

96022

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Orthobaric densities and molar volumes of liquids

Esters of monobasic acids

2: Branched chain alkyl esters

Endorsed by
The Institution of Chemical Engineers



ESDU DATA ITEM No. 96022

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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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ORTHOBARIC DENSITIES and MOLAR VOLUMES OF LIQUIDS ESTERS OF MONOBASIC ACIDS - 2: BRANCHED CHAIN ALKYL ALKANOATES

CONTENTS

CONTENTS				Page
1.	INTRODUCTION			1
2.	NOTATION AND UNITS			1
3.	THE CRITICAL DENSITY			2
4.	EVALUATION AND CORRELATION			2
5.	UNCERTAINTIES			2
6.	REFERENCES			2
	TABLE 1 Summary of constants in the liquid density equation			3
	TABLES for each compound are given on data sheets in the following order			
1	C ₄ H ₈ O ₂	1-Methylethyl methanoate	Isopropyl formate	5
2	C ₅ H ₁₀ O ₂	1-Methylpropyl methanoate	sec-Butyl formate	7
3	C ₅ H ₁₀ O ₂	2-Methylpropyl methanoate	Isobutyl formate	9
4	C ₅ H ₁₀ O ₂	1,1-Dimethylethyl methanoate	tert-Butyl formate	11
5	C ₆ H ₁₂ O ₂	3-Methylbutyl methanoate	Isopentyl formate	13
6	C ₅ H ₁₀ O ₂	1-Methylethyl ethanoate	Isopropyl acetate	15
7	C ₆ H ₁₂ O ₂	1-Methylpropyl ethanoate	sec-Butyl acetate	17
8	C ₆ H ₁₂ O ₂	2-Methylpropyl ethanoate	Isobutyl acetate	19
9	C ₆ H ₁₂ O ₂	1,1-Dimethylethyl ethanoate	tert-Butyl acetate	21
10	C ₇ H ₁₄ O ₂	3-Methylbutyl ethanoate	Isopentyl acetate	23
11	C ₆ H ₁₂ O ₂	1-Methylethyl propanoate	Isopropyl propionate	25
12	C ₇ H ₁₄ O ₂	1-Methylpropyl propanoate	sec-Butyl propionate	27
13	C ₇ H ₁₄ O ₂	2-Methylpropyl propanoate	Isobutyl propionate	29
	C ₇ H ₁₄ O ₂	1,1-Dimethylethyl propanoate (not issued)		
14	C ₈ H ₁₆ O ₂	3-Methylbutyl propanoate	Isopentyl propionate	31
15	C ₇ H ₁₄ O ₂	1-Methylethyl butanoate	Isopropyl butyrate	33
16	C ₈ H ₁₆ O ₂	1-Methylpropyl butanoate	sec-Butyl butyrate	35
17	C ₈ H ₁₆ O ₂	2-Methylpropyl butanoate	Isobutyl butyrate	37
	C ₈ H ₁₆ O ₂	1,1-Dimethylethyl butanoate (not issued)		
18	C ₉ H ₁₈ O ₂	3-Methylbutyl butanoate	Isopentyl butyrate	39
19	C ₈ H ₁₆ O ₂	1-Methylethyl pentanoate	Isopropyl valerate	41
20	C ₉ H ₁₈ O ₂	1-Methylpropyl pentanoate	sec-Butyl valerate	43
21	C ₉ H ₁₈ O ₂	2-Methylpropyl pentanoate	Isobutyl valerate	45
22	C ₉ H ₁₈ O ₂	1-Methylethyl hexanoate	Isopropyl caproate	47
	C ₁₁ H ₂₂ O ₂	3-Methylbutyl hexanoate (not issued)		
23	C ₅ H ₁₀ O ₂	Methyl 2-methylpropanoate	Methyl isobutyrate	49
24	C ₆ H ₁₂ O ₂	Ethyl 2-methylpropanoate	Ethyl isobutyrate	51
25	C ₇ H ₁₄ O ₂	Propyl 2-methylpropanoate	Propyl isobutyrate	53
26	C ₇ H ₁₄ O ₂	1-Methylethyl 2-methylpropanoate	Isopropyl isobutyrate	55
27	C ₈ H ₁₆ O ₂	Butyl 2-methylpropanoate	Butyl isobutyrate	57
28	C ₈ H ₁₆ O ₂	2-Methylpropyl 2-methylpropanoate	Isobutyl isobutyrate	59
	C ₈ H ₁₆ O ₂	1,1-Dimethylethyl 2-methylpropanoate (not issued)		
29	C ₉ H ₁₈ O ₂	3-Methylbutyl 2-methylpropanoate	Isopentyl isobutyrate	61
30	C ₆ H ₁₂ O ₂	Methyl 2-methylbutanoate		63
31	C ₆ H ₁₂ O ₂	Methyl 3-methylbutanoate	Methyl isovalerate	65
32	C ₇ H ₁₄ O ₂	Ethyl 3-methylbutanoate	Ethyl isovalerate	67
33	C ₈ H ₁₆ O ₂	Propyl 3-methylbutanoate	Propyl isovalerate	69
34	C ₈ H ₁₆ O ₂	1-Methylethyl 3-methylbutanoate	Isopropyl isovalerate	71
35	C ₉ H ₁₈ O ₂	Butyl 3-methylbutanoate	Butyl isovalerate	73
36	C ₉ H ₁₈ O ₂	2-Methylpropyl 3-methylbutanoate	Isobutyl isovalerate	75
	C ₉ H ₁₈ O ₂	1,1-Dimethylethyl 3-methylbutanoate (not issued)		
37	C ₁₀ H ₂₀ O ₂	3-Methylbutyl 3-methylbutanoate	Isopentyl isovalerate	77

96022

ORTHOBARIC DENSITIES AND MOLAR VOLUMES OF LIQUIDS ESTERS OF MONOBASIC ACIDS - 2: BRANCHED CHAIN ALKYL ALKANOATES

1. INTRODUCTION

This Data Item presents orthobaric densities and molar volumes of the branched chain alkyl alkanoates arranged in the order shown on the Contents page.

Table 1, page 5, 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 96021, 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. 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.

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
T	temperature in kelvins
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

3. THE CRITICAL DENSITY

Reliable critical densities, based on liquid and vapour density measurements at high reduced temperatures, have been reported for ten of the compounds considered here and in Part 1. Estimates of the critical density of each compound were 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 critical temperature and critical pressure but neither represents experimental data over a wide range of temperature as satisfactorily as does the equation 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.

Both estimates of the critical density were in good agreement the reported values, where available, and were generally in good agreement with each other for all the compounds, for some compounds there being no significant difference. The Rackett equation tended to give higher estimates than the Riedel equation as the carbon number increased. The mean of the two estimates gave the best fits to the data for the majority of compounds.

4. EVALUATION AND CORRELATION

As explained in Part 1 the coefficients of the ten compounds for which there are reliable high temperature density and critical density values were used to derive a reduced temperature - reduced density correlation analogous to that derived for vapour pressures, see Item 96021. To ensure that the correlation merged into the correlation for alkanes the equation for hexadecane was included in the present correlation which was then used to fit the data of the remaining compounds. In fitting the data for each compound considered here care was taken to ensure that the value of critical density was compatible with the value for the corresponding straight chain compound.

For all of the compounds considered here vapour pressure data were available, see Item 96021, and for some of the compounds the critical temperature, the critical pressure and the critical density were adjusted until they were optimum values for both properties.

