

91034

Issued November 1991

Orthobaric densities and molar volumes of liquids

Halogenated Methanes

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ESDU DATA ITEM No.91034

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THE PREPARATION OF THIS DATA ITEM

The work on this particular Data Item was monitored and guided by the Physical Data and Reaction Kinetics Committee, which first met in 1966 and now has the following membership:

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The technical work involved in the assessment of the available information and the construction and subsequent development of the Data Item was undertaken (under contract to ESDU) by

Mr J.Walton — Independent

in consultation with Dr D.Ambrose.

The person with overall responsibility for the work in this subject area is Mr G.H.Walter, Head of Heat Transfer, Internal Flow and Physical Data.

KEEPING UP TO DATE

We are constantly striving to develop new work and review data already issued. Any comments arising out of your use of our data, or any suggestions for new topics or information that might lead to improvements, will help us to provide a better service.

(Continued on inside back cover)

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ORTHOBARIC DENSITIES AND MOLAR VOLUMES OF LIQUIDS
HALOGENATED METHANES

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	COMPOUND TABLES in the following order	

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MONOHALOMETHANES			
1.1	CH ₃ F	Fluoromethane	Methyl fluoride Refrigerant 41
1.2	CH ₃ Cl	Chloromethane	Methyl chloride Refrigerant 40
	CH ₃ Br	Bromomethane (to be issued)	
	CH ₃ I	Iodomethane (to be issued)	
DIHALOMETHANES			
2.1	CH ₂ F ₂	Difluoromethane	Methylene difluoride Refrigerant 32
2.2	CH ₂ ClF	Chlorofluoromethane	Methylene chlorofluoride Refrigerant 31
2.3	CH ₂ Cl ₂	Dichloromethane	Methylene dichloride Refrigerant 30
	CH ₂ BrCl	Bromochloromethane (to be issued)	
	CH ₂ Br ₂	Dibromomethane (to be issued)	
	CH ₂ I ₂	Diiodomethane (to be issued)	
TRIALOMETHANES			
3.1	CHF ₃	Trifluoromethane	Fluoroform Refrigerant 23
3.2	CHClF ₂	Chlorodifluoromethane	Refrigerant 22
	CHBrF ₂	Bromodifluoromethane (to be issued)	
	CHI ₂ F ₂	Iododifluoromethane (to be issued)	
3.3	CHCl ₂ F	Dichlorofluoromethane	Refrigerant 21
	CHIBrF	Iodobromofluoromethane (not issued)	
	CHI ₂ F	Diiodofluoromethane (to be issued)	
3.4	CHCl ₃	Trichloromethane	Chloroform Refrigerant 20
	CHICl ₂	Iododichloromethane (to be issued)	
	CHI ₂ Cl	Diiodochloromethane (to be issued)	
	CHBr ₃	Tribromomethane (to be issued)	
TETRAHALOMETHANES			
4.1	CF ₄	Tetrafluoromethane	Carbon tetrafluoride Refrigerant 14
4.2	CClF ₃	Chlorotrifluoromethane	Refrigerant 13
4.2a	CBrF ₃	Bromotrifluoromethane	Refrigerant 13B1
4.3	CCl ₂ F ₂	Dichlorodifluoromethane	Refrigerant 12
4.3a	CBrClF ₂	Bromochlorodifluoromethane	Refrigerant 12B1
4.3c	CBr ₂ F ₂	Dibromodifluoromethane	Refrigerant 12B2
4.4	CCl ₃ F	Trichlorofluoromethane	Refrigerant 11
	CI ₂ ClF	Iododichlorofluoromethane (not issued)	
4.5	CCl ₄	Tetrachloromethane	Carbon tetrachloride Refrigerant 10
	CBrCl ₃	Bromotrichloromethane (to be issued)	
	CBr ₄	Tetrabromomethane (to be issued)	

NB. To allow for the future issue of other compounds sheet numbers are not always consecutive.

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ORTHOBARIC DENSITIES AND MOLAR VOLUMES OF LIQUIDS
HALOGENATED METHANES

1. INTRODUCTION

This Data Item presents orthobaric densities and molar volumes of the halogenated methanes arranged in the order shown on the Contents page. Table 1 is the Compound Name Index which lists alternative names of the compounds with, in bold, the first name used for each compound on the Contents page and at the head of each Table.

