

Orthobaric densities and molar volumes of liquids Halogenated alkylbenzenes and halogenated styrenes

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The Institution of Chemical Engineers

ESDU DATA ITEM No. 99008

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THE PREPARATION OF THIS DATA ITEM

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ORTHOBARIC DENSITIES and MOLAR VOLUMES OF LIQUIDS HALOGENATED AKYLBENZENES AND HALOGENATED STYRENES

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MONOHALOGENATED TOLUENES

1 $C_6H_5CH_2F$	(Fluoromethyl)benzene	Benzyl fluoride	5
2 $2-FC_6H_4CH_3$	2-Fluorotoluene	<i>o</i> -Fluorotoluene	7
3 $3-FC_6H_4CH_3$	3-Fluorotoluene	<i>m</i> -Fluorotoluene	9
4 $4-FC_6H_4CH_3$	4-Fluorotoluene	<i>p</i> -Fluorotoluene	11
5 $C_6H_5CH_2Cl$	(Chloromethyl)benzene	Benzyl chloride	13
6 $2-ClC_6H_4CH_3$	2-Chlorotoluene	<i>o</i> -Chlorotoluene	15
7 $3-ClC_6H_4CH_3$	3-Chlorotoluene	<i>m</i> -Chlorotoluene	17
8 $4-ClC_6H_4CH_3$	4-Chlorotoluene	<i>p</i> -Chlorotoluene	19
9 $C_6H_5CH_2Br$	(Bromomethyl)benzene	Benzyl bromide	21
10 $2-BrC_6H_4CH_3$	2-Bromotoluene	<i>o</i> -Bromotoluene	23
11 $3-BrC_6H_4CH_3$	3-Bromotoluene	<i>m</i> -Bromotoluene	25
12 $4-BrC_6H_4CH_3$	4-Bromotoluene	<i>p</i> -Bromotoluene	27
13 $C_6H_5CH_2I$	(Iodomethyl)benzene	Benzyl iodide	29
14 $2-IC_6H_4CH_3$	2-Iodotoluene	<i>o</i> -Iodotoluene	31
15 $3-IC_6H_4CH_3$	3-Iodotoluene	<i>m</i> -Iodotoluene	33
16 $4-IC_6H_4CH_3$	4-Iodotoluene	<i>p</i> -Iodotoluene	35

DIHALOGENATED TOLUENES

17 $C_6H_5CHF_2$	(Difluoromethyl)benzene	Benzal fluoride	37
18 $C_6H_5CHCl_2$	(Dichloromethyl)benzene	Benzal chloride	39
19 $2-ClC_6H_4CH_2Cl$	2-Chloro-1-(chloromethyl)benzene	2-Chlorobenzyl chloride	41
20 $3-ClC_6H_4CH_2Cl$	3-Chloro-1-(chloromethyl)benzene	3-Chlorobenzyl chloride	43
21 $4-ClC_6H_4CH_2Cl$	4-Chloro-1-(chloromethyl)benzene	4-Chlorobenzyl chloride	45
22 $2,3-Cl_2C_6H_3CH_3$	2,3-Dichlorotoluene (not issued)		
23 $2,4-Cl_2C_6H_3CH_3$	2,4-Dichlorotoluene	2,4-Dichloro-1-methylbenzene	47
24 $2,5-Cl_2C_6H_3CH_3$	2,5-Dichlorotoluene	1,4-Dichloro-2-methylbenzene	49
25 $2,6-Cl_2C_6H_3CH_3$	2,6-Dichlorotoluene	2,6-Dichloro-1-methylbenzene	51
26 $3,4-Cl_2C_6H_3CH_3$	3,4-Dichlorotoluene	1,2-Dichloro-4-methylbenzene	53
27 $3,5-Cl_2C_6H_3CH_3$	3,5-Dichlorotoluene (not issued)		

Continued overleaf

HIGHER HALOGENATED TOLUENES

26	$C_6H_5CF_3$	(Trifluoromethyl)benzene	Benzotrifluoride	55
27	$C_6H_5CCl_3$	(Trichloromethyl)benzene	Benzotrichloride	57
28	$3-FC_6H_4CF_3$	3-Fluoro-1-(trifluoromethyl)benzene	3-Fluorobenzotrifluoride	59
29	$C_6F_5CH_3$	2,3,4,5,6-Pentafluorotoluene		61
30	$C_6F_5CF_3$	Octafluorotoluene	Perfluorotoluene	63

HALOGENATED HIGHER ALKYL BENZENES

31	$C_6H_5C_2H_4Cl$	(2-Chloroethyl)benzene	β -Phenethyl chloride	65
32	$2-ClC_6H_4C_2H_5$	2-Chloro-1-ethylbenzene	2-Ethylchlorobenzene	67
33	$3-ClC_6H_4C_2H_5$	3-Chloro-1-ethylbenzene	3-Ethylchlorobenzene	69
34	$4-ClC_6H_4C_2H_5$	4-Chloro-1-ethylbenzene	4-Ethylchlorobenzene	71
35	$C_6H_5C_2H_4Br$	(2-Bromoethyl)benzene	β -Phenethyl bromide	73
36	$2-BrC_6H_4C_2H_5$	2-Bromo-1-ethylbenzene	2-Ethylbromobenzene	75
37	$4-BrC_6H_4C_2H_5$	4-Bromo-1-ethylbenzene	4-Ethylbromobenzene	77
38	$2-ClC_6H_4CH(CH_3)_2$	2-Chloro-1-isopropylbenzene	2-Chlorocumene	79
39	$4-ClC_6H_4CH(CH_3)_2$	4-Chloro-1-isopropylbenzene	4-Chlorocumene	81
40	$2-BrC_6H_4CH(CH_3)_2$	2-Bromo-1-isopropylbenzene	2-Bromocumene	83
41	$4-BrC_6H_4CH(CH_3)_2$	4-Bromo-1-isopropylbenzene	4-Bromocumene	85

HALOGENATED STYRENES

42	$2-ClC_6H_4CH=CH_2$	2-Chloro-1-vinylbenzene	2-Chlorostyrene	87
43	$4-ClC_6H_4CH=CH_2$	4-Chloro-1-vinylbenzene	4-Chlorostyrene	89
44	$2-BrC_6H_4CH=CH_2$	2-Bromo-1-vinylbenzene	2-Bromostyrene	91
45	$4-BrC_6H_4CH=CH_2$	4-Bromo-1-vinylbenzene	4-Bromostyrene	93

ORTHOBARIC DENSITIES AND MOLAR VOLUMES OF LIQUIDS HALOGENATED ALKYL BENZENES AND HALOGENATED STYRENES

1. INTRODUCTION

This Data Item presents orthobaric densities and molar volumes of the halogenated alkylbenzenes and halogenated styrenes arranged in the order shown on the Contents page.

Table 1 gives the constants in the liquid density equation for all the compounds. On the following Sheets the values of density and molar volume for each compound have been obtained by calculation from the equation given, with its numerical coefficients, at the top of each Sheet. This equation was fitted to the data that had been selected after critical assessment of all the data. The value of the critical temperature for each compound was taken from Item 99007, which gives the vapour pressures. For completeness all the critical parameters of each compound are given in the Tables which also show the density at 298.15 K, where applicable, and for convenience, the normal boiling point and the approximate melting point rounded to the nearest K or °C. Brackets enclose the data at those temperatures which are outside the range of supporting experimental data.

The table of Data at Specified Temperatures for each compound gives the density, the molar volume and their derivatives with respect to temperature. In addition this table also gives an assessment of the data quality indicated, in decreasing order, by one of the letters 'A', 'B' or 'C', at each temperature. The estimated uncertainties in density and molar volume are shown below each letter in the units of density and molar volume rounded to 1, 2 or 5 times a power of 10.

In the main tables the uncertainties in the tabulated values of density and molar volume are shown for each value. The number of decimal places in each value is adjusted to be consistent with the uncertainty. Data quality and uncertainties are discussed at greater length in Section 5.

The sources of information which give liquid density or liquid molar volume data for the compound considered are listed on the reverse side of each sheet. Those sources that were used to derive the critical density and the coefficients of the liquid density/molar volume equation are shown together with the temperature ranges (ambient, low, medium, high or critical) of their data. These temperature ranges correspond to low, medium, high and pressure ranges referred to in Item 99007.

2. NOTATION AND UNITS

All temperatures are based on the International Temperature Scale (ITS-90).

N_1, N_2, N_3, N_4	non-dimensional coefficients of the density/molar volume equation
T	kelvin temperature
t	Celsius temperature ($T-273.15$)
V	liquid molar volume
ρ	liquid density
τ	$(1-T/T_c)^{1/3}$

Note. The units of temperature, density and molar volume are shown in each table.

Subscripts

b	denotes value at normal boiling point
c	denotes value at critical point
m	denotes value at normal melting point
r	denotes reduced quantity, e.g. $T_r = T/T_c$

3. THE CRITICAL DENSITY

Estimates of the critical density of a compound may be made using both the Riedel equation, see Reference 1, and the latest form of Rackett equation, see References 2, 3 and 4. Both these equations require reliable values of the critical temperature and the critical pressure but neither represents experimental data over a wide range of temperature as satisfactorily as does the equation, see Table 1, which is used in this Item. However, provided the use

of the Riedel equation is limited to non-associated liquids, both equations usually yield reliable values of the critical density for a wide variety of compounds. It may be noted that the Rackett equation usually gives a higher estimate than the Riedel equation and that for a homologous series this difference increases with increasing molecular weight.

For the compounds considered here estimates of the critical density of each compound were made using both the Riedel and the Rackett equations. Critical densities, based on liquid density measurements and estimates of vapour density at high reduced temperatures, have been reported for several of the compounds and these values are in reasonable agreement with the mean of values estimated by the Riedel equation and the Rackett equation.

4. EVALUATION AND CORRELATION

For five polyfluoro-benzenes and two polyfluoro-toluenes there are extensive reliable medium pressure range data which extend some way into the high pressure range (above the normal boiling point). Reliable data for the remaining compounds considered here are, in general, confined to shorter temperature ranges in the medium pressure range. The data for the above seven compounds were fitted by the liquid density equation, with the third coefficient constrained to be zero, and the coefficients of their equations were used to derive a reduced temperature - reduced density correlation analogous to that derived for vapour pressures, see Item 99007. This correlation was then used here to fit the data of the remaining fluoro compounds. The correlation for the alkanes was used to fit the data of the chloro, bromo and iodo compounds

The liquid density equations presented here were derived in parallel with the vapour pressure equations presented in Item 99007, and where necessary the estimated values of critical temperature, critical pressure and critical density for some compounds were adjusted until they were optimum values for both vapour pressure and liquid density.

5. UNCERTAINTIES

At any temperature, the estimated uncertainties in the tabulated values of density and molar volume are dependent upon the rates of change of these properties with temperature and the quality of the experimental or estimated data upon which they are based. The table of Data at Specified Temperatures shows these derivatives, the assessed data quality (indicated by one of the letters 'A', 'B' or 'C') and the corresponding uncertainties at various points of the liquid range. At low and medium reduced temperatures average quality data, denoted by the letter 'B', have uncertainties varying from 0.1 to 1 per cent, increasing to between 1 and 10 per cent at the critical point. Data with lower or higher uncertainties than these bands are graded 'A' and 'C' respectively. When the data quality is 'C' it will be appreciated that the uncertainties are necessarily rather speculative and that for some compounds they may be underestimated.