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

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

Name	T_c K	ρ_c kg/m ³	N_1	N_2	N_3	N_4
1 1-Methylethyl methanoate	518.	305.	1.77004	-0.61775	0	0.20750
2 1-Methylpropyl methanoate	545.	299.	1.80258	-0.65111	0	0.22255
3 2-Methylpropyl methanoate	551.	297.	1.80975	-0.65871	0	0.22603
4 1,1-Dimethylethyl methanoate	533.	302.	1.77341	-0.62112	0	0.20900
5 3-Methylbutyl methanoate	576.	288.	1.84271	-0.69465	0	0.24266
6 1-Methylethyl ethanoate	531.00	295.	1.82613	-0.67638	0	0.23417
7 1-Methylpropyl ethanoate	563.	291.	1.80115	-0.64961	0	0.22186
8 2-Methylpropyl ethanoate	565.	289.	1.83063	-0.68129	0	0.23644
9 1,1-Dimethylethyl ethanoate	545.	296.	1.77286	-0.62056	0	0.20876
10 3-Methylbutyl ethanoate	592.	283.	1.84745	-0.69994	0	0.24513
11 1-Methylethyl propanoate	557.	289.	1.82150	-0.67134	0	0.23184
12 1-Methylpropyl propanoate	579.	284.	1.83673	-0.68801	0	0.23957
13 2-Methylpropyl propanoate	586.	282.	1.85609	-0.70966	0	0.24969
14 1,1-Dimethylethyl propanoate (not issued)						
14 3-Methylbutyl propanoate	609.	277.	1.87824	-0.73501	0	0.26164
15 1-Methylethyl butanoate	577.	281.	1.84347	-0.69550	0	0.24305
16 1-Methylpropyl butanoate	600.	277.	1.86080	-0.71500	0	0.25219
17 2-Methylpropyl butanoate	606.	276.	1.87397	-0.73007	0	0.25930
18 1,1-Dimethylethyl butanoate (not issued)						
18 3-Methylbutyl butanoate	627.	270.	1.91782	-0.78165	0	0.28387
19 1-Methylethyl pentanoate	600.	275.	1.87382	-0.72990	0	0.25922
20 1-Methylpropyl pentanoate	623.	271.	1.88947	-0.74807	0	0.26784
21 2-Methylpropyl pentanoate	628.	270.	1.90867	-0.77073	0	0.27864
22 1-Methylethyl hexanoate	620.	269.	1.90819	-0.77016	0	0.27836
22 3-Methylbutyl hexanoate (not issued)						
23 Methyl 2-methylpropanoate	540.70	301.	1.80944	-0.65874	0	0.22582
24 Ethyl 2-methylpropanoate	558.	289.	1.82949	-0.68005	0	0.23587
25 Propyl 2-methylpropanoate	581.	282.	1.84931	-0.70202	0	0.24611
26 1-Methylethyl 2-methylpropanoate	567.	282.	1.81619	-0.66561	0	0.22920
27 Butyl 2-methylpropanoate	606.	275.	1.87881	-0.73567	0	0.26195
28 2-Methylpropyl 2-methylpropanoate	597.	276.	1.85017	-0.70299	0	0.24656
29 1,1-Dimethylethyl 2-methylpropanoate (not issued)						
29 3-Methylbutyl 2-methylpropanoate	617.	272.	1.89280	-0.75197	0	0.26969
30 Methyl 2-methylbutanoate	567.	292.	1.83878	-0.69028	0	0.24062
31 Methyl 3-methylbutanoate	569.	291.	1.83057	-0.68123	0	0.23641
32 Ethyl 3-methylbutanoate	584.	283.	1.83575	-0.68693	0	0.23906
33 Propyl 3-methylbutanoate	604.	276.	1.87145	-0.72718	0	0.25794
34 1-Methylethyl 3-methylbutanoate	588.	277.	1.84415	-0.69625	0	0.24341

96022

35	Butyl 3-methylbutanoate	623.	270.	1.91072	-0.77316	0	0.27980
36	2-Methylpropyl 3-methylbutanoate	620.	272.	1.86492	-0.71970	0	0.25440
	1,1-Dimethylethyl 3-methylbutanoate (not issued)						
37	3-Methylbutyl 3-methylbutanoate	640.	266.	1.91291	-0.77578	0	0.28105

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**C₄H₈O₂ 1-Methylethyl methanoate; Isopropyl methanoate; Isopropyl formate**

CAS Reg. No. 625-55-8

Mol. Wt. 88.11

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

Critical Temperature	T_c	= 518. K	(t_c	= 244.85°C)
Critical Pressure	p_c	= 4000. kPa	(p_c	= 39.48 atm)
Critical Density	ρ_c	= 305. kg/m ³	(V_c	= 288.89 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.268		

$$N_1 = 1.77004 \quad N_2 = -0.61775 \quad N_3 = 0.00000 \quad N_4 = 0.20750$$

Density at 298.15 K (25°C)	ρ_{25}	= 869.40 kg/m ³	(V_{25}	= 101.35 cm ³ /mol)
Normal Boiling Point	T_b	= 340.619 K	(t_b	= 67.469°C)
Melting Point	T_m	= -	(t_m	= -)

Data at Specified Temperatures

$t/^{\circ}\text{C}$	-100	0	25	50	67.47	100	244.85
T/K	173.15	273.15	298.15	323.15	340.62	373.15	518.00
$\rho/(\text{kg/m}^3)$	(1007.77)	898.46	869.40	(839.23)	(817.30)	(774.00)	(305.00)
$(d\rho/dT)/(\text{kg/m}^3 \text{ K})$	(-1.06)	-1.14	-1.18	(-1.23)	(-1.28)	(-1.39)	$-\infty$
$V/(\text{cm}^3/\text{mol})$	(87.43)	98.07	101.35	(104.99)	(107.81)	(113.84)	(288.89)
$(dV/dT)/(\text{cm}^3/\text{mol K})$	(0.09)	0.12	0.14	(0.15)	(0.17)	(0.20)	∞
Data Quality	(B)	B	B	(B)	(B)	(B)	(B)
Uncertainty in ρ (kg/m ³)	(2.)	2.	2.	(2.)	(2.)	(5.)	(10.)
Uncertainty in V (cm ³ /mol)	(0.2)	0.2	0.2	(0.2)	(0.2)	(0.5)	(10.)

Orthobaric Liquid Density of 1-Methylethyl methanoate

Units: kg/m ³ v. °C											
t	ρ	Uncert.	t	ρ	Uncert.	t	ρ	Uncert.	t	ρ	Uncert.
°C	kg/m ³	kg/m ³	°C	kg/m ³	kg/m ³	°C	kg/m ³	kg/m ³	°C	kg/m ³	kg/m ³
-100	(1008.)	2.	0	898.	2.	100	(774.)	5.	200	(596.)	10.
-95	(1002.)	2.	5	893.	2.	105	(767.)	5.	205	(583.)	10.
-90	(997.)	2.	10	887.	2.	110	(760.)	5.	210	(569.)	10.
-85	(992.)	2.	15	881.	2.	115	(753.)	5.	215	(554.)	10.
-80	(987.)	2.	20	875.	2.	120	(745.)	5.	220	(537.)	10.
-75	(981.)	2.	25	869.	2.	125	(738.)	5.	225	(518.)	10.
-70	(976.)	2.	30	863.	2.	130	(730.)	5.	230	(496.)	10.
-65	(970.)	2.	35	857.	2.	135	(722.)	5.	235	(469.)	10.
-60	(965.)	2.	40	(851.)	2.	140	(714.)	5.	240	(431.)	10.
-55	(960.)	2.	45	(845.)	2.	145	(706.)	5.			
-50	(954.)	2.	50	(839.)	2.	150	(698.)	5.			
-45	(949.)	2.	55	(833.)	2.	155	(689.)	5.			
-40	(943.)	2.	60	(827.)	2.	160	(680.)	5.			
-35	(938.)	2.	65	(820.)	2.	165	(671.)	5.			
-30	(932.)	2.	70	(814.)	2.	170	(662.)	5.			
-25	(927.)	2.	75	(808.)	2.	175	(652.)	5.			
-20	(921.)	2.	80	(801.)	2.	180	(642.)	5.			
-15	(915.)	2.	85	(794.)	2.	185	(631.)	10.			
-10	(910.)	2.	90	(788.)	5.	190	(620.)	10.			
-5	(904.)	2.	95	(781.)	5.	195	(608.)	10.			

Orthobaric Liquid Molar Volume of 1-Methylethyl methanoate

Units: cm ³ /mol v. K											
T	V	Uncert.		T	V	Uncert.		T	V	Uncert.	
K	cm ³ /mol	cm ³ /mol		K	cm ³ /mol	cm ³ /mol		K	cm ³ /mol	cm ³ /mol	
175	(87.6)	0.2		275	98.3	0.2		375	(114.2)	0.5	
180	(88.1)	0.2		280	98.9	0.2		380	(115.3)	1.	
185	(88.5)	0.2		285	99.6	0.2		385	(116.4)	1.	
190	(89.0)	0.2		290	100.2	0.2		390	(117.5)	1.	
195	(89.5)	0.2		295	100.9	0.2		395	(118.7)	1.	
200	(90.0)	0.2		300	101.6	0.2		400	(119.9)	1.	
205	(90.5)	0.2		305	102.3	0.2		405	(121.2)	1.	
210	(91.0)	0.2		310	103.0	0.2		410	(122.)	1.	
215	(91.5)	0.2		315	(103.8)	0.2		415	(124.)	1.	
220	(92.0)	0.2		320	(104.5)	0.2		420	(125.)	1.	
225	(92.5)	0.2		325	(105.3)	0.2		425	(127.)	1.	
230	(93.1)	0.2		330	(106.1)	0.2		430	(128.)	1.	
235	(93.6)	0.2		335	(106.9)	0.2		435	(130.)	1.	
240	(94.2)	0.2		340	(107.7)	0.2		440	(132.)	1.	
245	(94.7)	0.2		345	(108.6)	0.2		445	(134.)	1.	
250	(95.3)	0.2		350	(109.4)	0.5		450	(136.)	2.	
255	(95.9)	0.2		355	(110.3)	0.5		455	(138.)	2.	
260	(96.5)	0.2		360	(111.3)	0.5		460	(141.)	2.	
265	(97.1)	0.2		365	(112.2)	0.5		465	(143.)	2.	
270	(97.7)	0.2		370	(113.2)	0.5		470	(146.)	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 PRIBRAM, -.; HANDL, -. *Monatsh. Chem.*, Vol.2, p.685, 1881.
- 2 LOWRY, T. M. *J. Chem. Soc.*, Vol.105, p.81, 1914.
- 3 VOGEL, A. I. *J. Chem. Soc.*, p.616, 1948.
- 4 SOLOV'EV, -.; BARATOV, -. *Zh. Fiz. Khim.*, Vol.34, p.1661, 1960.
- 5 KALASHNIKOV, S. M.; IMASHEV, U. B. *J. Gen. Chem. USSR*, Vol.50, p.2267, 1980.
- 6 TRC Thermodynamic Tables, Texas A & M Univ., Loose leaf data sheets extant 1996.* A