The values of density and molar volume for each compound have been obtained by calculation from the equation given, with the coefficients, at the top of each Table. 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, unless otherwise stated, taken from the relevant Data Item giving the vapour pressure. For completeness all the critical parameters of each compound are given in the Tables which also show the density at 25 deg.C, where applicable, and for convenience, the approximate normal boiling and melting points.

The table of Data at Specified Temperatures 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 'X', 'A', 'B' or 'C', at each temperature. Brackets enclose the letters at those temperatures which are outside the range of supporting experimental data. 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 and in Section 4 of the Introductory Data Item, Reference 4.

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 arbitrary temperature ranges are defined more precisely in Section 2 of the Introductory Data Item, Reference 4.

2. NOTATION AND UNITS

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

b_1, b_2, b_3, b_4	non-dimensional coefficients of the density/molar volume equation
d	liquid density
q	$(1-T/T_c)$
T	kelvin temperature
t	Celsius temperature ($T-273.15$)
V	liquid molar volume

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

3. THE CRITICAL DENSITY

The Rackett equation, one of many equations developed to estimate or correlate saturated liquid densities, is described, with its subsequent modifications, in References 1, 2 and 3. This equation does not represent the experimental data over the full range of temperature as well as does the equation used in this Item. However, in its latest form, when fitted to experimental data, it yields reliable values of critical density for a wide variety of compounds, provided the critical temperature and the critical pressure for each compound are reliably known.

For this Item, the critical density was initially taken as the value given by the modified Rackett equation and, where necessary, slightly adjusted to give a smooth variation between compounds. This value was, in general, found to be in good agreement with the reported critical densities.

4. EVALUATION AND CORRELATION

Reliable data over the greater part of the liquid range up to the critical point are available for seven of the compounds considered here. Reliable data for the remainder of the compounds are mainly confined to low and medium reduced temperatures.

The data of the seven compounds with reliable extensive data were fitted by the liquid density equation used here with the critical density adjusted to the value obtained as described in Section 3. It should be noted that in this Item three independent coefficients in the equation were sufficient to adequately represent the experimental data of each compound.

The equations for these compounds, together with the equations for five haloethanes obtained in exactly the same way, were then used to derive a correlation similar to that derived for alkanes which is described in Item 87010. This correlation was then used to derive the density/molar volume equations of the remainder of the compounds. The derived values were checked to confirm that they varied smoothly across each relevant chemical series.

5. UNCERTAINTIES

At any temperature, the estimated uncertainties in density and molar volume are dependent upon the rates of change of these properties with temperature and the data quality. The table of Data at Specified Temperatures shows these gradients, the assessed data quality (indicated by one of the letters 'X', 'A', 'B' or 'C') and the corresponding uncertainties at various points of the liquid range.

There is a tenfold increase in uncertainty with each successive data quality letter. Thus if, for example, an uncertainty is given as 10 (in the units of density or molar volume) it should be assumed that the uncertainty is greater than 1 but not necessarily as high as 10. However, 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.

Comparison of the tabulated values given here with those given in Reference 5 shows good agreement for most compounds, the differences generally being comparable with the estimated uncertainties. In the few cases where agreement is poor the experimental data is usually limited to one unconfirmed set from one Source only and appears to be questionable.

6. REFERENCES

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DANNER, R.P. Improved equation for prediction of saturated liquid density. J. Chem. Eng. Data, Vol.17, No.2, pp.236-241, 1972.
3. 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.
4. ESDU Orthobaric densities and molar volumes of liquids. Introduction to Data Items issued after July 1989. Item No. 89018, ESDU International, 1989.
5. TRC TRC Thermodynamic Tables - Non-Hydrocarbons. Thermodynamics Research Center, Texas A & M University System, College Station, Texas, USA. Loose leaf data sheets extant 1991.