For those compounds for which the data quality at the critical pressure is denoted by 'C' the values of critical temperature and critical density given in the Tables should be regarded only as correlating parameters.

6. REFERENCES

1. RIEDEL, L. Liquid density in the saturation state. Investigations on an extension of the theorem of corresponding states. Part 2 (in German). *Chem.-Ingr.-Tech.*, Vol.26, pp.259-264, 1954.
2. RACKETT, H.G. Equation of state for saturated liquids. *J. Chem. Eng. Data*, Vol.15, No.4, pp.514-517, 1970.
3. SPENCER, C.F.,
DANNER, R.P.J. Improved equation for prediction of saturated liquid density. *J. Chem. Eng. Data*, Vol.17, No.2, pp.236-241, 1972.
4. CAMPBELL, S.W.
THODOS, G. Prediction of saturated-liquid densities and critical volumes for polar and non-polar substances. *J. Chem. Eng. Data*, Vol.30, No.1, pp.102-111, 1985.

TABLE 1
Summary of Constants in the Liquid Density equation

$$\ln \rho = \ln \rho_c + N_1 \tau + N_2 \tau^2 + N_3 \tau^3 + N_4 \tau^4 \quad \text{where } \tau = (1 - T/T_c)^{1/3}$$

No.	Name	T_c K	ρ_c kg/m ³	N_1	N_2	N_3	N_4
MONOHALOGENATED TOLUENES							
1	(Fluoromethyl)benzene	620.	333.	1.83017	-0.68952	0	0.23232
2	2-Fluorotoluene	589.	335.	1.78275	-0.64565	0	0.21491
3	3-Fluorotoluene	593.	333.	1.78266	-0.64558	0	0.21489
4	4-Fluorotoluene	594.	333.	1.78064	-0.64385	0	0.21426
5	(Chloromethyl)benzene	681.	348.	1.82304	-0.68255	0	0.22939
6	2-Chlorotoluene	658.	348.	1.80459	-0.66510	0	0.22230
7	3-Chlorotoluene	662.	346.	1.79046	-0.65236	0	0.21739
8	4-Chlorotoluene	664.	344.	1.79601	-0.65729	0	0.21926
9	(Bromomethyl)benzene	720.	450.	1.81734	-0.67707	0	0.22713
10	2-Bromotoluene	692.	451.	1.80907	-0.66926	0	0.22396
11	3-Bromotoluene	696.	446.	1.80884	-0.66904	0	0.22387
12	4-Bromotoluene	697.	446.	1.79880	-0.65981	0	0.22023
13	(Iodomethyl)benzene	765.	533.	1.84109	-0.70041	0	0.23699
14	2-Iodotoluene	737.	535.	1.80129	-0.66207	0	0.22111
15	3-Iodotoluene	740.	531.	1.80709	-0.66741	0	0.22322
16	4-Iodotoluene	742.	533.	1.79469	-0.65611	0	0.21881
DIHALOGENATED TOLUENES							
17	(Difluoromethyl)benzene	611.	363.	1.89400	-0.76515	0	0.26783
18	(Dichloromethyl)benzene	717.	391.	1.82643	-0.68585	0	0.23077
19	2-Chloro-1-(chloromethyl)benzene	732.	394.	1.85801	-0.71780	0	0.24464
20	3-Chloro-1-(chloromethyl)benzene	730.	390.	1.84603	-0.70543	0	0.23917
21	4-Chloro-1-(chloromethyl)benzene	740.	390.	1.83848	-0.69779	0	0.23585
22	2,3-Dichlorotoluene (not issued)						
23	2,4-Dichlorotoluene	704.	394.	1.80915	-0.66933	0	0.22399
24	2,5-Dichlorotoluene	709.	394.	1.81458	-0.67444	0	0.22605
25	2,6-Dichlorotoluene	706.	398.	1.82262	-0.68215	0	0.22922
25	3,4-Dichlorotoluene	723.	391.	1.82082	-0.68040	0	0.22850
	3,5-Dichlorotoluene (not issued)						
HIGHER HALOGENATED TOLUENES							
26	(Trifluoromethyl)benzene	551.	396.	1.85880	-0.71863	0	0.24501
27	(Trichloromethyl)benzene	733.	423.	1.84769	-0.70713	0	0.23992
28	3-Fluoro-1-(trifluoromethyl)benzene	544.	433.	1.86756	-0.72787	0	0.24917
29	2,3,4,5,6-Pentafluorotoluene	566.48	474.	1.90150	-0.77386	0	0.25774
30	Octafluorotoluene	534.43	556.	1.94051	-0.82418	0	0.28358

Continued on next page

TABLE 1 continued

No.	Name	T_c K	ρ_c kg/m ³	N_1	N_2	N_3	N_4
HALOGENATED HIGHER ALKYL BENZENES							
31	(2-Chloroethyl)benzene	697.	334.	1.85595	-0.71565	0	0.24368
32	2-Chloro-1-ethylbenzene	671.	335.	1.82970	-0.68906	0	0.23212
33	3-Chloro-1-ethylbenzene	679.	332.	1.83582	-0.69513	0	0.23471
34	4-Chloro-1-ethylbenzene	680.	331.	1.82280	-0.68232	0	0.22929
35	(2-Bromoethyl)benzene	727.	420.	1.84534	-0.70473	0	0.23886
36	2-Bromo-1-ethylbenzene	704.	425.	1.83322	-0.69253	0	0.23360
37	4-Bromo-1-ethylbenzene	711.	419.	1.83165	-0.69098	0	0.23294
38	2-Chloro-1-isopropylbenzene	679.	325.	1.84585	-0.70524	0	0.23909
39	4-Chloro-1-isopropylbenzene	690.	320.	1.84069	-0.70002	0	0.23682
40	2-Bromo-1-isopropylbenzene	707.	406.	1.83865	-0.69796	0	0.23593
41	4-Bromo-1-isopropylbenzene	719.	399.	1.84017	-0.69949	0	0.23659
HALOGENATED STYRENES							
42	2-Chloro-1-vinylbenzene	693.	345.	1.83802	-0.69733	0	0.23566
43	4-Chloro-1-vinylbenzene	697.	341.	1.83434	-0.69365	0	0.23408
44	2-Bromo-1-vinylbenzene	726.	439.	1.83743	-0.69674	0	0.23540
45	4-Bromo-1-vinylbenzene	728.	433.	1.84070	-0.70002	0	0.23682

C₆H₅CH₂F
 (Fluoromethyl)benzene; Benzyl fluoride

C₇H₇F

CAS Reg. No. 350-50-5

Mol. Wt. 110.13

Orthobaric Liquid Density and Molar Volume $\ln(\rho/\rho_c) = -\ln(V/V_c) = N_1\tau + N_2\tau^2 + N_3\tau^3 + N_4\tau^4$

where ρ is the density, ρ_c is the critical density, V is the molar volume, V_c is the critical molar volume and $\tau = (1-T/T_c)^{1/3}$, where T is the temperature and T_c is the critical temperature in kelvins.

Critical Temperature	T_c	= 620. K	(t_c	= 346.85 °C)
Critical Pressure	p_c	= 4150. kPa	(p_c	= 40.96 atm)
Critical Density	ρ_c	= 333. kg/m ³	(V_c	= 330.72 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.266		

$N_1 = 1.83017$ $N_2 = -0.68952$ $N_3 = 0.00000$ $N_4 = 0.23232$

Density at 298.15 K (25 °C)	ρ_{25}	= 1023.09 kg/m ³	(V_{25}	= 107.64 cm ³ /mol)
Normal Boiling Point	T_b	= 412.850 K	(t_b	= 139.700 °C)
Approximate Melting Point	T_m	= 238. K	(t_m	= -35. °C)

Data at Specified Temperatures

$t/^\circ\text{C}$ T/K	-35 238.15	0 273.15	25 298.15	50 323.15	139.70 412.85	200 473.15	346.85 620.00
$\rho/(\text{kg/m}^3)$ ($d\rho/dT/(\text{kg/m}^3 \text{ K})$)	(1083.42) (-0.99)	(1048.50) (-1.01)	1023.09 -1.03	(997.18) (-1.05)	(897.81) (-1.19)	(821.06) (-1.38)	(333.00) ∞
$V/(\text{cm}^3/\text{mol})$ ($dV/dT/(\text{cm}^3/\text{mol K})$)	(101.65) (0.09)	(105.04) (0.10)	107.64 0.11	(110.44) (0.12)	(122.67) (0.16)	(134.13) (0.23)	(330.72) ∞
Data Quality	(B)	(B)	B	(B)	(B)	(B)	(B)
Uncertainty in ρ (per cent)	(0.1)	(0.1)	0.1	(0.1)	(0.2)	(0.2)	(2.)
Uncertainty in V (per cent)	(0.1)	(0.1)	0.1	(0.1)	(0.2)	(0.2)	(2.)

Orthobaric Liquid Density of (Fluoromethyl)benzene

Units: kg/m³ v. K

T K cent	ρ kg/m ³	Uncert. in ρ per cent	T K cent	ρ kg/m ³	Uncert. in ρ per cent	T K cent	ρ kg/m ³	Uncert. in ρ per cent	T K cent	ρ kg/m ³	Uncert. in ρ per cent
			350	(968.7)	0.1	500	(782.2)	0.2			
			360	(957.8)	0.1	510	(766.6)	0.5			
			370	(946.8)	0.2	520	(750.3)	0.5			
			380	(935.7)	0.2	530	(733.1)	0.5			
240	(1081.59)	0.1	390	(924.4)	0.2	540	(714.8)	0.5			
250	(1071.67)	0.1	400	(912.9)	0.2	550	(695.3)	0.5			
260	(1061.70)	0.1	410	(901.2)	0.2	560	(674.1)	0.5			
270	(1051.67)	0.1	420	(889.3)	0.2	570	(650.8)	1.			
280	(1041.58)	0.1	430	(877.1)	0.2	580	(624.7)	1.			
290	(1031.42)	0.1	440	(864.7)	0.2	590	(594.)	1.			
300	(1021.19)	0.1	450	(851.9)	0.2	600	(557.)	1.			
310	(1010.88)	0.1	460	(838.8)	0.2	610	(506.)	1.			
320	(1000.48)	0.1	470	(825.4)	0.2	620	(333.)	2.			
330	(990.0)	0.1	480	(811.5)	0.2						
340	(979.4)	0.1	490	(797.1)	0.2						

C₇H₇F

Orthobaric Liquid Molar Volume of (Fluoromethyl)benzene

Units: cm³/mol v. K

T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent
			350	(113.7)	0.1	500	(140.8)	0.2			
			360	(115.0)	0.1	510	(143.7)	0.5			
			370	(116.3)	0.2	520	(146.8)	0.5			
			380	(117.7)	0.2	530	(150.2)	0.5			
240	(101.82)	0.1	390	(119.1)	0.2	540	(154.1)	0.5			
250	(102.76)	0.1	400	(120.6)	0.2	550	(158.4)	0.5			
260	(103.73)	0.1	410	(122.2)	0.2	560	(163.4)	0.5			
270	(104.72)	0.1	420	(123.8)	0.2	570	(169.2)	1.			
280	(105.73)	0.1	430	(125.6)	0.2	580	(176.3)	1.			
290	(106.77)	0.1	440	(127.4)	0.2	590	(185.)	1.			
300	(107.84)	0.1	450	(129.3)	0.2	600	(198.)	1.			
310	(108.94)	0.1	460	(131.3)	0.2	610	(217.)	1.			
320	(110.08)	0.1	470	(133.4)	0.2	620	(331.)	2.			
330	(111.2)	0.1	480	(135.7)	0.2						
340	(112.4)	0.1	490	(138.2)	0.2						

The following Sources give liquid density or liquid molar volume data for this compound. Those Sources used to derive the coefficients of the liquid density/molar volume equation are indicated by the temperature range (ambient 'A', low 'L', medium 'M', high 'H' or critical 'C') of their data. An asterisk (*) indicates that the Source is not a primary source of experimental data.