**C₅H₁₀O₂ 1-Methylpropyl methanoate; *sec*-Butyl methanoate; *sec*-Butyl formate**

CAS Reg. No. 589-40-2

Mol. Wt. 102.13

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

Critical Temperature	T_c	= 545. K	(t_c	= 271.85 °C)
Critical Pressure	p_c	= 3500. kPa	(p_c	= 34.54 atm)
Critical Density	ρ_c	= 299. kg/m ³	(V_c	= 341.57 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.264		

$$N_1 = 1.80258 \quad N_2 = -0.65111 \quad N_3 = 0.00000 \quad N_4 = 0.22255$$

Density at 298.15 K (25 °C)	ρ_{25}	= 878.46 kg/m ³	(V_{25}	= 116.26 cm ³ /mol)
Normal Boiling Point	T_b	= 367.336 K	(t_b	= 94.186 °C)
Melting Point	T_m	= -	(t_m	= -)

Data at Specified Temperatures

$t/^\circ\text{C}$	-100	0	25	50	94.19	150	271.85
T/K	173.15	273.15	298.15	323.15	367.34	423.15	545.00
$\rho/(\text{kg/m}^3)$	(1008.69)	(905.54)	878.46	850.55	(798.36)	(724.04)	(299.00)
$(d\rho/dT)/(\text{kg/m}^3 \text{ K})$	(-1.01)	(-1.07)	-1.10	-1.14	(-1.23)	(-1.46)	$-\infty$
$V/(\text{cm}^3/\text{mol})$	(101.25)	(112.78)	116.26	120.08	(127.92)	(141.06)	(341.57)
$(dV/dT)/(\text{cm}^3/\text{mol K})$	(0.10)	(0.13)	0.15	0.16	(0.20)	(0.28)	∞
Data Quality	(B)	(B)	B	B	(C)	(C)	(C)
Uncertainty in ρ (kg/m ³)	(5.)	(2.)	2.	5.	(5.)	(10.)	(10.)
Uncertainty in V (cm ³ /mol)	(0.5)	(0.2)	0.2	0.5	(1.)	(2.)	(10.)

Orthobaric Liquid Density of 1-Methylpropyl methanoate

Units: kg/m ³ v. °C								
t	ρ	Uncert.	t	ρ	Uncert.	t	ρ	Uncert.
°C	kg/m ³	kg/m ³	°C	kg/m ³	kg/m ³	°C	kg/m ³	kg/m ³
-100	(1009.)	5.	0	(906.)	2.	100	(791.)	5.
-95	(1004.)	5.	5	(900.)	2.	105	(785.)	5.
-90	(999.)	5.	10	(895.)	2.	110	(778.)	5.
-85	(994.)	5.	15	(889.)	2.	115	(772.)	5.
-80	(988.)	5.	20	884.	2.	120	(765.)	5.
-75	(983.)	5.	25	878.	2.	125	(759.)	5.
-70	(978.)	5.	30	873.	2.	130	(752.)	5.
-65	(973.)	5.	35	867.	2.	135	(745.)	5.
-60	(968.)	2.	40	862.	2.	140	(738.)	10.
-55	(963.)	2.	45	856.	2.	145	(731.)	10.
-50	(958.)	2.	50	851.	5.	150	(724.)	10.
-45	(953.)	2.	55	845.	5.	155	(717.)	10.
-40	(948.)	2.	60	839.	5.	160	(709.)	10.
-35	(942.)	2.	65	833.	5.	165	(702.)	10.
-30	(937.)	2.	70	827.	5.	170	(694.)	10.
-25	(932.)	2.	75	822.	5.	175	(686.)	10.
-20	(927.)	2.	80	816.	5.	180	(677.)	10.
-15	(921.)	2.	85	810.	5.	185	(669.)	10.
-10	(916.)	2.	90	803.	5.	190	(660.)	10.
-5	(911.)	2.	95	(797.)	5.	195	(651.)	10.

Orthobaric Liquid Molar Volume of 1-Methylpropyl methanoate

Units: cm ³ /mol v. K											
T	V	Uncert.		T	V	Uncert.		T	V	Uncert.	
K	cm ³ /mol	cm ³ /mol		K	cm ³ /mol	cm ³ /mol		K	cm ³ /mol	cm ³ /mol	
175	(101.4)	0.5		275	(113.0)	0.2		375	(129.)	1.	
180	(101.9)	0.5		280	(113.7)	0.2		380	(131.)	1.	
185	(102.5)	0.5		285	(114.4)	0.2		385	(132.)	1.	
190	(103.0)	0.5		290	(115.1)	0.2		390	(133.)	1.	
195	(103.5)	0.5		295	115.8	0.2		395	(134.)	1.	
200	(104.0)	0.5		300	116.5	0.2		400	(135.)	1.	
205	(104.6)	0.5		305	117.3	0.2		405	(136.)	1.	
210	(105.1)	0.5		310	118.0	0.5		410	(138.)	1.	
215	(105.7)	0.5		315	118.8	0.5		415	(139.)	1.	
220	(106.3)	0.5		320	119.6	0.5		420	(140.)	2.	
225	(106.8)	0.2		325	120.4	0.5		425	(142.)	2.	
230	(107.4)	0.2		330	121.2	0.5		430	(143.)	2.	
235	(108.0)	0.2		335	122.0	0.5		435	(145.)	2.	
240	(108.6)	0.2		340	122.9	0.5		440	(146.)	2.	
245	(109.2)	0.2		345	123.8	0.5		445	(148.)	2.	
250	(109.8)	0.2		350	124.6	1.		450	(150.)	2.	
255	(110.4)	0.2		355	125.6	1.		455	(151.)	2.	
260	(111.1)	0.2		360	126.5	1.		460	(153.)	2.	
265	(111.7)	0.2		365	127.5	1.		465	(155.)	2.	
270	(112.4)	0.2		370	(128.5)	1.		470	(158.)	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 PICKARD, R. H.; KENYON, J.; HUNTER, H. *J.Chem.Soc.*, Vol.123, p.9, 1923.
- 2 PALOMAA, -. et al., *Chem.Ber.*, Vol.68, p.306, 1935.
- 3 TRC Thermodynamic Tables, Texas A & M Univ., Loose leaf data sheets extant 1996.* A

**C₅H₁₀O₂ 2-Methylpropyl methanoate; Isobutyl methanoate; Isobutyl formate**

CAS Reg. No. 542-55-2

Mol. Wt. 102.13

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

Critical Temperature	T_c	= 551. K	(t_c	= 277.85°C)
Critical Pressure	p_c	= 3550. kPa	(p_c	= 35.04 atm)
Critical Density	ρ_c	= 297. kg/m ³	(V_c	= 343.87 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.266		

$$N_1 = 1.80975 \quad N_2 = -0.65871 \quad N_3 = 0.00000 \quad N_4 = 0.22603$$

Density at 298.15 K (25°C)	ρ_{25}	= 878.09 kg/m ³	(V_{25}	= 116.31 cm ³ /mol)
Normal Boiling Point	T_b	= 371.45 K	(t_b	= 98.300°C)
Melting Point	T_m	= 177.	(t_m	= -96.°C)

Data at Specified Temperatures

$t/^\circ\text{C}$	-96	0	25	50	98.30	150	277.85
T/K	177.15	273.15	298.15	323.15	371.45	423.15	551.00
$\rho/(\text{kg/m}^3)$	(1002.38)	904.70	878.09	850.69	794.61	(727.28)	(297.00)
$(d\rho/dT)/(\text{kg/m}^3 \text{ K})$	(-0.99)	-1.05	-1.08	-1.11	-1.22	(-1.41)	$-\infty$
$V/(\text{cm}^3/\text{mol})$	(101.89)	112.89	116.31	120.06	128.53	(140.43)	(343.87)
$(dV/dT)/(\text{cm}^3/\text{mol K})$	(0.10)	0.13	0.14	0.16	0.20	(0.27)	∞
Data Quality	(B)	B	B	B	C	(C)	(C)
Uncertainty in ρ (kg/m ³)	(5.)	2.	2.	5.	5.	(10.)	(10.)
Uncertainty in V (cm ³ /mol)	(0.5)	0.2	0.2	0.5	1.	(2.)	(10.)