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COMPOUND NAME INDEX

The first name given for each compound on the Contents page and at the head of each Table is in bold type

Name		Sheet No.
Bromochlorodifluoromethane		4.3a
Bromotrifluoromethane		4.2a
Carbon tetrachloride	see Tetrachloromethane	4.5
Carbon tetrafluoride	see Tetrafluoromethane	4.1
Chlorodifluoromethane		3.2
Chloroform	see Trichloromethane	3.4
Chlorofluoromethane		2.2
Chloromethane		1.2
Chlorotrifluoromethane		4.2
Dibromodifluoromethane		4.3c
Dichlorodifluoromethane		4.3
Dichlorofluoromethane		3.3
Dichloromethane		2.3
Difluoromethane		2.1
Fluoroform	see Trifluoromethane	3.1
Fluoromethane		1.1
Methyl chloride	see Chloromethane	1.2
Methyl fluoride	see Fluoromethane	1.1
Methylene chlorofluoride	see Chlorofluoromethane	2.2
Methylene dichloride	see Dichloromethane	2.3
Methylene difluoride	see Difluoromethane	2.1
Tetrachloromethane		4.5
Tetrafluoromethane		4.1
Trichlorofluoromethane		4.4
Trichloromethane		3.4
Trifluoromethane		3.1

Refrigerant Number Index

Refrigerant	Name	Sheet No.
Refrigerant 10	see Tetrachloromethane	4.5
Refrigerant 11	see Trichlorofluoromethane	4.4
Refrigerant 12	see Dichlorodifluoromethane	4.3
Refrigerant 12B1	see Bromochlorodifluoromethane	4.3a
Refrigerant 12B2	see Dibromodifluoromethane	4.3c
Refrigerant 13	see Chlorotrifluoromethane	4.2
Refrigerant 13B1	see Bromotrifluoromethane	4.2a
Refrigerant 14	see Tetrafluoromethane	4.1
Refrigerant 20	see Trichloromethane	3.4
Refrigerant 21	see Dichlorofluoromethane	3.3
Refrigerant 22	see Chlorodifluoromethane	3.2
Refrigerant 23	see Trifluoromethane	3.1
Refrigerant 30	see Dichloromethane	2.3
Refrigerant 31	see Chlorofluoromethane	2.2
Refrigerant 32	see Difluoromethane	2.1
Refrigerant 40	see Chloromethane	1.2
Refrigerant 41	see Fluoromethane	1.1

CH₃F Fluoromethane (Methyl fluoride, Refrigerant 41)

Orthobaric Liquid Density and Molar Volume

$$\ln(d/d_c) = -\ln(V/V_c) = b_1q + b_2q^2 + b_3q^3 + b_4q^4$$

where d is the density, d_c the critical density, V the molar volume, V_c the critical molar volume and $q = (1-T/T_c)^{1/3}$, T being the temperature and T_c the critical temperature in kelvins.

Molecular Weight	MW =	78.11	
Critical Temperature	$T_c =$	317.5 K	($t_c = 44.35\text{ }^\circ\text{C}$)
Critical Pressure	$p_c =$	6.000 MPa	($= 59.22\text{ atm}$)
Critical Density	$d_c =$	307 kg/m ³	($V_c = 111\text{ cm}^3/\text{mol}$)
Critical Compression Factor	$Z_c =$	0.252	
$b_1 = 1.84315$	$b_2 = -0.66531$	$b_3 = 0.00000$	$b_4 = 0.22055$
Density at 298.15 K (25 °C)	$d_{25} =$	575.04 kg/m ³	($V_{25} = 135.84\text{ cm}^3/\text{mol}$)
Normal Boiling Point	$T_b =$	194.83 K	($t_b = -78.32\text{ }^\circ\text{C}$)
Normal Melting Point	$T_m =$	131 K	($t_m = -142\text{ }^\circ\text{C}$)

Data at Specified Temperatures

$t/^\circ\text{C}$	-142	-100	-78	-50	0	25	44
T/K	131.15	173.15	195.15	223.15	273.15	298.15	317.15
$d/(\text{kg}/\text{m}^3)$	1004.30	923.20	878.00	815.89	678.62	575.04	368.77
$(d(d)/dT)/(\text{kg}/\text{m}^3\text{ K})$	-1.88	-2.00	-2.11	-2.34	-3.38	-5.35	-61.92
$V/(\text{cm}^3/\text{mol})$	77.78	84.61	88.97	95.74	115.11	135.84	211.82
$(dV/dT)/(\text{cm}^3/\text{mol K})$	0.15	0.18	0.21	0.27	0.57	1.26	35.57
Data Quality	B	B	B	B	B	B	B
Uncertainty in d (kg/m ³)	1	1	1	1	2	5	10
Uncertainty in V (cm ³ /mol)	0.1	0.1	0.1	0.1	0.2	1	5