1 INGOLD, C.K.; INGOLD, E.H.;

J.Chem.Soc.,

p.2257, 1928.

A

2-FC₆H₄CH₃
 2-Fluorotoluene; *o*-Fluorotoluene; *o*-Tolylfluoride

C₇H₇F

CAS Reg. No. 95-52-3

Mol. Wt. 110.13

Orthobaric Liquid Density and Molar Volume $\ln(\rho/\rho_c) = -\ln(V/V_c) = N_1 \tau + N_2 \tau^2 + N_3 \tau^3 + N_4 \tau^4$

where ρ is the density, ρ_c is the critical density, V is the molar volume, V_c is the critical molar volume and $\tau = (1-T/T_c)^{1/3}$, where T is the temperature and T_c is the critical temperature in kelvins.

Critical Temperature	T_c	= 589. K	(t_c	= 315.85 °C)
Critical Pressure	p_c	= 3930. kPa	(p_c	= 38.79 atm)
Critical Density	ρ_c	= 335. kg/m ³	(V_c	= 328.75 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.264		

$N_1 = 1.78275$ $N_2 = -0.64565$ $N_3 = 0.00000$ $N_4 = 0.21491$

Density at 298.15 K (25 °C)	ρ_{25}	= 996.00 kg/m ³	(V_{25}	= 110.57 cm ³ /mol)
Normal Boiling Point	T_b	= 386.75 K	(t_b	= 113.600 °C)
Approximate Melting Point	T_m	= 211. K	(t_m	= -62. °C)

Data at Specified Temperatures

$t/^\circ\text{C}$	-62	0	25	50	113.60	200	315.85
T/K	211.15	273.15	298.15	323.15	386.75	473.15	589.00
$\rho/(\text{kg/m}^3)$	(1086.07)	(1022.46)	996.00	(968.88)	(895.69)	(778.31)	(335.00)
$(d\rho/dT)/(\text{kg/m}^3 \text{ K})$	(-1.01)	(-1.05)	-1.07	(-1.10)	(-1.21)	(-1.56)	$-\infty$
$V/(\text{cm}^3/\text{mol})$	(101.40)	(107.71)	110.57	(113.67)	(122.96)	(141.50)	(328.75)
$(dV/dT)/(\text{cm}^3/\text{mol K})$	(0.09)	(0.11)	0.12	(0.13)	(0.17)	(0.28)	∞
Data Quality	(B)	(B)	B	(B)	(B)	(B)	(B)
Uncertainty in ρ (per cent)	(0.2)	(0.2)	0.2	(0.2)	(0.2)	(0.5)	(1.)
Uncertainty in V (per cent)	(0.2)	(0.2)	0.2	(0.2)	(0.2)	(0.5)	(1.)

Orthobaric Liquid Density of 2-Fluorotoluene

Units: kg/m³ v. K

T	ρ	Uncert.	T	ρ	Uncert.	T	ρ	Uncert.	T	ρ	Uncert.
°C	kg/m ³	per cent	°C	kg/m ³	per cent	°C	kg/m ³	per cent	°C	kg/m ³	per cent
220	(1077.1)	0.2	300	(994.0)	0.2	400	(879.4)	0.5	500	(733.5)	0.5
230	(1067.0)	0.2	310	(983.2)	0.2	410	(866.8)	0.5	510	(715.0)	0.5
240	(1056.8)	0.2	320	(972.3)	0.2	420	(853.9)	0.5	520	(695.2)	1.
			330	(961.3)	0.2	430	(840.6)	0.5	530	(673.7)	1.
			340	(950.2)	0.2	440	(827.0)	0.5	540	(650.1)	1.
250	(1046.5)	0.2	350	(938.8)	0.2	450	(812.9)	0.5	550	(624.)	1.
260	(1036.2)	0.2	360	(927.4)	0.2	460	(798.3)	0.5	560	(593.)	1.
270	(1025.8)	0.2	370	(915.7)	0.2	470	(783.2)	0.5	570	(555.)	1.
280	(1015.3)	0.2	380	(903.8)	0.2	480	(767.4)	0.5	580	(501.)	1.
290	1004.7	0.2	390	(891.7)	0.2	490	(750.9)	0.5			

C₇H₇F

Orthobaric Liquid Molar Volume of 2-Fluorotoluene

Units: cm³/mol v. K

T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent
220	(102.2)	0.2	300	(110.8)	0.2	400	(125.2)	0.5	500	(150.1)	0.5
230	(103.2)	0.2	310	(112.0)	0.2	410	(127.1)	0.5	510	(154.0)	0.5
240	(104.2)	0.2	320	(113.3)	0.2	420	(129.0)	0.5	520	(158.4)	1.
250	(105.2)	0.2	330	(114.6)	0.2	430	(131.0)	0.5	530	(163.5)	1.
260	(106.3)	0.2	340	(115.9)	0.2	440	(133.2)	0.5	540	(169.4)	1.
270	(107.4)	0.2	350	(117.3)	0.2	450	(135.5)	0.5	550	(177.)	1.
280	(108.5)	0.2	360	(118.8)	0.2	460	(138.0)	0.5	560	(186.)	1.
290	109.6	0.2	370	(120.3)	0.2	470	(140.6)	0.5	570	(199.)	1.
			380	(121.8)	0.2	480	(143.5)	0.5	580	(220.)	1.
			390	(123.5)	0.2	490	(146.7)	0.5			

The following Sources give liquid density or liquid molar volume data for this compound. Those Sources used to derive the coefficients of the liquid density/molar volume equation are indicated by the temperature range (ambient 'A', low 'L', medium 'M', high 'H' or critical 'C') of their data. An asterisk (*) indicates that the Source is not a primary source of experimental data.

- | | | | |
|---|------------------------------------|---|---|
| 1 | HOLLEMAN, A.F.; | <i>Rec.Trav.Chim.</i> , Vol.25, p.331, 1906. | |
| 2 | SWARTS, F.; | <i>J.Chim.Phys.</i> , Vol.20, p.60, 1923. | A |
| 3 | SCHIEMANN, G.; | <i>Z.Phys.Chem.(Leipzig)</i> , A, Vol.156, p.397, 1931. | A |
| 4 | HUDLICKY, M.; | <i>Coll.Czech.Chem.Comm.</i> , Vol.25, p.1199, 1960. | A |
| 5 | TERRY, T.D.; KEPNER, R.E.; et al.; | <i>J.Chem.Eng.Data</i> , Vol.5, p.403, 1960. | A |

3-FC₆H₄CH₃
 3-Fluorotoluene; *m*-Fluorotoluene; *m*-Tolylfluoride

C₇H₇F

CAS Reg. No. 352-70-5

Mol. Wt. 110.13

Orthobaric Liquid Density and Molar Volume $\ln(\rho/\rho_c) = -\ln(V/V_c) = N_1 \tau + N_2 \tau^2 + N_3 \tau^3 + N_4 \tau^4$

where ρ is the density, ρ_c is the critical density, V is the molar volume, V_c is the critical molar volume and $\tau = (1 - T/T_c)^{1/3}$, where T is the temperature and T_c is the critical temperature in kelvins.

Critical Temperature	T_c	= 593. K	(t_c	= 319.85 °C)
Critical Pressure	p_c	= 3950. kPa	(p_c	= 38.98 atm)
Critical Density	ρ_c	= 333. kg/m ³	(V_c	= 330.72 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.265		

$N_1 = 1.78266$ $N_2 = -0.64558$ $N_3 = 0.00000$ $N_4 = 0.21489$

Density at 298.15 K (25 °C)	ρ_{25}	= 992.15 kg/m ³	(V_{25}	= 111.00 cm ³ /mol)
Normal Boiling Point	T_b	= 389.150 K	(t_b	= 116. °C)
Approximate Melting Point	T_m	= 185. K	(t_m	= -88. °C)

Data at Specified Temperatures							
$t/^\circ\text{C}$	-89	0	25	50	116	200	319.85
T/K	184.15	273.15	298.15	323.15	389.15	473.15	593.00
$\rho/(\text{kg}/\text{m}^3)$	(1107.70)	(1018.24)	992.15	965.44	(890.58)	(778.56)	(333.00)
$(d\rho/dT)/(\text{kg}/\text{m}^3 \text{ K})$	(-0.99)	(-1.03)	-1.05	-1.08	(-1.20)	(-1.52)	$-\infty$
$V/(\text{cm}^3/\text{mol})$	(99.42)	(108.16)	111.00	114.07	(123.66)	(141.45)	(330.72)
$(dV/dT)/(\text{cm}^3/\text{mol K})$	(0.09)	(0.11)	0.12	0.13	(0.17)	(0.28)	∞
Data Quality	(B)	(B)	B	B	(B)	(B)	(B)
Uncertainty in ρ (per cent)	(0.1)	(0.1)	0.1	0.1	(0.2)	(0.2)	(2.)
Uncertainty in V (per cent)	(0.1)	(0.1)	0.1	0.1	(0.2)	(0.2)	(2.)

Orthobaric Liquid Density of 3-Fluorotoluene

Units: kg/m³ v. K

T	ρ	Uncert.	T	ρ	Uncert.	T	ρ	Uncert.	T	ρ	Uncert.
K	kg/m ³	per cent	K	kg/m ³	per cent	K	kg/m ³	per cent	K	kg/m ³	per
			300	990.2	0.1	450	(812.3)	0.2			
			310	979.6	0.1	460	(798.1)	0.2			
			320	968.8	0.1	470	(783.3)	0.2			
			330	958.0	0.1	480	(768.0)	0.2			
190	(1101.93)	0.1	340	947.0	0.1	490	(751.9)	0.2			
200	(1092.04)	0.1	350	(935.9)	0.1	500	(735.0)	0.5			
210	(1082.12)	0.1	360	(924.6)	0.2	510	(717.2)	0.5			
220	(1072.15)	0.1	370	(913.1)	0.2	520	(698.1)	0.5			
230	(1062.13)	0.1	380	(901.4)	0.2	530	(677.5)	0.5			
240	(1052.07)	0.1	390	(889.6)	0.2	540	(655.0)	0.5			
250	(1041.94)	0.1	400	(877.4)	0.2	550	(630.0)	1.			
260	(1031.75)	0.1	410	(865.1)	0.2	560	(601.4)	1.			
270	(1021.48)	0.1	420	(852.4)	0.2	570	(567.)	1.			
280	(1011.14)	0.1	430	(839.4)	0.2	580	(522.)	1.			
290	1000.72	0.1	440	(826.1)	0.2	590	(444.)	1.			