Orthobaric Liquid Density of 2-Methylpropyl methanoateUnits: kg/m³ v. °C

t	ρ	Uncert.	t	ρ	Uncert.	t	ρ	Uncert.	t	ρ	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
-95	(1001.)	5.	0	905.	2.	100	(793.)	5.	200	(648.)	10.
-90	(996.)	5.	5	899.	2.	105	(786.)	5.	205	(639.)	10.
-85	(991.)	5.	10	894.	2.	110	(780.)	5.	210	(629.)	10.
-80	(986.)	5.	15	889.	2.	115	(774.)	5.	215	(620.)	10.
			20	883.	2.	120	(768.)	5.	220	(609.)	10.
-75	(981.)	5.	25	878.	2.	125	(761.)	5.	225	(598.)	10.
-70	(976.)	5.	30	873.	2.	130	(755.)	5.	230	(587.)	10.
-65	(971.)	5.	35	867.	2.	135	(748.)	5.	235	(575.)	10.
-60	(966.)	5.	40	862.	2.	140	(741.)	10.	240	(562.)	10.
-55	(961.)	2.	45	856.	2.	145	(734.)	10.	245	(548.)	10.
-50	(956.)	2.	50	851.	5.	150	(727.)	10.	250	(532.)	10.
-45	(951.)	2.	55	845.	5.	155	(720.)	10.	255	(515.)	10.
-40	(946.)	2.	60	839.	5.	160	(713.)	10.	260	(496.)	10.
-35	(941.)	2.	65	834.	5.	165	(706.)	10.	265	(473.)	10.
-30	(936.)	2.	70	828.	5.	170	(698.)	10.	270	(443.)	10.
-25	(931.)	2.	75	822.	5.	175	(690.)	10.	275	(398.)	10.
-20	(926.)	2.	80	816.	5.	180	(682.)	10.			
-15	(920.)	2.	85	811.	5.	185	(674.)	10.			
-10	(915.)	2.	90	805.	5.	190	(666.)	10.			
-5	(910.)	2.	95	799.	5.	195	(657.)	10.			

Orthobaric Liquid Molar Volume of 2-Methylpropyl methanoate

Units: cm ³ /mol v. K											
T	V	Uncert.		T	V	Uncert.		T	V	Uncert.	
K	cm ³ /mol	cm ³ /mol		K	cm ³ /mol	cm ³ /mol		K	cm ³ /mol	cm ³ /mol	
180	(102.2)	0.5		275	113.1	0.2		375	(129.)	1.	
185	(102.7)	0.5		280	113.8	0.2		380	(130.)	1.	
190	(103.2)	0.5		285	114.5	0.2		385	(131.)	1.	
195	(103.7)	0.5		290	115.2	0.2		390	(132.)	1.	
				295	115.9	0.2		395	(133.)	1.	
200	(104.3)	0.5		300	116.6	0.2		400	(135.)	1.	
205	(104.8)	0.5		305	117.3	0.2		405	(136.)	1.	
210	(105.3)	0.5		310	118.0	0.5		410	(137.)	1.	
215	(105.9)	0.5		315	118.8	0.5		415	(138.)	1.	
220	(106.4)	0.5		320	119.6	0.5		420	(140.)	1.	
225	(107.0)	0.5		325	120.3	0.5		425	(141.)	2.	
230	(107.6)	0.2		330	121.1	0.5		430	(142.)	2.	
235	(108.2)	0.2		335	122.0	0.5		435	(144.)	2.	
240	(108.8)	0.2		340	122.8	0.5		440	(145.)	2.	
245	(109.4)	0.2		345	123.7	0.5		445	(147.)	2.	
250	(110.0)	0.2		350	124.5	1.		450	(149.)	2.	
255	(110.6)	0.2		355	125.4	1.		455	(150.)	2.	
260	(111.2)	0.2		360	126.3	1.		460	(152.)	2.	
265	(111.8)	0.2		365	127.3	1.		465	(154.)	2.	
270	(112.5)	0.2		370	128.2	1.		470	(156.)	2.	
								475	(158.)	2.	
								480	(161.)	2.	
								485	(163.)	2.	
								490	(166.)	2.	
								495	(169.)	2.	
								500	(172.)	2.	
								505	(175.)	2.	
								510	(179.)	2.	
								515	(184.)	2.	
								520	(188.)	5.	
								525	(194.)	5.	
								530	(201.)	5.	
								535	(209.)	5.	
								540	(221.)	5.	
								545	(238.)	5.	
								550	(278.)	10.	

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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|----|---|---|----------|
| 1 | PIERRE, -.; PUCHOT, -. | <i>Liebigs Ann.Chem.</i> , Vol.163, p.281, 1872. | |
| 2 | ELSAESSER, E. | <i>Liebigs Ann.Chem.</i> , Vol.218, p.324, 1883. | |
| 3 | SCHIFF, R. | <i>Liebigs Ann.Chem.</i> , Vol.220, p.71, 1883. | |
| 4 | SCHIFF, R. | <i>Liebigs Ann.Chem.</i>, Vol.234, p.309, 1886. | M |
| 5 | BIRON, E. B. | <i>J.Russ.Phys.Chem.Soc.</i> , Vol.42, p.178, 1910. | |
| 6 | EISENLOHR, F. | <i>Zh.Phys.Chem.Stoekh.Verw.</i> , Vol.75, p.592, 1911. | |
| 7 | MATHEWS, J. H.; FAVILLE, K. E. | <i>J.Phys.Chem.</i>, Vol.22, p.6, 1918. | A |
| 8 | UNKOVSKAYA, -.; VOLOVA, -. | <i>J.Russ.Phys.Chem.Soc.</i> , Vol.57, p.113, 1925. | |
| 9 | HANNOTTE, T. | <i>Bull.Soc.Chim.Belges</i> , Vol.35, p.86, 1926. | |
| 10 | MATHEWS, J. H. | <i>J.Am.Chem.Soc.</i> , Vol.48, p.562, 1926. | |
| 11 | MUNCH, J. C. | <i>J.Am.Chem.Soc.</i> , Vol.48, p.994, 1926. | |
| 12 | FRIEND, J. N.; HARGREAVES, W. D. | <i>Phil.Mag.</i>, Vol.34, p.649, 1943. | M |
| 13 | VOGEL, A. I. | <i>J.Chem.Soc.</i> , p.616, 1948. | |
| 14 | POLIEVKA, -.; MISTRIK, -. | <i>Chem.Zvesti</i> , Vol.26, p.149, 1972. | |
| 15 | LINEK, -. | <i>Coll.Czech.Chem.Comm.</i> , Vol.44, p.3501, 1979. | |
| 16 | AMBROSE, D. | in <i>Hndbk.Chem.Phys.</i> , CRC Press, 72nd.ed., pp.6-49 to 6-63, 1991.* | |
| 17 | TRC Thermodynamic Tables, | Texas A & M Univ., Loose leaf data sheets extant 1996.* | |



C₅H₁₀O₂ 1,1-Dimethylethyl methanoate; *tert*-Butyl methanoate; *tert*-Butyl formate

CAS Reg. No. 762-75-4

Mol. Wt. 102.13

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

Critical Temperature	T_c	= 533. K	(t_c	= 259.85 °C)
Critical Pressure	p_c	= 3600. kPa	(p_c	= 35.53 atm)
Critical Density	ρ_c	= 302. kg/m ³	(V_c	= 338.18 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.275		

$$N_1 = 1.77341 \quad N_2 = -0.62112 \quad N_3 = 0.00000 \quad N_4 = 0.20900$$

Density at 298.15 K (25 °C)	ρ_{25}	= 871.59 kg/m ³	(V_{25}	= 117.18 cm ³ /mol)
Normal Boiling Point	T_b	= 356.05 K	(t_b	= 82.900 °C)
Melting Point	T_m	= -	(t_m	= -)

Data at Specified Temperatures

$t/^\circ\text{C}$	-100	0	25	50	82.90	150	259.85
T/K	173.15	273.15	298.15	323.15	356.05	423.15	533.00
$\rho/(\text{kg/m}^3)$	(1004.21)	(899.31)	871.59	(842.91)	(803.22)	(711.01)	(302.00)
$(d\rho/dT)/(\text{kg/m}^3 \text{ K})$	(-1.02)	(-1.09)	-1.13	(-1.17)	(-1.25)	(-1.54)	$-\infty$
$V/(\text{cm}^3/\text{mol})$	(101.70)	(113.57)	117.18	(121.16)	(127.15)	(143.64)	(338.18)
$(dV/dT)/(\text{cm}^3/\text{mol K})$	(0.10)	(0.14)	0.15	(0.17)	(0.20)	(0.31)	∞
Data Quality	(B)	(B)	B	(B)	(B)	(B)	(B)
Uncertainty in ρ (kg/m ³)	(5.)	(2.)	1.	(2.)	(5.)	(5.)	(10.)
Uncertainty in V (cm ³ /mol)	(0.5)	(0.2)	0.1	(0.2)	(0.5)	(1.)	(10.)