Orthobaric Liquid Density of Fluoromethane

Units: kg/m³ v. °C

t	d	Uncert. in d	t	d	Uncert. in d	t	d	Uncert. in d	t	d	Uncert. in d
$^\circ\text{C}$	kg/m ³	kg/m ³	$^\circ\text{C}$	kg/m ³	kg/m ³	$^\circ\text{C}$	kg/m ³	kg/m ³	$^\circ\text{C}$	kg/m ³	kg/m ³
-140	1001.	1	-30	767.	1	20	600.	5	40	460.	10
-130	982.	1	-25	753.	1	22	590.	5	41	446.	10
-120	962.	1	-20	740.	1	24	580.	5	42	429.	10
-110	943.	1	-15	725.	1	26	570.	5	43	407.	10
			-10	711.	1	28	558.	5	44	369.	10
-100	923.	1	-5	695.	2	30	546.	5			
-90	903.	1	0	679.	2	32	533.	10			
-80	882.	1	5	661.	2	34	518.	10			
-70	861.	1	10	643.	5	36	502.	10			
-60	839.	1	15	622.	5	38	483.	10			
-50	816.	1									
-40	792.	1									

Orthobaric Liquid Molar Volume of Fluoromethane

Units: cm^3/mol v. K

T	V	Uncert.	T	V	Uncert.	T	V	Uncert.	T	V	Uncert.
K	cm^3/mol	in cm^3/mol	K	cm^3/mol	in cm^3/mol	K	cm^3/mol	in cm^3/mol	K	cm^3/mol	in cm^3/mol
			240	100.8	0.2	290	127.	1	310	158.	2
			245	102.5	0.2	292	129.	1	311	161.	2
			250	104.4	0.2	294	131.	1	312	165.	2
			255	106.4	0.2	296	133.	1	313	169.	2
140	79.1	0.1	260	108.5	0.2	298	136.	1	314	174.	5
150	80.7	0.1	265	110.8	0.2	300	138.	2	315	181.	5
160	82.3	0.1	270	113.4	0.2	302	141.	2	316	190.	5
170	84.0	0.1	275	116.2	0.2	304	145.	2	317	207.	5
180	85.9	0.1	280	119.	0.5	306	148.	2			
190	87.9	0.1	285	123.	0.5	308	153.	2			
200	90.0	0.1									
210	92.3	0.1									
220	94.9	0.1									
230	97.7	0.1									

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 | LEDUC, A., | C.R. Acad. Sci., Vol. 155, p. 206, 1912. | |
| 2 | CAWOOD, W., PATTERSON, H. S., | J. Chem. Soc., p. 2180, 1932. | C |
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| 5 | AMBROSE, D., | NPL Report Chem 107, Nat. Phys. Lab., Teddington, Middlesex, UK, 1980.* | |
| 6 | SHINAKA, K., GEE, N., FREEMAN, G. R., | J. Chem. Thermodynamics, Vol. 17, p. 1111, 1985. | M |
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| 8 | TRC Thermodynamic Tables, | Texas A & M Univ., Loose leaf data sheets extant 1991.* | |

CH₃Cl Chloromethane (Methyl chloride, Refrigerant 40)

Orthobaric Liquid Density and Molar Volume

$$\ln(d/d_c) = -\ln(V/V_c) = b_1q + b_2q^2 + b_3q^3 + b_4q^4$$

where d is the density, d_c the critical density, V the molar volume, V_c the critical molar volume and $q = (1-T/T_c)^{1/3}$, T being the temperature and T_c the critical temperature in kelvins.