C₇H₇F

Orthobaric Liquid Molar Volume of 3-Fluorotoluene

Units: cm³/mol v. K

T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent
			300	111.2	0.1	450	(135.6)	0.2			
			310	112.4	0.1	460	(138.0)	0.2			
			320	113.7	0.1	470	(140.6)	0.2			
			330	115.0	0.1	480	(143.4)	0.2			
190	(99.94)	0.1	340	116.3	0.1	490	(146.5)	0.2			
200	(100.85)	0.1	350	(117.7)	0.1	500	(149.8)	0.5			
210	(101.77)	0.1	360	(119.1)	0.2	510	(153.6)	0.5			
220	(102.72)	0.1	370	(120.6)	0.2	520	(157.8)	0.5			
230	(103.69)	0.1	380	(122.2)	0.2	530	(162.5)	0.5			
240	(104.68)	0.1	390	(123.8)	0.2	540	(168.1)	0.5			
250	(105.70)	0.1	400	(125.5)	0.2	550	(174.8)	1.			
260	(106.74)	0.1	410	(127.3)	0.2	560	(183.1)	1.			
270	(107.81)	0.1	420	(129.2)	0.2	570	(194.)	1.			
280	(108.92)	0.1	430	(131.2)	0.2	580	(211.)	1.			
290	110.05	0.1	440	(133.3)	0.2	590	(248.)	1.			

The following Sources give liquid density or liquid molar volume data for this compound. Those Sources used to derive the coefficients of the liquid density/molar volume equation are indicated by the temperature range (ambient 'A', low 'L', medium 'M', high 'H' or critical 'C') of their data. An asterisk (*) indicates that the Source is not a primary source of experimental data.

- | | | | |
|---|-----------------|--|---|
| 1 | HOLLEMAN, A.F.; | <i>Rec.Trav.Chim.</i> , Vol.25, p.331, 1906. | |
| 2 | JAEGER, F.M.; | <i>Z.Anorg.Allg.Chem.</i> , Vol.101, p.125, 1917. | |
| 3 | SWARTS, F.; | <i>J.Chim.Phys.</i> , Vol.20, p.60, 1923. | A |
| 4 | SCHIEHMANN, G.; | <i>Z.Phys.Chem.(Leipzig)</i> , Vol.156, p.397, 1931. | A |
| 5 | DESREUX, V.; | <i>Bull.Soc.Chim.Belg.</i> , Vol.44, p.249, 1935. | A |
| 6 | HUDLICKY, M.; | <i>Coll.Czech.Chem.Comm.</i> , Vol.25, p.1199, 1960. | |

4-FC₆H₄CH₃
 4-Fluorotoluene; *p*-Fluorotoluene; *p*-Tolylfluoride

C₇H₇F

CAS Reg. No. 352-32-9

Mol. Wt. 110.13

Orthobaric Liquid Density and Molar Volume $\ln(\rho/\rho_c) = -\ln(V/V_c) = N_1 \tau + N_2 \tau^2 + N_3 \tau^3 + N_4 \tau^4$

where ρ is the density, ρ_c is the critical density, V is the molar volume, V_c is the critical molar volume and $\tau = (1-T/T_c)^{1/3}$, where T is the temperature and T_c is the critical temperature in kelvins.

Critical Temperature	T_c	= 594. K	(t_c	= 320.85 °C)
Critical Pressure	p_c	= 3950. kPa	(p_c	= 38.98 atm)
Critical Density	ρ_c	= 333. kg/m ³	(V_c	= 330.72 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.265		

$N_1 = 1.78064$ $N_2 = -0.64385$ $N_3 = 0.00000$ $N_4 = 0.21426$

Density at 298.15 K (25 °C)	ρ_{25}	= 991.93 kg/m ³	(V_{25}	= 111.03 cm ³ /mol)
Normal Boiling Point	T_b	= 389.790 K	(t_b	= 116.640 °C)
Approximate Melting Point	T_m	= 216. K	(t_m	= -57. °C)

Data at Specified Temperatures

$t/^\circ\text{C}$	-57	0	25	50	116.64	200	320.85
T/K	216.15	273.15	298.15	323.15	389.79	473.15	594.00
$\rho/(\text{kg/m}^3)$	(1075.49)	(1017.92)	991.93	965.31	(889.96)	(779.26)	(333.00)
$(d\rho/dT)/(\text{kg/m}^3 \text{ K})$	(-0.99)	(-1.03)	-1.05	-1.08	(-1.19)	(-1.51)	$-\infty$
$V/(\text{cm}^3/\text{mol})$	(102.40)	(108.19)	111.03	114.09	(123.75)	(141.33)	(330.72)
$(dV/dT)/(\text{cm}^3/\text{mol K})$	(0.09)	(0.11)	0.12	0.13	(0.17)	(0.27)	∞
Data Quality	(B)	(B)	B	B	(B)	(B)	(B)
Uncertainty in ρ (per cent)	(0.1)	(0.1)	0.1	0.1	(0.2)	(0.2)	(2.)
Uncertainty in V (per cent)	(0.1)	(0.1)	0.1	0.1	(0.2)	(0.2)	(2.)

Orthobaric Liquid Density of 4-Fluorotoluene

Units: kg/m³ v. K

T	ρ	Uncert.	T	ρ	Uncert.	T	ρ	Uncert.	T	ρ	Uncert.
K	kg/m ³	per cent	K	kg/m ³	per cent	K	kg/m ³	per cent	K	kg/m ³	per
cent											
220	(1071.66)	0.1	300	990.0	0.1	400	(877.6)	0.2	500	(736.0)	0.5
230	(1061.68)	0.1	310	979.4	0.1	410	(865.3)	0.2	510	(718.3)	0.5
240	(1051.64)	0.1	320	968.7	0.1	420	(852.7)	0.2	520	(699.4)	0.5
			330	957.9	0.1	430	(839.8)	0.2	530	(679.0)	0.5
			340	946.9	0.1	440	(826.5)	0.2	540	(656.8)	0.5
250	(1041.55)	0.1	350	935.8	0.1	450	(812.8)	0.2	550	(632.1)	1.
260	(1031.39)	0.1	360	924.6	0.2	460	(798.7)	0.2	560	(603.9)	1.
270	(1021.16)	0.1	370	913.2	0.2	470	(784.0)	0.2	570	(570.)	1.
280	(1010.85)	0.1	380	(901.5)	0.2	480	(768.7)	0.2	580	(527.)	1.
290	1000.46	0.1	390	(889.7)	0.2	490	(752.8)	0.2	590	(456.)	1.

C₇H₇F

Orthobaric Liquid Molar Volume of 4-Fluorotoluene

Units: cm³/mol v. K

T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent
220	(102.77)	0.1	300	111.2	0.1	400	(125.5)	0.2	500	(149.6)	0.5
230	(103.73)	0.1	310	112.4	0.1	410	(127.3)	0.2	510	(153.3)	0.5
240	(104.72)	0.1	320	113.7	0.1	420	(129.2)	0.2	520	(157.5)	0.5
			330	115.0	0.1	430	(131.1)	0.2	530	(162.2)	0.5
			340	116.3	0.1	440	(133.2)	0.2	540	(167.7)	0.5
250	(105.74)	0.1	350	117.7	0.1	450	(135.5)	0.2	550	(174.2)	1.
260	(106.78)	0.1	360	119.1	0.2	460	(137.9)	0.2	560	(182.4)	1.
270	(107.85)	0.1	370	120.6	0.2	470	(140.5)	0.2	570	(193.)	1.
280	(108.95)	0.1	380	(122.2)	0.2	480	(143.3)	0.2	580	(209.)	1.
290	110.08	0.1	390	(123.8)	0.2	490	(146.3)	0.2	590	(242.)	1.

The following Sources give liquid density or liquid molar volume data for this compound. Those Sources used to derive the coefficients of the liquid density/molar volume equation are indicated by the temperature range (ambient 'A', low 'L', medium 'M', high 'H' or critical 'C') of their data. An asterisk (*) indicates that the Source is not a primary source of experimental data.

1	WALLACH, O.;	<i>Liebigs Ann.Chem.</i> , Vol.235, p.261, 1886.	
2	HOLLEMAN, A.F.;	<i>Rec.Trav.Chim.</i> , Vol.25, p.331, 1906.	
3	SWARTS, F.;	<i>J.Chim.Phys.</i> , Vol.20, p.60, 1923.	
4	SCHIEMANN, G.;	<i>Z.Phys.Chem.(Leipzig)</i> , Vol.156, p.397, 1931.	
5	ALLEN, E.C.; SUGDEN, S.;	<i>J.Chem.Soc.</i> , p.760, 1932.	M
6	VOGEL, A.I.;	<i>J.Chem.Soc.</i> , p.644, 1948.	
7	RUTLEGE, G.P.; SMITH, W.T.;	<i>J.Am.Chem.Soc.</i> , Vol.75, p.5762, 1953.	M
8	HUDLICKY, M.;	<i>Coll.Czech.Chem.Comm.</i> , Vol.25, p.1199, 1960.	
9	GOOD, W.D.; et al.;	<i>J.Phys.Chem.</i> , Vol.66, p.1529, 1962.	
10	MECHTIEV, -.; et al.;	<i>Azerb.Khim.Zh.</i> , Vol.1, p.21, 1971.	A
11	HUANG, H.H.;	<i>J.Chem.Soc.,Perkin Trans.,2</i> , p.903, 1975.	A
12	COLNAY, M.E.; VASSEUR, A.; et al.;	<i>J.Chem.Res.Miniprint</i> , p.2050, 1983.	A

C₆H₅CH₂Cl
 (Chloromethyl)benzene; Benzyl chloride

C₇H₇Cl

CAS Reg. No. 100-44-7

Mol. Wt. 126.59

Orthobaric Liquid Density and Molar Volume $\ln(\rho/\rho_c) = -\ln(V/V_c) = N_1\tau + N_2\tau^2 + N_3\tau^3 + N_4\tau^4$

where ρ is the density, ρ_c is the critical density, V is the molar volume, V_c is the critical molar volume and $\tau = (1-T/T_c)^{1/3}$, where T is the temperature and T_c is the critical temperature in kelvins.

Critical Temperature	T_c	= 681. K	(t_c	= 407.85 °C)
Critical Pressure	p_c	= 4100. kPa	(p_c	= 40.46 atm)
Critical Density	ρ_c	= 348. kg/m ³	(V_c	= 363.76 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.263		

$N_1 = 1.82304$ $N_2 = -0.68255$ $N_3 = 0.00000$ $N_4 = 0.22939$

Density at 298.15 K (25 °C)	ρ_{25}	= 1094.79 kg/m ³	(V_{25}	= 115.63 cm ³ /mol)
Normal Boiling Point	T_b	= 452.475 K	(t_b	= 179.325 °C)
Approximate Melting Point	T_m	= 234. K	(t_m	= -39. °C)

Data at Specified Temperatures							
$t/^\circ\text{C}$	-40	0	25	50	179.32	300	407.85
T/K	233.15	273.15	298.15	323.15	452.47	573.15	681.00
$\rho/(\text{kg/m}^3)$	(1155.82)	1118.47	1094.79	1070.76	(937.24)	(779.29)	(348.00)
$(d\rho/dT)/(\text{kg/m}^3 \text{ K})$	(-0.93)	-0.94	-0.95	-0.97	(-1.12)	(-1.60)	$-\infty$
$V/(\text{cm}^3/\text{mol})$	(109.52)	113.18	115.63	118.22	(135.07)	(162.44)	(363.76)
$(dV/dT)/(\text{cm}^3/\text{mol K})$	(0.09)	0.10	0.10	0.11	(0.16)	(0.33)	∞
Data Quality	(B)	B	B	B	(B)	(B)	(B)
Uncertainty in ρ (per cent)	(0.1)	0.1	0.1	0.1	(0.2)	(0.2)	(1.)
Uncertainty in V (per cent)	(0.1)	0.1	0.1	0.1	(0.2)	(0.2)	(1.)

