
		$CH_3(CH_2)_3CH_3$

Mole % Pur. 99.86	Ref. 2	Molecular Formula C_5H_{12}	Molecular Weight 72.146

		Ref.
F.P. °C	-129.721	2
F.P. 100%		
B.P. °C		
760 mm	36.074	2
100	-12.59	2
30	-33.93	4
10	-50.1	4
1	-76.63	5
Pressure mm 25°C	512.5	4
t_w	825.9	5
Density g/ml 20°C	0.62624	2
d_4^{t} 25	0.62139	2
d_4^{t} 30	0.61649	4
a	0.64604	4
b	-0.03904	4
Ref. Index n_D 20°C	1.35748	2
25	1.35472	2
30	1.35194	4
"C"	0.7664	4
MR (Obs.)	25.266	2
MR (Calc.)	25.29	5
(nD-d/2)	1.04436	2
Dielectric	1.843	5
A | -35 to	6.85221	2
B | 80 °C	1064.63	2
C	232.0	2
A* | -35 to	1.18695	5
B* | 60 °C	995.37	5
K	24.0	4
c	-0.16075	4
t_k | 60 to	185.	4
t_x | 160 °C	243.6	5
A' | to		
B' | °C		
C'		
A'* to		
B'* °C		
Ac | 80 to	7.37001	5
Bc | t_c °C	1411.3	5
Cc	279.1	5
Cryos. A*	0.04906	2
consts. B*	0.0042	2
t_e °C	38.54	5

		Ref.
dt/dP °C/mm		
25°C	0.05257	4
BP	0.03856	2
t_e	0.03631	5
30 mm	0.5334	4
ΔHm cal/g	27.805	2
ΔHv cal/g		
25°C	87.54	2
30 mm	98.53	5
BP	85.38	2
t_s	84.92	5
t_c (d, e)	84.92	5
$\Delta Hv/T_e$	19.65	5
d | -35 to	92.16	5
e | 40 °C	0.1879	5
d' | to		
e' | °C		
d_c g/ml	0.232	2
v_c ml/g	4.311	2
t_c °C	196.62	2
P_c mm	25316.	2
PV/RT		
25°C	0.9662	5
30 mm	1.0000	5
BP	0.9547	4
t_s	0.9523	5
t_c	0.268	2
ΔHc kcal/m	782.04	2
ΔHf	-41.36	2
ΔFf	-2.25	2
Viscosity centistokes		
η 0 °C	0.432	2
10	0.401	2
20	0.375	2
30	0.351	2
B^V | -10 to	251.11	4
A^V | 40 °C	Σ.71711	4
(B^V) | -70 to	261.39	4
(A^V) | -10 °C	Σ.67863	4
c_p liq. °K		
c_p vap. 300°K	0.40016	2
400	0.50633	2
c_v vap.		

			Ref.
f |	to		
g |	°K		
h			
f' |	to		
g' |	°K		
h'			
m |	300 to	0.0310	4
n |	600 °K	0.0014	4
o		-0.0_642	4
m' |	700 to	0.0976	4
n' |	1000 °K	0.0012	4
o'		-0.0_641	4
Surface tension dynes/cm.	20°C	16.00	2
γ	30	14.95	2
	40	13.8*	2
Parachor [P]	20°C	231.0	4
	30	231.0	4
	40	230.5	4
	Sugd.	229.2	5
Exp. L.1.%/wt.		3.6	3
u.		18.6	3
Dispersion		98.0	2
Flash Point °C		-40.0	3
Fire Point			
M Spec.			
Ultra V.			
X-Ray Dif.			
Infrared		727.	1
Solubility in +			
Acetone		∞	
Carbon tet.		∞	
Benzene		∞	
Ether		∞	
n-Heptane		∞	
Ethanol		∞	
Water			
Water in			
Viscosity centistokes			
η -60°C		0.803	2
-20		0.514	2
-10		0.469	2

$T_R = 0.75\ T_c$

* at saturation pressure

+ 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 NFPA 325