Molecular Weight	MW =	50.49	
Critical Temperature	$T_c =$	416.3 K	($t_c = 143.15\text{ }^\circ\text{C}$)
Critical Pressure	$p_c =$	6.675 MPa	(= 65.88 atm)
Critical Density	$d_c =$	362 kg/m ³	($V_c = 139\text{ cm}^3/\text{mol}$)
Critical Compression Factor	$Z_c =$	0.268	
$b_1 = 1.74939$	$b_2 = -0.62023$	$b_3 = 0.00000$	$b_4 = 0.22623$
Density at 298.15 K (25 °C)	$d_{25} =$	911.98 kg/m ³	($V_{25} = 55.36\text{ cm}^3/\text{mol}$)
Normal Boiling Point	$T_b =$	248.97 K	($t_b = -24.17\text{ }^\circ\text{C}$)
Normal Melting Point	$T_m =$	175 K	($t_m = -98\text{ }^\circ\text{C}$)

Data at Specified Temperatures

$t/^\circ\text{C}$	-98	-24	0	20	30	100	143
T/K	175.15	249.15	273.15	293.15	303.15	373.15	416.15
$d/(\text{kg/m}^3)$	1127.99	1003.93	960.37	921.97	901.82	726.01	408.71
$(d(d)/dT)/(\text{kg/m}^3\text{ K})$	-1.61	-1.77	-1.87	-1.98	-2.05	-3.32	-107.38
$V/(\text{cm}^3/\text{mol})$	44.76	50.29	52.57	54.76	55.98	69.54	123.53
$(dV/dT)/(\text{cm}^3/\text{mol K})$	0.06	0.09	0.10	0.12	0.13	0.32	32.45
Data Quality	(B)	B	B	B	B	B	B
Uncertainty in d (kg/m ³)	1	1	1	1	1	5	10
Uncertainty in V (cm ³ /mol)	0.05	0.05	0.05	0.05	0.05	0.5	2

Orthobaric Liquid Density of Chloromethane

Units: kg/m³ v. °C

t	d	Uncert.	t	d	Uncert.	t	d	Uncert.	t	d	Uncert.
$^\circ\text{C}$	kg/m ³	kg/m ³	$^\circ\text{C}$	kg/m ³	kg/m ³	$^\circ\text{C}$	kg/m ³	kg/m ³	$^\circ\text{C}$	kg/m ³	kg/m ³
-90	1115.	1	50	859.	2	120	648.	5	140	498.	10
-80	1099.	1	55	848.	2	122	638.	5	141	481.	10
-70	1082.	1	60	836.	2	124	628.	5	142	457.	10
-60	1066.	1	65	824.	2	126	617.	10	143	409.	10
			70	812.	2	128	605.	10			
-50	1049.	1	75	799.	2	130	593.	10			
-40	1032.	1	80	786.	2	132	579.	10			
-30	1014.	1	85	772.	2	134	564.	10			
-20	997.	1	90	757.	2	136	546.	10			
-10	979.	1	95	742.	5	138	525.	10			
0	960.	1	100	726.	5						
10	941.	1	105	709.	5						
20	922.	1	110	690.	5						
30	902.	1	115	670.	5						
40	881.	1									

Orthobaric Liquid Molar Volume of Chloromethane

Units: cm^3/mol v. K

T	V	Uncert. in V	T	V	Uncert. in V	T	V	Uncert. in V	T	V	Uncert. in V
K	cm^3/mol	cm^3/mol	K	cm^3/mol	cm^3/mol	K	cm^3/mol	cm^3/mol	K	cm^3/mol	cm^3/mol
			300	55.59	0.05	372	69.	0.5	401	83.	1
			305	56.2	0.05	374	70.	0.5	402	84.	1
			310	56.9	0.1	376	70.	0.5	403	85.	1
180	(45.1)	0.05	315	57.6	0.1	378	71.	0.5	404	86.	1
190	45.7	0.05	320	58.3	0.1	380	72.	0.5	405	87.	1
200	46.4	0.05	325	59.1	0.1	382	73.	0.5	406	88.	1
210	47.1	0.05	330	59.9	0.1	384	73.	0.5	407	89.	1
220	47.9	0.05	335	60.7	0.2	386	74.	0.5	408	91.	1
230	48.7	0.05	340	61.6	0.2	388	75.	0.5	409	92.	2
240	49.5	0.05	345	62.6	0.2	390	76.	0.5	410	94.	2
250	50.4	0.05	350	63.6	0.2	392	77.	1	411	96.	2
260	51.3	0.05	355	64.7	0.2	394	78.	1	412	98.	2
270	52.3	0.05	360	65.9	0.2	396	80.	1	413	101.	2
280	53.3	0.05	365	67.2	0.2	398	81.	1	414	104.	2
290	54.39	0.05	370	68.6	0.2	400	82.	1	415	109.	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.

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