Orthobaric Liquid Density of (Chloromethyl)benzene

Units: kg/m³ v. K

T	ρ	Uncert.	T	ρ	Uncert.	T	ρ	Uncert.	T	ρ	Uncert.
K	kg/m ³	per cent	K	kg/m ³	per cent	K	kg/m ³	per cent	K	kg/m ³	per
cent											
			350	1044.5	0.1	500	(881.3)	0.2	650	(613.9)	1.
			360	1034.6	0.1	510	(868.7)	0.2	660	(578.)	1.
			370	1024.5	0.1	520	(855.8)	0.2	670	(529.)	1.
			380	1014.4	0.1	530	(842.5)	0.2	680	(424.)	1.
240	(1149.47)	0.1	390	1004.2	0.1	540	(828.8)	0.2			
250	(1140.16)	0.1	400	993.8	0.2	550	(814.5)	0.2			
260	(1130.81)	0.1	410	983.4	0.2	560	(799.7)	0.2			
270	(1121.43)	0.1	420	972.8	0.2	570	(784.3)	0.2			
280	1112.01	0.1	430	962.0	0.2	580	(768.1)	0.2			
290	1102.54	0.1	440	951.1	0.2	590	(751.1)	0.2			
300	1093.02	0.1	450	(940.0)	0.2	600	(733.0)	0.5			
310	1083.45	0.1	460	(928.7)	0.2	610	(713.6)	0.5			
320	1073.81	0.1	470	(917.2)	0.2	620	(692.6)	0.5			
330	1064.11	0.1	480	(905.5)	0.2	630	(669.5)	0.5			
340	1054.3	0.1	490	(893.5)	0.2	640	(643.7)	0.5			

C₇H₇Cl

Orthobaric Liquid Molar Volume of (Chloromethyl)benzene

Units: cm³/mol v. K

T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent
			350	121.2	0.1	500	(143.6)	0.2	650	(206.2)	1.
			360	122.4	0.1	510	(145.7)	0.2	660	(219.)	1.
			370	123.6	0.1	520	(147.9)	0.2	670	(239.)	1.
			380	124.8	0.1	530	(150.3)	0.2	680	(298.)	1.
240	(110.13)	0.1	390	126.1	0.1	540	(152.7)	0.2			
250	(111.03)	0.1	400	127.4	0.2	550	(155.4)	0.2			
260	(111.95)	0.1	410	128.7	0.2	560	(158.3)	0.2			
270	(112.88)	0.1	420	130.1	0.2	570	(161.4)	0.2			
280	113.84	0.1	430	131.6	0.2	580	(164.8)	0.2			
290	114.82	0.1	440	133.1	0.2	590	(168.5)	0.2			
300	115.82	0.1	450	(134.7)	0.2	600	(172.7)	0.5			
310	116.84	0.1	460	(136.3)	0.2	610	(177.4)	0.5			
320	117.89	0.1	470	(138.0)	0.2	620	(182.8)	0.5			
330	118.96	0.1	480	(139.8)	0.2	630	(189.1)	0.5			
340	120.1	0.1	490	(141.7)	0.2	640	(196.7)	0.5			

The following Sources give liquid density or liquid molar volume data for this compound. Those Sources used to derive the coefficients of the liquid density/molar volume equation are indicated by the temperature range (ambient 'A', low 'L', medium 'M', high 'H' or critical 'C') of their data. An asterisk (*) indicates that the Source is not a primary source of experimental data.

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2	GLADSTONE, J.H.;	<i>J.Chem.Soc.</i> , Vol.45, p.241, 1884.	
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15	SHREIBERT, A.L.; et al.;	<i>J.Appl.Chem.</i> , Vol.41, p.2201, 1968.	
16	CURRAN, D.J.; CURLEY, J.E.;	<i>Anal.Chem.</i> , Vol.43, p.118, 1971.	
17	KAJUWARA, -.; SATO, -.;	<i>Kogyo Kagaku Zasshi</i> , Vol.74, p.619, 1971.	
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2-ClC₆H₄CH₃
 2-Chlorotoluene; *o*-Chlorotoluene; *o*-Tolylchloride

C₇H₇Cl

CAS Reg. No. 95-49-8

Mol. Wt. 126.59

Orthobaric Liquid Density and Molar Volume $\ln(\rho/\rho_c) = -\ln(V/V_c) = N_1 \tau + N_2 \tau^2 + N_3 \tau^3 + N_4 \tau^4$

where ρ is the density, ρ_c is the critical density, V is the molar volume, V_c is the critical molar volume and $\tau = (1-T/T_c)^{1/3}$, where T is the temperature and T_c is the critical temperature in kelvins.

Critical Temperature	T_c	= 658. K	(t_c	= 384.85 °C)
Critical Pressure	p_c	= 3850. kPa	(p_c	= 38.00 atm)
Critical Density	ρ_c	= 348. kg/m ³	(V_c	= 363.76 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.256		

$N_1 = 1.80459$ $N_2 = -0.66510$ $N_3 = 0.00000$ $N_4 = 0.22230$

Density at 298.15 K (25 °C)	ρ_{25}	= 1077.69 kg/m ³	(V_{25}	= 117.46 cm ³ /mol)
Normal Boiling Point	T_b	= 432.450 K	(t_b	= 159.300 °C)
Approximate Melting Point	T_m	= 238. K	(t_m	= -35. °C)

Data at Specified Temperatures

$t/^\circ\text{C}$	-35	0	25	50	159.30	300	384.85
T/K	238.15	273.15	298.15	323.15	432.45	573.15	658.00
$\rho/(\text{kg/m}^3)$	(1135.64)	1102.06	1077.69	1052.92	937.03	(741.46)	(348.00)
$(d\rho/dT)/(\text{kg/m}^3 \text{ K})$	(-0.95)	-0.97	-0.98	-1.00	-1.14	(-1.84)	$-\infty$
$V/(\text{cm}^3/\text{mol})$	(111.47)	114.87	117.46	120.23	135.10	(170.73)	(363.76)
$(dV/dT)/(\text{cm}^3/\text{mol K})$	(0.09)	0.10	0.11	0.11	0.16	(0.42)	∞
Data Quality	(B)	B	B	B	B	(B)	(B)
Uncertainty in ρ (per cent)	(0.1)	0.1	0.1	0.1	0.2	(0.2)	(1.)
Uncertainty in V (per cent)	(0.1)	0.1	0.1	0.1	0.2	(0.2)	(1.)

Orthobaric Liquid Density of 2-Chlorotoluene

Units: kg/m³ v. K

T	ρ	Uncert.	T	ρ	Uncert.	T	ρ	Uncert.	T	ρ	Uncert.
K	kg/m ³	per cent	K	kg/m ³	per cent	K	kg/m ³	per cent	K	kg/m ³	per
cent											
			350	1025.8	0.1	500	(854.1)	0.2	650	(509.)	1.
			360	1015.5	0.1	510	(840.6)	0.2			
			370	1005.1	0.1	520	(826.6)	0.2			
			380	994.6	0.1	530	(812.1)	0.2			
240	(1133.88)	0.1	390	983.9	0.2	540	(797.0)	0.2			
250	(1124.33)	0.1	400	973.1	0.2	550	(781.2)	0.2			
260	(1114.74)	0.1	410	962.2	0.2	560	(764.7)	0.2			
270	(1105.10)	0.1	420	951.1	0.2	570	(747.2)	0.2			
280	1095.42	0.1	430	939.8	0.2	580	(728.6)	0.2			
290	1085.68	0.1	440	(928.3)	0.2	590	(708.7)	0.5			
300	1075.87	0.1	450	(916.7)	0.2	600	(687.0)	0.5			
310	1066.01	0.1	460	(904.7)	0.2	610	(663.1)	0.5			
320	1056.07	0.1	470	(892.5)	0.2	620	(636.1)	0.5			
330	1046.05	0.1	480	(880.1)	0.2	630	(604.5)	1.			
340	1036.0	0.1	490	(867.3)	0.2	640	(565.)	1.			

Units: cm³/mol v. K

T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent
			350	123.4	0.1	500	(148.2)	0.2	650	(249.)	1.
			360	124.7	0.1	510	(150.6)	0.2			
			370	126.0	0.1	520	(153.1)	0.2			
			380	127.3	0.1	530	(155.9)	0.2			
240	(111.64)	0.1	390	128.7	0.2	540	(158.8)	0.2			
250	(112.59)	0.1	400	130.1	0.2	550	(162.0)	0.2			
260	(113.56)	0.1	410	131.6	0.2	560	(165.5)	0.2			
270	(114.55)	0.1	420	133.1	0.2	570	(169.4)	0.2			
280	115.56	0.1	430	134.7	0.2	580	(173.7)	0.2			
290	116.60	0.1	440	(136.4)	0.2	590	(178.6)	0.5			
300	117.66	0.1	450	(138.1)	0.2	600	(184.3)	0.5			
310	118.75	0.1	460	(139.9)	0.2	610	(190.9)	0.5			
320	119.87	0.1	470	(141.8)	0.2	620	(199.0)	0.5			
330	121.02	0.1	480	(143.8)	0.2	630	(209.4)	1.			
340	122.2	0.1	490	(146.0)	0.2	640	(224.)	1.			

The following Sources give liquid density or liquid molar volume data for this compound. Those Sources used to derive the coefficients of the liquid density/molar volume equation are indicated by the temperature range (ambient 'A', low 'L', medium 'M', high 'H' or critical 'C') of their data. An asterisk (*) indicates that the Source is not a primary source of experimental data.

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3-ClC₆H₄CH₃
 3-Chlorotoluene; *m*-Chlorotoluene; *m*-Tolylchloride

C₇H₇Cl

CAS Reg. No. 108-41-8

Mol. Wt. 126.59

Orthobaric Liquid Density and Molar Volume $\ln(\rho/\rho_c) = -\ln(V/V_c) = N_1\tau + N_2\tau^2 + N_3\tau^3 + N_4\tau^4$

where ρ is the density, ρ_c is the critical density, V is the molar volume, V_c is the critical molar volume and $\tau = (1-T/T_c)^{1/3}$, where T is the temperature and T_c is the critical temperature in kelvins.

Critical Temperature	T_c	= 662. K	(t_c	= 388.85 °C)
Critical Pressure	p_c	= 3975. kPa	(p_c	= 39.23 atm)
Critical Density	ρ_c	= 346. kg/m ³	(V_c	= 365.87 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.264		

$N_1 = 1.79046$ $N_2 = -0.65236$ $N_3 = 0.00000$ $N_4 = 0.21739$

Density at 298.15 K (25 °C)	ρ_{25}	= 1067.65 kg/m ³	(V_{25}	= 118.57 cm ³ /mol)
Normal Boiling Point	T_b	= 435.350 K	(t_b	= 162.200 °C)
Approximate Melting Point	T_m	= 225. K	(t_m	= -48. °C)

Data at Specified Temperatures

$t/^\circ\text{C}$ T/K	-50 223.15	0 273.15	25 298.15	50 323.15	162.20 435.35	300 573.15	388.85 662.00
$\rho/(\text{kg/m}^3)$ ($d\rho/dT/(\text{kg/m}^3 \text{ K})$)	(1138.30) (-0.93)	(1091.50) (-0.95)	1067.65 -0.96	1043.41 -0.98	926.85 -1.12	(740.31) (-1.76)	(346.00) -∞
$V/(\text{cm}^3/\text{mol})$ ($dV/dT/(\text{cm}^3/\text{mol K})$)	(111.21) (0.09)	(115.98) (0.10)	118.57 0.11	121.32 0.11	136.58 0.17	(170.99) (0.41)	(365.87) ∞
Data Quality	(B)	(B)	B	B	B	(B)	(B)
Uncertainty in ρ (per cent)	(0.1)	(0.1)	0.1	0.1	0.2	(0.2)	(1.)
Uncertainty in V (per cent)	(0.1)	(0.1)	0.1	0.1	0.2	(0.2)	(1.)