Orthobaric Liquid Density of 1,1-Dimethylethyl methanoate

Units: kg/m ³ v. °C											
t	ρ	Uncert.	t	ρ	Uncert.	t	ρ	Uncert.	t	ρ	Uncert.
°C	kg/m ³	kg/m ³	°C	kg/m ³	kg/m ³	°C	kg/m ³	kg/m ³	°C	kg/m ³	kg/m ³
-100	(1004.)	5.	0	(899.)	2.	100	(781.)	5.	200	(622.)	10.
-95	(999.)	5.	5	(894.)	2.	105	(775.)	5.	205	(611.)	10.
-90	(994.)	5.	10	(888.)	2.	110	(768.)	5.	210	(600.)	10.
-85	(989.)	5.	15	(883.)	2.	115	(762.)	5.	215	(588.)	10.
-80	(984.)	5.	20	877.	1.	120	(755.)	5.	220	(575.)	10.
-75	(979.)	5.	25	872.	1.	125	(748.)	5.	225	(561.)	10.
-70	(973.)	5.	30	(866.)	1.	130	(741.)	5.	230	(546.)	10.
-65	(968.)	5.	35	(860.)	1.	135	(733.)	5.	235	(529.)	10.
-60	(963.)	2.	40	(855.)	2.	140	(726.)	5.	240	(511.)	10.
-55	(958.)	2.	45	(849.)	2.	145	(719.)	5.	245	(489.)	10.
-50	(953.)	2.	50	(843.)	2.	150	(711.)	5.	250	(463.)	10.
-45	(947.)	2.	55	(837.)	2.	155	(703.)	5.	255	(426.)	10.
-40	(942.)	2.	60	(831.)	2.	160	(695.)	5.			
-35	(937.)	2.	65	(825.)	2.	165	(687.)	5.			
-30	(932.)	2.	70	(819.)	2.	170	(679.)	5.			
-25	(926.)	2.	75	(813.)	2.	175	(670.)	10.			
-20	(921.)	2.	80	(807.)	5.	180	(661.)	10.			
-15	(916.)	2.	85	(801.)	5.	185	(652.)	10.			
-10	(910.)	2.	90	(794.)	5.	190	(642.)	10.			
-5	(905.)	2.	95	(788.)	5.	195	(632.)	10.			

Units: $\text{cm}^3/\text{mol v. K}$

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.

- J.Org.Chem.*, Vol.19, p.1316, 1954.

**C₆H₁₂O₂ 3-Methylbutyl methanoate; Isopentyl methanoate; Isopentyl formate**

CAS Reg. No. 110-45-2

Mol. Wt. 116.16

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

Critical Temperature	T_c	= 576. K	(t_c	= 302.85 °C)
Critical Pressure	p_c	= 3150. kPa	(p_c	= 31.09 atm)
Critical Density	ρ_c	= 288. kg/m ³	(V_c	= 403.33 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.265		

$$N_1 = 1.84271 \quad N_2 = -0.69465 \quad N_3 = 0.00000 \quad N_4 = 0.24266$$

Density at 298.15 K (25 °C)	ρ_{25}	= 873.65 kg/m ³	(V_{25}	= 132.96 cm ³ /mol)
Normal Boiling Point	T_b	= 397.25 K	(t_b	= 124.100 °C)
Melting Point	T_m	= 180.	(t_m	= -93. °C)

Data at Specified Temperatures

$t/^\circ\text{C}$	-93	0	25	50	124.10	200	302.85
T/K	180.15	273.15	298.15	323.15	397.25	473.15	576.00
$\rho/(\text{kg/m}^3)$	(987.63)	898.47	873.65	848.23	(767.48)	(668.30)	(288.00)
$(d\rho/dT)/(\text{kg/m}^3 \text{ K})$	(-0.94)	-0.98	-1.00	-1.03	(-1.17)	(-1.50)	$-\infty$
$V/(\text{cm}^3/\text{mol})$	(117.62)	129.29	132.96	136.94	(151.35)	(173.81)	(403.33)
$(dV/dT)/(\text{cm}^3/\text{mol K})$	(0.11)	0.14	0.15	0.17	(0.23)	(0.39)	∞
Data Quality	(B)	B	B	B	(B)	(B)	(B)
Uncertainty in ρ (kg/m ³)	(5.)	2.	1.	2.	(5.)	(5.)	(10.)
Uncertainty in V (cm ³ /mol)	(0.5)	0.2	0.2	0.2	(1.)	(2.)	(10.)

Orthobaric Liquid Density of 3-Methylbutyl methanoate

Units: kg/m ³ v. °C								
t	ρ	Uncert.	t	ρ	Uncert.	t	ρ	Uncert.
°C	kg/m ³	kg/m ³	°C	kg/m ³	kg/m ³	°C	kg/m ³	kg/m ³
			0	898.	2.	100	795.	2.
			5	894.	2.	105	789.	2.
-90	(985.)	5.	10	889.	2.	110	784.	5.
-85	(980.)	5.	15	884.	1.	115	778.	5.
-80	(975.)	5.	20	879.	1.	120	(772.)	5.
-75	(971.)	5.	25	874.	1.	125	(766.)	5.
-70	(966.)	5.	30	869.	1.	130	(761.)	5.
-65	(961.)	5.	35	864.	1.	135	(755.)	5.
-60	(956.)	5.	40	858.	2.	140	(749.)	5.
-55	(952.)	2.	45	853.	2.	145	(742.)	5.
-50	(947.)	2.	50	848.	2.	150	(736.)	5.
-45	(942.)	2.	55	843.	2.	155	(730.)	5.
-40	(937.)	2.	60	838.	2.	160	(724.)	5.
-35	(932.)	2.	65	833.	2.	165	(717.)	5.
-30	(928.)	2.	70	827.	2.	170	(711.)	5.
-25	(923.)	2.	75	822.	2.	175	(704.)	5.
-20	(918.)	2.	80	817.	2.	180	(697.)	5.
-15	(913.)	2.	85	811.	2.	185	(690.)	5.
-10	(908.)	2.	90	806.	2.	190	(683.)	5.
-5	(903.)	2.	95	800.	2.	195	(676.)	5.
						200	(668.)	5.
						205	(661.)	5.
						210	(653.)	5.
						215	(645.)	5.
						220	(637.)	10.
						225	(628.)	10.
						230	(619.)	10.
						235	(610.)	10.
						240	(600.)	10.
						245	(590.)	10.
						250	(580.)	10.
						255	(569.)	10.
						260	(557.)	10.
						265	(545.)	10.
						270	(531.)	10.
						275	(516.)	10.
						280	(500.)	10.
						285	(481.)	10.
						290	(459.)	10.
						295	(430.)	10.

Orthobaric Liquid Molar Volume of 3-Methylbutyl methanoate

Units: cm ³ /mol v. K											
T	V	Uncert.	T	V	Uncert.	T	V	Uncert.	T	V	Uncert.
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
185	(118.2)	0.5	275	129.5	0.2	375	146.5	0.5	475	(175.)	2.
190	(118.7)	0.5	280	130.3	0.2	380	147.6	0.5	480	(177.)	2.
195	(119.3)	0.5	285	131.0	0.2	385	148.6	0.5	485	(179.)	2.
			290	131.7	0.2	390	149.7	0.5	490	(181.)	2.
			295	132.5	0.2	395	(150.8)	1.	495	(183.)	2.
200	(119.9)	0.5	300	133.2	0.2	400	(152.0)	1.	500	(186.)	2.
205	(120.5)	0.5	305	134.0	0.2	405	(153.2)	1.	505	(189.)	2.
210	(121.1)	0.5	310	134.8	0.2	410	(154.4)	1.	510	(192.)	2.
215	(121.7)	0.5	315	135.6	0.2	415	(155.6)	1.	515	(195.)	2.
220	(122.3)	0.5	320	136.4	0.2	420	(157.)	1.	520	(198.)	2.
225	(122.9)	0.5	325	137.3	0.2	425	(158.)	1.	525	(202.)	2.
230	(123.5)	0.5	330	138.1	0.5	430	(160.)	1.	530	(206.)	2.
235	(124.2)	0.5	335	139.0	0.5	435	(161.)	1.	535	(210.)	2.
240	(124.8)	0.5	340	139.8	0.5	440	(163.)	1.	540	(215.)	5.
245	(125.5)	0.5	345	140.7	0.5	445	(164.)	1.	545	(221.)	5.
250	(126.1)	0.2	350	141.6	0.5	450	(166.)	1.	550	(228.)	5.
255	(126.8)	0.2	355	142.6	0.5	455	(167.)	1.	555	(236.)	5.
260	(127.5)	0.2	360	143.5	0.5	460	(169.)	2.	560	(246.)	5.
265	(128.1)	0.2	365	144.5	0.5	465	(171.)	2.	565	(259.)	5.
270	(128.8)	0.2	370	145.5	0.5	470	(173.)	2.	570	(279.)	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 ELSAESSER, E. *Liebigs Ann.Chem.*, Vol.218, p.324, 1883.
- 2 SCHIFF, R. *Liebigs Ann.Chem.*, Vol.220, p.71, 1883.
- 3 GLADSTONE, J. H. *Chem.Soc.*, Vol.59, p.293, 1891.
- 4 RICHARDS, T. W.; MATHEWS, J. H. *Z.Phys.Chem.Stoech.Verw.*, Vol.61, p.452, 1908.
- 5 KREMANN, -; MEINGAST, -; GUGL, -. *Monatsh.Chem.*, Vol.35, p.1297, 1914.
- 6 MATHEWS, J. H.; FAVILLE, K. E. *J.Phys.Chem.*, Vol.22, p.6, 1918.
- 7 HANNOTTE, T. *Bull.Soc.Chim.Belges*, Vol.35, p.86, 1926.
- 8 MATHEWS, J. H. *J.Am.Chem.Soc.*, Vol.48, p.562, 1926.
- 9 MUNCH, J. C. *J.Am.Chem.Soc.*, Vol.48, p.994, 1926.
- 10 GERRARD, W. *J.Chem.Soc.*, p.103, 1939.
- 11 VOGEL, A. I. *J.Chem.Soc.*, p.616, 1948.
- 12 LYSENKO, -. *Zh.Obshch.Khim.*, Vol.26, p.2965, 1956.
- 13 SOLOV'EV, -; BARATOV, -. *Zh.Fiz.Khim.*, Vol.34, p.1661, 1960.
- 14 KARPOV, -; FEDOSYUK, -. *J.Appl.Chem.USSR*, Vol.40, p.2718, 1967.
- 15 RAJYAM, -; MURTY, -. *Ind.J.Pure Appl.Phys.*, Vol.11, p.23, 1973.
- 16 TRC Thermodynamic Tables, Texas A & M Univ., Loose leaf data sheets extant 1996.* A