Orthobaric Liquid Density of 3-Chlorotoluene

Units: kg/m³ v. K

T K cent	ρ kg/m ³	Uncert. in ρ per cent	T K cent	ρ kg/m ³	Uncert. in ρ per cent	T K cent	ρ kg/m ³	Uncert. in ρ per cent	T K cent	ρ kg/m ³	Uncert. in ρ per
			350	1016.8	0.1	500	(849.3)	0.2	650	(530.)	1.
			360	1006.8	0.1	510	(836.1)	0.2	660	(442.)	1.
			370	996.6	0.1	520	(822.5)	0.2			
230	(1131.95)	0.1	380	986.3	0.1	530	(808.5)	0.2			
240	(1122.64)	0.1	390	975.9	0.2	540	(793.8)	0.2			
250	(1113.29)	0.1	400	965.4	0.2	550	(778.6)	0.2			
260	(1103.91)	0.1	410	954.7	0.2	560	(762.6)	0.2			
270	(1094.48)	0.1	420	943.8	0.2	570	(745.8)	0.2			
280	(1085.00)	0.1	430	932.8	0.2	580	(728.0)	0.2			
290	1075.46	0.1	440	921.6	0.2	590	(708.9)	0.5			
300	1065.87	0.1	450	910.2	0.2	600	(688.3)	0.5			
310	1056.22	0.1	460	(898.6)	0.2	610	(665.7)	0.5			
320	1046.49	0.1	470	(886.7)	0.2	620	(640.5)	0.5			
330	1036.7	0.1	480	(874.5)	0.2	630	(611.5)	1.			
340	1026.8	0.1	490	(862.1)	0.2	640	(576.5)	1.			

C₇H₇Cl

Orthobaric Liquid Molar Volume of 3-Chlorotoluene

Units: cm³/mol v. K

T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent
			350	124.5	0.1	500	(149.1)	0.2	650	(239.)	1.
			360	125.7	0.1	510	(151.4)	0.2	660	(286.)	1.
			370	127.0	0.1	520	(153.9)	0.2			
230	(111.83)	0.1	380	128.3	0.1	530	(156.6)	0.2			
240	(112.76)	0.1	390	129.7	0.2	540	(159.5)	0.2			
250	(113.71)	0.1	400	131.1	0.2	550	(162.6)	0.2			
260	(114.67)	0.1	410	132.6	0.2	560	(166.0)	0.2			
270	(115.66)	0.1	420	134.1	0.2	570	(169.7)	0.2			
280	(116.67)	0.1	430	135.7	0.2	580	(173.9)	0.2			
290	117.71	0.1	440	137.4	0.2	590	(178.6)	0.5			
300	118.77	0.1	450	139.1	0.2	600	(183.9)	0.5			
310	119.85	0.1	460	(140.9)	0.2	610	(190.1)	0.5			
320	120.97	0.1	470	(142.8)	0.2	620	(197.6)	0.5			
330	122.1	0.1	480	(144.8)	0.2	630	(207.0)	1.			
340	123.3	0.1	490	(146.8)	0.2	640	(219.6)	1.			

The following Sources give liquid density or liquid molar volume data for this compound. Those Sources used to derive the coefficients of the liquid density/molar volume equation are indicated by the temperature range (ambient 'A', low 'L', medium 'M', high 'H' or critical 'C') of their data. An asterisk (*) indicates that the Source is not a primary source of experimental data.

1	FEITLER, S.;	<i>Z.Phys.Chem.</i> , Vol.4, p.68, 1889.	
2	SEUBERT, K.;	<i>Chem.Ber.</i> , Vol.22, p.2520, 1889.	
3	DOBROSSERDOV, D.K.;	<i>J.Russ.Phys.Chem.Soc.</i> , Vol.43, p.115, 1911.	
4	VON AUWERS, K.;	<i>Liebigs Ann.Chem.</i> , Vol.422, p.164, 1921.	
5	KERR, R.N.;	<i>Phil.Mag.</i> , Vol.3, p.332, 1927.	
6	LAGEMAN, R.T.; McMILLAN, D.R.; et al.;	<i>J.Phys.Chem.</i> , Vol.17, p.369, 1949.	M
7	SKVARCHENKO, V.R.; et al.;	<i>J.Gen.Chem.USSR</i> , Vol.30, p.3502, 1960.	
8	MECHTIEV, -.; et al.;	<i>Azerb.Khim.Zh.</i> , No.1, p.21, 1971.	
9	TMENOV, D.N.; et al.;	<i>J.Appl.Chem.USSR</i> , Vol.50, p.127, 1977.	A
10	GOUD, B.B.; VENKATESU, P.; et al.;	<i>J.Chem.Eng.Data</i> , Vol.40, p.1211, 1995.	A

4-ClC₆H₄CH₃
 4-Chlorotoluene; *p*-Chlorotoluene; *p*-Tolylchloride

C₇H₇Cl

CAS Reg. No. 106-43-4

Mol. Wt. 126.59

Orthobaric Liquid Density and Molar Volume $\ln(\rho/\rho_c) = -\ln(V/V_c) = N_1 \tau + N_2 \tau^2 + N_3 \tau^3 + N_4 \tau^4$

where ρ is the density, ρ_c is the critical density, V is the molar volume, V_c is the critical molar volume and $\tau = (1-T/T_c)^{1/3}$, where T is the temperature and T_c is the critical temperature in kelvins.

Critical Temperature	T_c	= 664. K	(t_c	= 390.85 °C)
Critical Pressure	p_c	= 3850. kPa	(p_c	= 38.00 atm)
Critical Density	ρ_c	= 344. kg/m ³	(V_c	= 367.99 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.257		

$N_1 = 1.79601$ $N_2 = -0.65729$ $N_3 = 0.00000$ $N_4 = 0.21926$

Density at 298.15 K (25 °C)	ρ_{25}	= 1064.55 kg/m ³	(V_{25}	= 118.91 cm ³ /mol)
Normal Boiling Point	T_b	= 435.600 K	(t_b	= 162.450 °C)
Approximate Melting Point	T_m	= 281. K	(t_m	= 8. °C)

Data at Specified Temperatures

$t/^\circ\text{C}$ T/K	0	25	50	100	162.45	300	390.85
	273.15	298.15	323.15	373.15	435.60	573.15	664.00
$\rho/(\text{kg/m}^3)$ ($d\rho/dT/(\text{kg/m}^3 \text{ K})$)	(1088.26) (-0.94)	1064.55 -0.96	1040.46 -0.97	990.75 -1.02	924.45 -1.11	(740.29) (-1.73)	(344.00) -∞
$V/(\text{cm}^3/\text{mol})$ ($dV/dT/(\text{cm}^3/\text{mol K})$)	(116.32) (0.10)	118.91 0.11	121.67 0.11	127.77 0.13	136.94 0.16	(171.00) (0.40)	(367.99) ∞
Data Quality	(B)	B	B	B	B	(B)	(B)
Uncertainty in ρ (per cent)	(0.1)	0.1	0.1	0.1	0.2	(0.2)	(1.)
Uncertainty in V (per cent)	(0.1)	0.1	0.1	0.1	0.2	(0.2)	(1.)

Orthobaric Liquid Density of 4-Chlorotoluene

Units: kg/m³ v. K

T K cent	ρ kg/m ³	Uncert. in ρ per cent	T K cent	ρ kg/m ³	Uncert. in ρ per cent	T K cent	ρ kg/m ³	Uncert. in ρ per cent	T K cent	ρ kg/m ³	Uncert. in ρ per cent
			400	962.9	0.1	550	(778.0)	0.2			
			410	952.3	0.2	560	(762.3)	0.2			
			420	941.6	0.2	570	(745.7)	0.2			
280	(1081.80)	0.1	430	930.7	0.2	580	(728.2)	0.2			
290	1072.32	0.1	440	(919.5)	0.2	590	(709.4)	0.5			
300	1062.78	0.1	450	(908.2)	0.2	600	(689.3)	0.5			
310	1053.18	0.1	460	(896.7)	0.2	610	(667.2)	0.5			
320	1043.52	0.1	470	(884.9)	0.2	620	(642.7)	0.5			
330	1033.78	0.1	480	(872.9)	0.2	630	(614.7)	1.			
340	1023.96	0.1	490	(860.5)	0.2	640	(581.3)	1.			
350	1014.05	0.1	500	(847.9)	0.2	650	(538.)	1.			
360	1004.06	0.1	510	(834.8)	0.2	660	(467.)	1.			
370	994.0	0.1	520	(821.4)	0.2						
380	983.7	0.1	530	(807.5)	0.2						
390	973.4	0.1	540	(793.0)	0.2						

C₇H₇Cl

Orthobaric Liquid Molar Volume of 4-Chlorotoluene

Units: cm³/mol v. K

T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent
280	(117.02)	0.1	400	131.5	0.1	550	(162.7)	0.2			
290	118.05	0.1	410	132.9	0.2	560	(166.1)	0.2			
			420	134.4	0.2	570	(169.8)	0.2			
			430	136.0	0.2	580	(173.8)	0.2			
			440	(137.7)	0.2	590	(178.4)	0.5			
300	119.11	0.1	450	(139.4)	0.2	600	(183.7)	0.5			
310	120.20	0.1	460	(141.2)	0.2	610	(189.7)	0.5			
320	121.31	0.1	470	(143.1)	0.2	620	(197.0)	0.5			
330	122.45	0.1	480	(145.0)	0.2	630	(205.9)	1.			
340	123.63	0.1	490	(147.1)	0.2	640	(217.8)	1.			
350	124.84	0.1	500	(149.3)	0.2	650	(235.)	1.			
360	126.08	0.1	510	(151.6)	0.2	660	(271.)	1.			
370	127.4	0.1	520	(154.1)	0.2						
380	128.7	0.1	530	(156.8)	0.2						
390	130.0	0.1	540	(159.6)	0.2						

The following Sources give liquid density or liquid molar volume data for this compound. Those Sources used to derive the coefficients of the liquid density/molar volume equation are indicated by the temperature range (ambient 'A', low 'L', medium 'M', high 'H' or critical 'C') of their data. An asterisk (*) indicates that the Source is not a primary source of experimental data.

1	SCHIFF, R.;	<i>Liebigs Ann.Chem.</i> , Vol.220, p.71, 1883.	
2	FEITLER, S.;	<i>Z.Phys.Chem.</i> , Vol.4, p.78, 1889.	
3	SEUBERT, K.;	<i>Chem.Ber.</i> , Vol.22, p.2520, 1889.	
4	PERKIN, H.;	<i>J.Chem.Soc.</i> , Vol.69, p.1201, 1896.	
5	KAHLBAUM, G.W.A.;	<i>Z.Phys.Chem.</i> , Vol.26, p.577, 1898.	
6	COHEN, J.B.; DAWSON, H.M.; et al.;	<i>J.Chem.Soc.</i> , Vol.97, p.1623, 1910.	
7	DOBROSSERDOV, D.K.;	<i>J.Russ.Phys.Chem.Soc.</i> , Vol.43, p.115, 1911.	
8	JAEGER, F.M.;	<i>Z.Anorg.Allg.Chem.</i> , Vol.101, p.125, 1917.	
9	VON AUWERS, K.;	<i>Liebigs Ann.Chem.</i> , Vol.422, p.164, 1921.	
10	WAHL, A.; NORMAND, G.; et al.;	<i>C.R.Hebd.Seances Acad.Sci.</i> , Vol.174, p.948, 1922.	A
11	WAHL, A.; VERMEYLEN, G.;	<i>Bull.Soc.Chim.France</i> , Vol.31, p.571, 1922.	
12	MATHEWS, J.H.;	<i>J.Am.Chem.Soc.</i> , Vol.48, p.562, 1926.	
13	KERR, R.N.;	<i>Phil.Mag.</i> , Vol.3, p.332, 1927.	
14	GINDRAUX, L.;	<i>Helv.Chem.Acta</i> , Vol.12, p.921, 1929.	
15	LAGEMAN, R.T.; EVANS, J.S.; et al.;	<i>J.Am.Chem.Soc.</i> , Vol.70, p.2996, 1948.	M
16	VOGEL, A.I.;	<i>J.Chem.Soc.</i> , p.644, 1948.	
17	CONRADI, J.J.; LI, N.C.;	<i>J.Am.Chem.Soc.</i> , Vol.75, p.785, 1953.	
18	PARTHASARATHY, P.S.; CHARL, S.S.; et al.;	<i>J.Phys.Radium</i> , Vol.14, p.541, 1953.	
19	PETRO, A.J.; SMYTH, C.P.;	<i>J.Am.Chem.Soc.</i> , Vol.79, p.6142, 1957.	M
20	MECHTIEV, -.; et al.;	<i>Azerb.Khim.Zh.</i> , No.1, p.21, 1971.	
21	SULEIMANKOV, -.; et al.;	<i>Azerb.Khim.Zh.</i> , No.1, p.36, 1976.	A
22	SREENIVASULU, B.; KUMAR, V.C.; et al.;	<i>J.Chem.Eng.Data</i> , Vol.37, p.47, 1992.	
23	KUMAR, K.S.; NAIDU, P.R.;	<i>J.Chem.Eng.Data</i> , Vol.38, p.156, 1993.	
24	GOUD, B.B.; VENKATESU, P.; et al.;	<i>J.Chem.Eng.Data</i> , Vol.40, p.1211, 1995.	A
25	PALAIIOLOGOU, M.M.; MOLINOU, I.E.;	<i>J.Chem.Eng.Data</i> , Vol.40, p.880, 1995.	M

C₆H₅CH₂Br
 (Bromomethyl)benzene; Benzyl bromide

C₇H₇Br

CAS Reg. No. 100-39-0

Mol. Wt. 171.04

Orthobaric Liquid Density and Molar Volume $\ln(\rho/\rho_c) = -\ln(V/V_c) = N_1\tau + N_2\tau^2 + N_3\tau^3 + N_4\tau^4$

where ρ is the density, ρ_c is the critical density, V is the molar volume, V_c is the critical molar volume and $\tau = (1-T/T_c)^{1/3}$, where T is the temperature and T_c is the critical temperature in kelvins.

Critical Temperature	T_c	= 720. K	(t_c	= 446.85 °C)
Critical Pressure	p_c	= 3950. kPa	(p_c	= 38.98 atm)
Critical Density	ρ_c	= 450. kg/m ³	(V_c	= 380.09 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.251		

$N_1 = 1.81734$ $N_2 = -0.67707$ $N_3 = 0.00000$ $N_4 = 0.22713$

Density at 298.15 K (25 °C)	ρ_{25}	= 1432.57 kg/m ³	(V_{25}	= 119.39 cm ³ /mol)
Normal Boiling Point	T_b	= 474.150 K	(t_b	= 201. °C)
Approximate Melting Point	T_m	= 271. K	(t_m	= -2. °C)

Data at Specified Temperatures

$t/^\circ\text{C}$ T/K	-2 271.15	0 273.15	25 298.15	100 373.15	201 474.15	300 573.15	446.85 720.00
$\rho/(\text{kg/m}^3)$ ($d\rho/dT/(\text{kg/m}^3 \text{ K})$)	(1463.50) (-1.14)	(1461.22) (-1.14)	1432.57 -1.15	(1344.24) (-1.21)	(1215.50) (-1.36)	(1066.00) (-1.72)	(450.00) -∞
$V/(\text{cm}^3/\text{mol})$ ($dV/dT/(\text{cm}^3/\text{mol K})$)	(116.87) (0.09)	(117.05) (0.09)	119.39 0.10	(127.24) (0.11)	(140.72) (0.16)	(160.45) (0.26)	(380.09) ∞
Data Quality	(B)	(B)	B	(B)	(B)	(B)	(B)
Uncertainty in ρ (per cent)	(0.05)	(0.05)	0.05	(0.05)	(0.2)	(0.2)	(1.)
Uncertainty in V (per cent)	(0.05)	(0.05)	0.05	(0.05)	(0.2)	(0.2)	(1.)

Orthobaric Liquid Density of (Bromomethyl)benzene

Units: kg/m³ v. K

T K cent	ρ kg/m ³	Uncert. in ρ per cent	T K cent	ρ kg/m ³	Uncert. in ρ per cent	T K cent	ρ kg/m ³	Uncert. in ρ per cent	T K cent	ρ kg/m ³	Uncert. in ρ per
			400	(1311.41)	0.1	550	(1104.3)	0.2	700	(734.7)	1.
			410	(1298.96)	0.1	560	(1088.1)	0.2	710	(670.3)	1.
			420	(1286.4)	0.1	570	(1071.4)	0.2	720	(450.)	1.
280	(1453.40)	0.05	430	(1273.7)	0.1	580	(1054.1)	0.2			
290	1441.95	0.05	440	(1260.8)	0.1	590	(1036.2)	0.2			
300	(1430.44)	0.05	450	(1247.8)	0.1	600	(1017.5)	0.2			
310	(1418.88)	0.05	460	(1234.5)	0.1	610	(998.1)	0.2			
320	(1407.26)	0.05	470	(1221.1)	0.2	620	(977.6)	0.2			
330	(1395.57)	0.05	480	(1207.5)	0.2	630	(956.1)	0.5			
340	(1383.81)	0.05	490	(1193.7)	0.2	640	(933.2)	0.5			
350	(1371.97)	0.05	500	(1179.5)	0.2	650	(908.6)	0.5			
360	(1360.06)	0.05	510	(1165.2)	0.2	660	(882.0)	0.5			
370	(1348.05)	0.05	520	(1150.5)	0.2	670	(852.6)	0.5			
380	(1335.94)	0.1	530	(1135.5)	0.2	680	(819.7)	0.5			
390	(1323.73)	0.1	540	(1120.1)	0.2	690	(781.5)	1.			

C₇H₇Br

Orthobaric Liquid Molar Volume of (Bromomethyl)benzene

Units: cm³/mol v. K

T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent
			400	(130.42)	0.1	550	(154.9)	0.2	700	(232.8)	1.
			410	(131.67)	0.1	560	(157.2)	0.2	710	(255.2)	1.
			420	(133.0)	0.1	570	(159.6)	0.2	720	(380.)	1.
280	(117.68)	0.05	430	(134.3)	0.1	580	(162.3)	0.2			
290	118.62	0.05	440	(135.7)	0.1	590	(165.1)	0.2			
300	(119.57)	0.05	450	(137.1)	0.1	600	(168.1)	0.2			
310	(120.55)	0.05	460	(138.5)	0.1	610	(171.4)	0.2			
320	(121.54)	0.05	470	(140.1)	0.2	620	(175.0)	0.2			
330	(122.56)	0.05	480	(141.6)	0.2	630	(178.9)	0.5			
340	(123.60)	0.05	490	(143.3)	0.2	640	(183.3)	0.5			
350	(124.67)	0.05	500	(145.0)	0.2	650	(188.2)	0.5			
360	(125.76)	0.05	510	(146.8)	0.2	660	(193.9)	0.5			
370	(126.88)	0.05	520	(148.7)	0.2	670	(200.6)	0.5			
380	(128.03)	0.1	530	(150.6)	0.2	680	(208.7)	0.5			
390	(129.21)	0.1	540	(152.7)	0.2	690	(218.9)	1.			

The following Sources give liquid density or liquid molar volume data for this compound. Those Sources used to derive the coefficients of the liquid density/molar volume equation are indicated by the temperature range (ambient 'A', low 'L', medium 'M', high 'H' or critical 'C') of their data. An asterisk (*) indicates that the Source is not a primary source of experimental data.

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|---|--------------------------------|---|---|
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2-BrC₆H₄CH₃
 2-Bromotoluene; *o*-Bromotoluene; *o*-Tolylbromide

C₇H₇Br

CAS Reg. No. 95-46-5

Mol. Wt. 171.04

Orthobaric Liquid Density and Molar Volume $\ln(\rho/\rho_c) = -\ln(V/V_c) = N_1 \tau + N_2 \tau^2 + N_3 \tau^3 + N_4 \tau^4$

where ρ is the density, ρ_c is the critical density, V is the molar volume, V_c is the critical molar volume and $\tau = (1 - T/T_c)^{1/3}$, where T is the temperature and T_c is the critical temperature in kelvins.

Critical Temperature	T_c	= 692. K	(t_c	= 418.85 °C)
Critical Pressure	p_c	= 3850. kPa	(p_c	= 38.00 atm)
Critical Density	ρ_c	= 451. kg/m ³	(V_c	= 379.25 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.254		

$$N_1 = 1.80907 \quad N_2 = -0.66926 \quad N_3 = 0.00000 \quad N_4 = 0.22396$$

Density at 298.15 K (25 °C)	ρ_{25}	= 1417.55 kg/m ³	(V_{25}	= 120.66 cm ³ /mol)
Normal Boiling Point	T_b	= 454.650 K	(t_b	= 181.5 °C)
Approximate Melting Point	T_m	= 245. K	(t_m	= -28. °C)

Data at Specified Temperatures

$t/^\circ\text{C}$	-30	0	25	100	181.50	300	418.85
T/K	243.15	273.15	298.15	373.15	454.65	573.15	692.00
$\rho/(\text{kg/m}^3)$	(1482.84)	(1447.42)	1417.55	1325.03	(1216.39)	(1024.18)	(451.00)
$(d\rho/dT)/(\text{kg/m}^3 \text{ K})$	(-1.17)	(-1.19)	-1.20	-1.27	(-1.41)	(-1.95)	$-\infty$
$V/(\text{cm}^3/\text{mol})$	(115.35)	(118.17)	120.66	129.08	(140.61)	(167.00)	(379.25)
$(dV/dT)/(\text{cm}^3/\text{mol K})$	(0.09)	(0.10)	0.10	0.12	(0.16)	(0.32)	∞
Data Quality	(B)	(B)	B	B	(B)	(B)	(B)
Uncertainty in ρ (per cent)	(0.05)	(0.05)	0.05	0.1	(0.2)	(0.2)	(1.)
Uncertainty in V (per cent)	(0.05)	(0.05)	0.05	0.1	(0.2)	(0.2)	(1.)