**C₅H₁₀O₂ 1-Methylethyl ethanoate; Isopropyl ethanoate; Isopropyl acetate**

CAS Reg. No. 108-21-4

Mol. Wt. 102.13

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

Critical Temperature	T_c	= 531.00 K	(t_c	= 257.85 °C)
Critical Pressure	p_c	= 3340. kPa	(p_c	= 32.96 atm)
Critical Density	ρ_c	= 295. kg/m ³	(V_c	= 346.20 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.262		

$$N_1 = 1.82613 \quad N_2 = -0.67638 \quad N_3 = 0.00000 \quad N_4 = 0.23417$$

Density at 298.15 K (25 °C)	ρ_{25}	= 864.33 kg/m ³	(V_{25}	= 118.16 cm ³ /mol)
Normal Boiling Point	T_b	= 361.726 K	(t_b	= 88.576 °C)
Melting Point	T_m	= 200.	(t_m	= -73. °C)

Data at Specified Temperatures

$t/^\circ\text{C}$ T/K	-73 200.15	0 273.15	25 298.15	50 323.15	88.58 361.73	200 473.15	257.85 531.00
$\rho/(\text{kg/m}^3)$ ($d\rho/dT/(\text{kg/m}^3 \text{ K})$)	(970.57) (-1.05)	892.32 -1.10	864.33 -1.14	835.41 -1.18	(788.24) (-1.27)	(612.19) (-2.16)	(295.00) -∞
$V/(\text{cm}^3/\text{mol})$ ($dV/dT/(\text{cm}^3/\text{mol K})$)	(105.23) (0.11)	114.45 0.14	118.16 0.16	122.25 0.17	(129.57) (0.21)	(166.83) (0.59)	(346.20) ∞
Data Quality	(B)	B	B	B	(B)	(B)	(C)
Uncertainty in ρ (kg/m ³)	(5.)	2.	1.	2.	(5.)	(5.)	(10.)
Uncertainty in V (cm ³ /mol)	(0.5)	0.2	0.1	0.2	(0.5)	(2.)	(10.)

Orthobaric Liquid Density of 1-Methylethyl ethanoate

Units: kg/m ³ v. °C											
t °C	ρ kg/m ³	Uncert. in ρ kg/m ³	t °C	ρ kg/m ³	Uncert. in ρ kg/m ³	t °C	ρ kg/m ³	Uncert. in ρ kg/m ³	t °C	ρ kg/m ³	Uncert. in ρ kg/m ³
-70	(967.)	5.	25	864.	1.	125	(740.)	5.	225	(550.)	10.
-65	(962.)	5.	30	859.	1.	130	(732.)	5.	230	(534.)	10.
-60	(957.)	5.	35	853.	1.	135	(725.)	5.	235	(517.)	10.
-55	(952.)	5.	40	847.	2.	140	(718.)	5.	240	(497.)	10.
			45	841.	2.	145	(710.)	5.	245	(474.)	10.
-50	(946.)	5.	50	835.	2.	150	(703.)	5.	250	(444.)	10.
-45	(941.)	5.	55	829.	2.	155	(695.)	5.	255	(398.)	10.
-40	(936.)	2.	60	824.	2.	160	(687.)	5.			
-35	(930.)	2.	65	(817.)	2.	165	(678.)	5.			
-30	(925.)	2.	70	(811.)	2.	170	(670.)	5.			
-25	(920.)	2.	75	(805.)	2.	175	(661.)	5.			
-20	(914.)	2.	80	(799.)	2.	180	(652.)	5.			
-15	(909.)	2.	85	(793.)	5.	185	(643.)	5.			
-10	(903.)	2.	90	(786.)	5.	190	(633.)	5.			
-5	(898.)	2.	95	(780.)	5.	195	(623.)	5.			
0	892.	2.	100	(773.)	5.	200	(612.)	5.			
5	887.	2.	105	(767.)	5.	205	(601.)	5.			
10	881.	2.	110	(760.)	5.	210	(589.)	10.			
15	876.	1.	115	(753.)	5.	215	(577.)	10.			
20	870.	1.	120	(747.)	5.	220	(564.)	10.			

Orthobaric Liquid Molar Volume of 1-Methylethyl ethanoate

Units: cm ³ /mol v. K								
T	V	Uncert.	T	V	Uncert.	T	V	Uncert.
K	cm ³ /mol	in V	K	cm ³ /mol	in V	K	cm ³ /mol	in V
		cm ³ /mol			cm ³ /mol			cm ³ /mol
205	(105.8)	0.5	300	118.4	0.1	400	(138.6)	1.
210	(106.4)	0.5	305	119.2	0.2	405	(140.0)	1.
215	(106.9)	0.5	310	120.0	0.2	410	(141.4)	1.
220	(107.5)	0.5	315	120.9	0.2	415	(143.)	1.
			320	121.7	0.2	420	(144.)	1.
225	(108.1)	0.5	325	122.6	0.2	425	(146.)	1.
230	(108.8)	0.5	330	123.5	0.2	430	(148.)	1.
235	(109.4)	0.5	335	(124.4)	0.5	435	(149.)	1.
240	(110.0)	0.5	340	(125.3)	0.5	440	(151.)	1.
245	(110.7)	0.2	345	(126.2)	0.5	445	(153.)	1.
250	(111.3)	0.2	350	(127.2)	0.5	450	(155.)	1.
255	(112.0)	0.2	355	(128.2)	0.5	455	(157.)	2.
260	(112.6)	0.2	360	(129.2)	0.5	460	(160.)	2.
265	(113.3)	0.2	365	(130.3)	0.5	465	(162.)	2.
270	(114.0)	0.2	370	(131.3)	0.5	470	(165.)	2.
275	114.7	0.2	375	(132.5)	0.5	475	(168.)	2.
280	115.4	0.2	380	(133.6)	1.	480	(171.)	2.
285	116.2	0.2	385	(134.8)	1.	485	(175.)	2.
290	116.9	0.2	390	(136.0)	1.	490	(178.)	2.
295	117.7	0.1	395	(137.3)	1.	495	(183.)	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 PRIBRAM, -.; HANDL, -. *Monatsh. Chem.*, Vol.2, p.686, 1881.
- 2 SMITH, -.; OLSSON, -. *Z.Phys.Chem.Stoech.Verw.*, Vol.102, p.28, 1922.
- 3 MUNCH, J. C. *J.Am.Chem.Soc.*, Vol.48, p.994, 1926.
- 4 SWARTS, F. *Bull.Soc.Chim.Belges*, Vol.38, p.99, 1929.
- 5 DORRIS, -.; SOWA, -.; NIEUWLAND, -. *J.Am.Chem.Soc.*, Vol.56, p.2689, 1934.
- 6 VOGEL, A. I. *J.Chem.Soc.*, p.616, 1948.
- 7 WADSOE, -. *Acta Chem.Scand.*, Vol.12, p.630, 1958.
- 8 ATAWIN, -.; et al. *Izv.Sib.Otd.Akad.Nauk SSSR,Khim.*, No.11, p.111, 1965.
- 9 ORLOVA, -.; KEIKO, -. *Izv.Sib.Otd.Akad.Nauk SSSR,Khim.*, No.3, p.111, 1965.
- 10 UNION CARBIDE CORP. *Chem.Plastics Physical Properties*, (Prod.Bull.), 1968.
- 11 GEISELER, -.; et al. *Z.Phys.Chem.(Leipzig)*, Vol.252, p.170, 1973.
- 12 LEMONDS, -.; McCLELLAN, -. *Anal.Chem.*, Vol.45, p.1455, 1973.
- 13 LINEK, -.; WICHTERLE, -. *Coll.Czech.Chem.Comm.*, Vol.38, p.1846, 1973.
- 14 GONZALEZ, -.; NIETA, -. *An.Quim.*, Vol.74, p.326, 1978.
- 15 MECHTIEV, -. et al. *Azerb.Khim.Zh.*, Vol.6, p.55, 1978. A
- 16 KHIMENKO, M. T.; ZHURAVEL, V. P. et al. *Russ.J.Phys.Chem.*, Vol.63, p.733, 1989.
- 17 KRISHNAIAH, A.; VISWANATH, D. S. *J.Chem.Eng.Data*, Vol.36, p.317, 1991.
- 18 TRC Thermodynamic Tables, Texas A & M Univ., Loose leaf data sheets extant 1996.*

**C₆H₁₂O₂ 1-Methylpropyl ethanoate; *sec*-Butyl ethanoate; *sec*-Butyl acetate**

CAS Reg. No. 105-46-4

Mol. Wt. 116.16

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

Critical Temperature	T_c	= 563. K	(t_c	= 289.85°C)
Critical Pressure	p_c	= 3200. kPa	(p_c	= 31.58 atm)
Critical Density	ρ_c	= 291. kg/m ³	(V_c	= 399.18 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.273		

$$N_1 = 1.80115 \quad N_2 = -0.64961 \quad N_3 = 0.00000 \quad N_4 = 0.22186$$

Density at 298.15 K (25°C)	ρ_{25}	= 864.70 kg/m ³	(V_{25}	= 134.34 cm ³ /mol)
Normal Boiling Point	T_b	= 385.113 K	(t_b	= 111.963°C)
Melting Point	T_m	= -	(t_m	= -)

Data at Specified Temperatures

$t/^{\circ}\text{C}$	-100	0	25	50	111.96	200	289.85
T/K	173.15	273.15	298.15	323.15	385.11	473.15	563.00
$\rho/(\text{kg/m}^3)$	(986.60)	889.94	864.70	838.76	(770.07)	(650.92)	(291.00)
$(d\rho/dT)/(\text{kg/m}^3 \text{ K})$	(-0.95)	-1.00	-1.02	-1.05	(-1.18)	(-1.62)	$-\infty$
$V/(\text{cm}^3/\text{mol})$	(117.74)	130.53	134.34	138.49	(150.84)	(178.46)	(399.18)
$(dV/dT)/(\text{cm}^3/\text{mol K})$	(0.11)	0.15	0.16	0.17	(0.23)	(0.44)	∞
Data Quality	(B)	B	B	B	(C)	(C)	(C)
Uncertainty in ρ (kg/m ³)	(5.)	2.	2.	5.	(5.)	(10.)	(10.)
Uncertainty in V (cm ³ /mol)	(0.5)	0.2	0.2	0.5	(1.)	(2.)	(20.)

Orthobaric Liquid Density of 1-Methylpropyl ethanoateUnits: kg/m³ v. °C

t	ρ	Uncert.	t	ρ	Uncert.	t	ρ	Uncert.	t	ρ	Uncert.
°C	kg/m ³	kg/m ³	°C	kg/m ³	kg/m ³	°C	kg/m ³	kg/m ³	°C	kg/m ³	kg/m ³
-100	(987.)	5.	0	890.	2.	100	(784.)	5.	200	(651.)	10.
-95	(982.)	5.	5	885.	2.	105	(778.)	5.	205	(643.)	10.
-90	(977.)	5.	10	880.	2.	110	(772.)	5.	210	(634.)	10.
-85	(972.)	5.	15	875.	2.	115	(766.)	5.	215	(625.)	10.
-80	(968.)	2.	20	870.	2.	120	(761.)	5.	220	(616.)	10.
-75	(963.)	2.	25	865.	2.	125	(754.)	5.	225	(607.)	10.
-70	(958.)	2.	30	860.	2.	130	(748.)	5.	230	(597.)	10.
-65	(953.)	2.	35	854.	2.	135	(742.)	5.	235	(587.)	10.
-60	(949.)	2.	40	849.	2.	140	(736.)	5.	240	(576.)	10.
-55	(944.)	2.	45	844.	2.	145	(730.)	5.	245	(564.)	10.
-50	(939.)	2.	50	839.	5.	150	(723.)	5.	250	(552.)	10.
-45	(934.)	2.	55	833.	5.	155	(716.)	5.	255	(539.)	10.
-40	(929.)	2.	60	828.	5.	160	(710.)	5.	260	(525.)	10.
-35	(924.)	2.	65	823.	5.	165	(703.)	5.	265	(509.)	10.
-30	(920.)	2.	70	817.	5.	170	(696.)	5.	270	(491.)	10.
-25	(915.)	2.	75	812.	5.	175	(689.)	5.	275	(470.)	10.
-20	(910.)	2.	80	806.	5.	180	(682.)	5.	280	(445.)	10.
-15	(905.)	2.	85	801.	5.	185	(674.)	10.	285	(410.)	10.
-10	(900.)	2.	90	(795.)	5.	190	(667.)	10.			
-5	(895.)	2.	95	(790.)	5.	195	(659.)	10.			

Orthobaric Liquid Molar Volume of 1-Methylpropyl ethanoate

Units: cm ³ /mol v. K											
T	V	Uncert.		T	V	Uncert.		T	V	Uncert.	
K	cm ³ /mol	cm ³ /mol		K	cm ³ /mol	cm ³ /mol		K	cm ³ /mol	cm ³ /mol	
175	(117.9)	0.5		275	130.8	0.2		375	(149.)	1.	
180	(118.5)	0.5		280	131.5	0.2		380	(150.)	1.	
185	(119.1)	0.5		285	132.3	0.2		385	(151.)	1.	
190	(119.7)	0.5		290	133.1	0.2		390	(152.)	1.	
195	(120.3)	0.5		295	133.8	0.2		395	(153.)	1.	
200	(120.9)	0.5		300	134.6	0.2		400	(154.)	1.	
205	(121.5)	0.5		305	135.4	0.5		405	(156.)	1.	
210	(122.1)	0.5		310	136.3	0.5		410	(157.)	1.	
215	(122.7)	0.5		315	137.1	0.5		415	(158.)	1.	
220	(123.3)	0.5		320	137.9	0.5		420	(160.)	1.	
225	(124.0)	0.5		325	138.8	0.5		425	(161.)	2.	
230	(124.6)	0.5		330	139.7	0.5		430	(163.)	2.	
235	(125.2)	0.5		335	140.6	0.5		435	(164.)	2.	
240	(125.9)	0.2		340	141.5	1.		440	(166.)	2.	
245	(126.6)	0.2		345	142.5	1.		445	(168.)	2.	
250	(127.3)	0.2		350	143.4	1.		450	(169.)	2.	
255	(127.9)	0.2		355	144.4	1.		455	(171.)	2.	
260	(128.6)	0.2		360	(145.4)	1.		460	(173.)	2.	
265	(129.3)	0.2		365	(146.4)	1.		465	(175.)	2.	
270	(130.1)	0.2		370	(147.)	1.		470	(177.)	2.	
								475	(179.)	2.	
								480	(182.)	2.	
								485	(184.)	2.	
								490	(187.)	2.	
								495	(190.)	2.	
								500	(193.)	2.	
								505	(196.)	2.	
								510	(199.)	2.	
								515	(203.)	2.	
								520	(207.)	2.	
								525	(212.)	5.	
								530	(218.)	5.	
								535	(224.)	5.	
								540	(231.)	5.	
								545	(240.)	5.	
								550	(252.)	5.	
								555	(268.)	5.	
								560	(297.)	10.	

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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|----|---------------------------------------|---|---|
| 1 | LIEBEN, -. | <i>Liebigs Ann.Chem.</i> , Vol.150, p.112, 1869. | |
| 2 | PICKARD, R. H.; KENYON, J. | <i>J.Chem.Soc.</i> , Vol.105, p.830, 1914. | |
| 3 | CLOUGH, -.; JONES, -. | <i>Ind.Eng.Chem.</i> , Vol.15, p.1032, 1923. | |
| 4 | SMITH, -.; OLSSON, -. | <i>Z.Phys.Chem.Stoech.Verw.</i> , Vol.118, p.99, 1925. | |
| 5 | MUNCH, J. C. | <i>J.Am.Chem.Soc.</i> , Vol.48, p.994, 1926. | |
| 6 | HUECKEL, W.; ACKERMANN, P. | <i>J.Prakt.Chem.</i> , Vol.136, p.15, 1933. | |
| 7 | KENYON, J.; PHILLIPS, -.; PITTMAN, -. | <i>J.Chem.Soc.</i> , p.1079, 1935. | |
| 8 | HOUTMAN, -.; VAN STEENIS, - et al. | <i>Rec.Trav.Khim.</i> , Vol.65, p.785, 1946. | |
| 9 | VOGEL, A. I. | <i>J.Chem.Soc.</i> , p.616, 1948. | |
| 10 | MYERS, - et al. | <i>J.Phys.Chem.</i> , Vol.56, p.461, 1952. | A |
| 11 | JAKOVLEV, -. | <i>Zh.Obshch.Khim.</i> , Vol.24, p.983, 1954. | |
| 12 | KLIMOV, - et al. | Soviet Patent SU 292957, 1971. | |
| 13 | FABEROV, - et al. | Soviet Patent SU 2182410, 1973. | |
| 14 | TRC Thermodynamic Tables, | Texas A & M Univ., Loose leaf data sheets extant 1996.* | |

**C₆H₁₂O₂ 2-Methylpropyl ethanoate; Isobutyl ethanoate; Isobutyl acetate**

CAS Reg. No. 110-19-0

Mol. Wt. 116.16

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

Critical Temperature	T_c	= 565. K	(t_c	= 291.85 °C)
Critical Pressure	p_c	= 3105. kPa	(p_c	= 30.64 atm)
Critical Density	ρ_c	= 289. kg/m ³	(V_c	= 401.94 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.266		

$$N_1 = 1.83063 \quad N_2 = -0.68129 \quad N_3 = 0.00000 \quad N_4 = 0.23644$$

Density at 298.15 K (25 °C)	ρ_{25}	= 867.69 kg/m ³	(V_{25}	= 133.87 cm ³ /mol)
Normal Boiling Point	T_b	= 390.15 K	(t_b	= 117. °C)
Melting Point	T_m	= 174. °C	(t_m	= -99. °C)

Data at Specified Temperatures

$t/^\circ\text{C}$	-99	0	25	50	117	200	291.85
T/K	174.15	273.15	298.15	323.15	390.15	473.15	565.00
$\rho/(\text{kg/m}^3)$	(989.52)	893.05	867.69	841.67	(766.98)	(654.31)	(289.00)
$(d\rho/dT)/(\text{kg/m}^3 \text{ K})$	(-0.96)	-1.00	-1.03	-1.06	(-1.19)	(-1.61)	$-\infty$
$V/(\text{cm}^3/\text{mol})$	(117.39)	130.07	133.87	138.01	(151.45)	(177.53)	(401.94)
$(dV/dT)/(\text{cm}^3/\text{mol K})$	(0.11)	0.15	0.16	0.17	(0.23)	(0.44)	∞
Data Quality	(B)	B	B	B	(C)	(C)	(C)
Uncertainty in ρ (kg/m ³)	(5.)	2.	2.	5.	(5.)	(10.)	(10.)
Uncertainty in V (cm ³ /mol)	(0.5)	0.2	0.2	0.5	(1.)	(2.)	(20.)