Orthobaric Liquid Density of 2-Bromotoluene

Units: kg/m³ v. K

T	ρ	Uncert.	T	ρ	Uncert.	T	ρ	Uncert.	T	ρ	Uncert.
K	kg/m ³	per cent	K	kg/m ³	per cent	K	kg/m ³	per cent	K	kg/m ³	per
250	(1474.79)	0.05	400	1290.44	0.1	550	(1067.2)	0.2			
260	(1463.00)	0.05	410	1277.3	0.1	560	(1049.1)	0.2			
270	(1451.16)	0.05	420	1264.0	0.1	570	(1030.3)	0.2			
280	1439.27	0.05	430	1250.5	0.1	580	(1010.6)	0.2			
290	1427.33	0.05	440	1236.8	0.1	590	(990.1)	0.2			
300	1415.32	0.05	450	1222.9	0.2	600	(968.4)	0.2			
310	1403.25	0.05	460	(1208.8)	0.2	610	(945.4)	0.2			
320	1391.10	0.05	470	(1194.5)	0.2	620	(920.8)	0.5			
330	1378.87	0.05	480	(1179.8)	0.2	630	(894.2)	0.5			
340	1366.56	0.05	490	(1164.9)	0.2	640	(865.1)	0.5			
350	1354.15	0.05	500	(1149.7)	0.2	650	(832.5)	0.5			
360	1341.65	0.05	510	(1134.0)	0.2	660	(795.0)	0.5			
370	1329.03	0.1	520	(1118.0)	0.2	670	(749.7)	1.			
380	1316.30	0.1	530	(1101.6)	0.2	680	(689.4)	1.			
390	1303.44	0.1	540	(1084.7)	0.2	690	(576.)	1.			

C₇H₇Br

Orthobaric Liquid Molar Volume of 2-Bromotoluene

Units: cm³/mol v. K

T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent
250	(115.98)	0.05	400	132.54	0.1	550	(160.3)	0.2			
260	(116.91)	0.05	410	133.9	0.1	560	(163.0)	0.2			
270	(117.86)	0.05	420	135.3	0.1	570	(166.0)	0.2			
280	118.84	0.05	430	136.8	0.1	580	(169.2)	0.2			
290	119.83	0.05	440	138.3	0.1	590	(172.8)	0.2			
300	120.85	0.05	450	139.9	0.2	600	(176.6)	0.2			
310	121.89	0.05	460	(141.5)	0.2	610	(180.9)	0.2			
320	122.95	0.05	470	(143.2)	0.2	620	(185.8)	0.5			
330	124.04	0.05	480	(145.0)	0.2	630	(191.3)	0.5			
340	125.16	0.05	490	(146.8)	0.2	640	(197.7)	0.5			
350	126.31	0.05	500	(148.8)	0.2	650	(205.5)	0.5			
360	127.49	0.05	510	(150.8)	0.2	660	(215.2)	0.5			
370	128.70	0.1	520	(153.0)	0.2	670	(228.1)	1.			
380	129.94	0.1	530	(155.3)	0.2	680	(248.1)	1.			
390	131.22	0.1	540	(157.7)	0.2	690	(297.)	1.			

The following Sources give liquid density or liquid molar volume data for this compound. Those Sources used to derive the coefficients of the liquid density/molar volume equation are indicated by the temperature range (ambient 'A', low 'L', medium 'M', high 'H' or critical 'C') of their data. An asterisk (*) indicates that the Source is not a primary source of experimental data.

1	GLADSTONE, J.H.;	<i>J.Chem.Soc.</i> , Vol.45, p.245, 1884.	
2	FEITLER, S.;	<i>Z.Phys.Chem.</i> , Vol.4, p.78, 1889.	
3	SEUBERT, K.;	<i>Chem.Ber.</i> , Vol.22, p.2520, 1889.	
4	PERKIN, H.;	<i>J.Chem.Soc.</i> , Vol.69, p.1201, 1896.	
5	VAN DER LAAN, M.F.H.;	<i>Rec.Trav.Chim.</i> , Vol.26, p.17, 1907.	
6	JAEGER, F.M.;	<i>Z.Anorg.Allg.Chem.</i> , Vol.101, p.125, 1917.	
7	KERR, R.N.;	<i>Phil.Mag.</i> , Vol.3, p.332, 1927.	
8	LEWINA, R.Ya.; GRINBERG, I.Kh.;	<i>Zh.Obshch.Khim.</i> , Vol.7, p.2306, 1937.	
9	LAGEMAN, R.T.; McMILLAN, D.R.; et al.;	<i>J.Phys.Chem.</i> , Vol.17, p.369, 1949.	M
10	HUSSEY, A.S.; DYER, J.R.;	<i>J.Am.Chem.Soc.</i> , Vol.73, p.603, 1951.	
11	LIBERMAN, A.L.; et al.;	<i>Dokl.Akad.Nauk SSSR</i> , Vol.91, p.845, 1953.	
12	DREISBACH, R. R.;	<i>Adv.Chem.Series</i> , No.15, p.134,2, 1955.	A
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14	MECHTIEV, -.; et al.;	<i>Azerb.Khim.Zh.</i> , No.1, p.21, 1971.	

3-BrC₆H₄CH₃
 3-Bromotoluene; *m*-Bromotoluene; *m*-Tolylbromide

C₇H₇Br

CAS Reg. No. 591-17-3

Mol. Wt. 171.04

Orthobaric Liquid Density and Molar Volume $\ln(\rho/\rho_c) = -\ln(V/V_c) = N_1\tau + N_2\tau^2 + N_3\tau^3 + N_4\tau^4$

where ρ is the density, ρ_c is the critical density, V is the molar volume, V_c is the critical molar volume and $\tau = (1-T/T_c)^{1/3}$, where T is the temperature and T_c is the critical temperature in kelvins.

Critical Temperature	T_c	= 696. K	(t_c	= 422.85 °C)
Critical Pressure	p_c	= 3850. kPa	(p_c	= 38.00 atm)
Critical Density	ρ_c	= 446. kg/m ³	(V_c	= 383.50 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.255		

$N_1 = 1.80884$ $N_2 = -0.66904$ $N_3 = 0.00000$ $N_4 = 0.22387$

Density at 298.15 K (25 °C)	ρ_{25}	= 1403.75 kg/m ³	(V_{25}	= 121.84 cm ³ /mol)
Normal Boiling Point	T_b	= 457.300 K	(t_b	= 184.150 °C)
Approximate Melting Point	T_m	= 233. K	(t_m	= -40. °C)

Data at Specified Temperatures

$t/^\circ\text{C}$ T/K	-40 233.15	0 273.15	25 298.15	100 373.15	184.15 457.30	300 573.15	422.85 696.00
$\rho/(\text{kg/m}^3)$ ($d\rho/dT/(\text{kg/m}^3 \text{ K})$)	(1479.41) (-1.15)	(1433.10) (-1.17)	1403.75 -1.18	1312.93 -1.25	(1202.79) (-1.39)	(1019.05) (-1.89)	(446.00) -∞
$V/(\text{cm}^3/\text{mol})$ ($dV/dT/(\text{cm}^3/\text{mol K})$)	(115.61) (0.09)	(119.35) (0.10)	121.84 0.10	130.27 0.12	(142.20) (0.16)	(167.84) (0.31)	(383.50) ∞
Data Quality	(B)	(B)	B	B	(B)	(B)	(B)
Uncertainty in ρ (per cent)	(0.05)	(0.05)	0.05	0.1	(0.2)	(0.2)	(1.)
Uncertainty in V (per cent)	(0.05)	(0.05)	0.05	0.1	(0.2)	(0.2)	(1.)

Orthobaric Liquid Density of 3-Bromotoluene

Units: kg/m³ v. K

T K cent	ρ kg/m ³	Uncert. in ρ per cent	T K cent	ρ kg/m ³	Uncert. in ρ per cent	T K cent	ρ kg/m ³	Uncert. in ρ per cent	T K cent	ρ kg/m ³	Uncert. in ρ per
			350	1341.51	0.05	500	(1141.2)	0.2	650	(835.7)	0.5
			360	1329.24	0.1	510	(1126.0)	0.2	660	(800.9)	0.5
			370	1316.86	0.1	520	(1110.3)	0.2	670	(759.8)	1.
			380	1304.36	0.1	530	(1094.3)	0.2	680	(707.7)	1.
240	(1471.53)	0.05	390	1291.75	0.1	540	(1077.8)	0.2	690	(629.)	1.
250	(1459.98)	0.05	400	1279.00	0.1	550	(1060.8)	0.2			
260	(1448.40)	0.05	410	1266.1	0.1	560	(1043.2)	0.2			
270	(1436.77)	0.05	420	1253.1	0.1	570	(1025.0)	0.2			
280	(1425.09)	0.05	430	1239.8	0.1	580	(1005.9)	0.2			
290	(1413.36)	0.05	440	1226.4	0.1	590	(986.0)	0.2			
300	1401.57	0.05	450	1212.8	0.2	600	(965.1)	0.2			
310	1389.71	0.05	460	(1199.0)	0.2	610	(943.0)	0.2			
320	1377.78	0.05	470	(1185.0)	0.2	620	(919.4)	0.5			
330	1365.77	0.05	480	(1170.7)	0.2	630	(894.0)	0.5			
340	1353.69	0.05	490	(1156.1)	0.2	640	(866.4)	0.5			

C₇H₇Br

Orthobaric Liquid Molar Volume of 3-Bromotoluene

Units: cm³/mol v. K

T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent	T K	V cm ³ /mol	Uncert. in V per cent
			350	127.50	0.05	500	(149.9)	0.2	650	(204.7)	0.5
			360	128.68	0.1	510	(151.9)	0.2	660	(213.6)	0.5
			370	129.89	0.1	520	(154.0)	0.2	670	(225.1)	1.
			380	131.13	0.1	530	(156.3)	0.2	680	(241.7)	1.
240	(116.23)	0.05	390	132.41	0.1	540	(158.7)	0.2	690	(272.)	1.
250	(117.15)	0.05	400	133.73	0.1	550	(161.2)	0.2			
260	(118.09)	0.05	410	135.1	0.1	560	(164.0)	0.2			
270	(119.04)	0.05	420	136.5	0.1	570	(166.9)	0.2			
280	(120.02)	0.05	430	138.0	0.1	580	(170.0)	0.2			
290	(121.02)	0.05	440	139.5	0.1	590	(173.5)	0.2			
300	122.03	0.05	450	141.0	0.2	600	(177.2)	0.2			
310	123.08	0.05	460	(142.6)	0.2	610	(181.4)	0.2			
320	124.14	0.05	470	(144.3)	0.2	620	(186.0)	0.5			
330	125.23	0.05	480	(146.1)	0.2	630	(191.3)	0.5			
340	126.35	0.05	490	(147.9)	0.2	640	(197.4)	0.5			

The following Sources give liquid density or liquid molar volume data for this compound. Those Sources used to derive the coefficients of the liquid density/molar volume equation are indicated by the temperature range (ambient 'A', low 'L', medium 'M', high 'H' or critical 'C') of their data. An asterisk (*) indicates that the Source is not a primary source of experimental data.

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3	KERR, R.N.;	<i>Phil.Mag.</i> ,	Vol.3, p.332, 1927.	
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