Orthobaric Liquid Density of 2-Methylpropyl ethanoate

Units: kg/m ³ v. °C											
t	ρ	Uncert.	t	ρ	Uncert.	t	ρ	Uncert.	t	ρ	Uncert.
°C	kg/m ³	kg/m ³	°C	kg/m ³	kg/m ³	°C	kg/m ³	kg/m ³	°C	kg/m ³	kg/m ³
-95	(986.)	5.	0	893.	2.	100	787.	5.	200	(654.)	10.
-90	(981.)	5.	5	888.	2.	105	781.	5.	205	(646.)	10.
-85	(976.)	5.	10	883.	2.	110	775.	5.	210	(638.)	10.
-80	(971.)	5.	15	878.	2.	115	(769.)	5.	215	(629.)	10.
			20	873.	2.	120	(763.)	5.	220	(620.)	10.
-75	(967.)	5.	25	868.	2.	125	(757.)	5.	225	(611.)	10.
-70	(962.)	5.	30	863.	2.	130	(751.)	5.	230	(601.)	10.
-65	(957.)	5.	35	857.	2.	135	(745.)	5.	235	(591.)	10.
-60	(952.)	2.	40	852.	2.	140	(739.)	5.	240	(580.)	10.
-55	(947.)	2.	45	847.	2.	145	(732.)	5.	245	(569.)	10.
-50	(942.)	2.	50	842.	5.	150	(726.)	5.	250	(557.)	10.
-45	(937.)	2.	55	836.	5.	155	(719.)	5.	255	(544.)	10.
-40	(933.)	2.	60	831.	5.	160	(713.)	5.	260	(530.)	10.
-35	(928.)	2.	65	826.	5.	165	(706.)	5.	265	(515.)	10.
-30	(923.)	2.	70	820.	5.	170	(699.)	5.	270	(498.)	10.
-25	(918.)	2.	75	815.	5.	175	(692.)	5.	275	(479.)	10.
-20	(913.)	2.	80	809.	5.	180	(685.)	5.	280	(455.)	10.
-15	(908.)	2.	85	804.	5.	185	(677.)	10.	285	(425.)	10.
-10	(903.)	2.	90	798.	5.	190	(670.)	10.	290	(374.)	10.
-5	(898.)	2.	95	793.	5.	195	(662.)	10.			

Orthobaric Liquid Molar Volume of 2-Methylpropyl ethanoate

			Units: cm ³ /mol v. K								
T	V	Uncert.	T	V	Uncert.	T	V	Uncert.	T	V	Uncert.
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
175	(117.5)	0.5	275	130.3	0.2	375	148.	1.	475	(178.)	2.
180	(118.1)	0.5	280	131.1	0.2	380	149.	1.	480	(181.)	2.
185	(118.6)	0.5	285	131.8	0.2	385	(150.)	1.	485	(183.)	2.
190	(119.2)	0.5	290	132.6	0.2	390	(151.)	1.	490	(186.)	2.
195	(119.8)	0.5	295	133.4	0.2	395	(153.)	1.	495	(188.)	2.
200	(120.4)	0.5	300	134.2	0.2	400	(154.)	1.	500	(191.)	2.
205	(121.0)	0.5	305	135.0	0.5	405	(155.)	1.	505	(194.)	2.
210	(121.6)	0.5	310	135.8	0.5	410	(156.)	1.	510	(198.)	2.
215	(122.2)	0.5	315	136.6	0.5	415	(158.)	1.	515	(202.)	2.
220	(122.9)	0.5	320	137.5	0.5	420	(159.)	1.	520	(206.)	2.
225	(123.5)	0.5	325	138.3	0.5	425	(161.)	2.	525	(210.)	5.
230	(124.1)	0.5	330	139.2	0.5	430	(162.)	2.	530	(215.)	5.
235	(124.8)	0.5	335	140.1	0.5	435	(164.)	2.	535	(221.)	5.
240	(125.5)	0.5	340	141.0	1.	440	(165.)	2.	540	(228.)	5.
245	(126.1)	0.5	345	142.0	1.	445	(167.)	2.	545	(236.)	5.
250	(126.8)	0.2	350	142.9	1.	450	(168.)	2.	550	(247.)	5.
255	(127.5)	0.2	355	143.9	1.	455	(170.)	2.	555	(261.)	5.
260	(128.2)	0.2	360	144.9	1.	460	(172.)	2.	560	(283.)	5.
265	(128.9)	0.2	365	145.9	1.	465	(174.)	2.	565	(402.)	20.
270	(129.6)	0.2	370	147.0	1.	470	(176.)	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 ELSAESSER, E. *Liebigs Ann.Chem.*, Vol.118, p.325, 1861.
- 2 SCHIFF, R. *Liebigs Ann.Chem.*, Vol.220, p.71, 1883.
- 3 RICHARDS, T. W.; MATHEWS, J. H. *J.Am.Chem.Soc.*, Vol.30, p.10, 1908.
- 4 RICHARDS, T. W.; MATHEWS, J. H. *Z.Phys.Chem.Stoech.Verw.*, Vol.61, p.449, 1908.
- 5 FALK, -. *J.Am.Chem.Soc.*, Vol.31, p.807, 1909.
- 6 BIRON, E. B. *J.Russ.Phys.Chem.Soc.*, Vol.42, p.171, 1910.
- 7 EISENLOHR, F. *Z.Phys.Chem.Stoech.Verw.*, Vol.75, p.592, 1911.
- 8 SMITH, -.; OLSSON, -. *Z.Phys.Chem.Stoech.Verw.*, Vol.118, p.99, 1925.
- 9 UNKOVSKAYA, -.; VOLOVA, -. *J.Russ.Phys.Chem.Soc.*, Vol.57, p.111, 1925.
- 10 HANNOTTE, T. *Bull.Soc.Chim.Belges*, Vol.35, p.90, 1926.
- 11 MATHEWS, J. H. *J.Am.Chem.Soc.*, Vol.48, p.562, 1926.
- 12 MUNCH, J. C. *J.Am.Chem.Soc.*, Vol.48, p.994, 1926.
- 13 HUECKEL, W.; ACKERMANN, P. *J.Prakt.Chem.*, Vol.136, p.15, 1933.
- 14 VOGEL, A. I. *J.Chem.Soc.*, p.616, 1948.
- 15 MUMFORD, S. A.; PHILLIPS, J. W. C. *J.Chem.Soc.*, p.75, 1950.
- 16 TUVOVA-POLJAK, -.; DENISOVA, -. *J.Gen.Chem.USSR*, Vol.34, p.2676, 1964.
- 17 PAUL, -. et al. *Indian J.Chem.*, Vol.3, p.243, 1965.
- 18 UNION CARBIDE CORP. *Chem.Plastics Physical Properties*, (Prod.Bull.), 1968.
- 19 LINEK, -. *Coll.Czech.Chem.Comm.*, Vol.41, p.1714, 1976.
- 20 MECHTIEV, -. et al. *Azerb.Khim.Zh.*, Vol.6, p.55, 1978.
- 21 AMBROSE, D. in *Hndbk.Chem.Phys.*, CRC Press, 72nd.ed., pp.6-49 to 6-63, 1991.*
- 22 TRC Thermodynamic Tables, Texas A & M Univ., Loose leaf data sheets extant 1996.* A

**C₆H₁₂O₂ 1,1-Dimethylethyl ethanoate; *tert*-Butyl ethanoate; *tert*-Butyl acetate**

CAS Reg. No. 540-88-5

Mol. Wt. 116.16

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

Critical Temperature	T_c	= 545. K	(t_c	= 271.85 °C)
Critical Pressure	p_c	= 3270. kPa	(p_c	= 32.27 atm)
Critical Density	ρ_c	= 296. kg/m ³	(V_c	= 392.43 cm ³ /mol)
Critical Compression Factor	Z_c	= 0.283		

$$N_1 = 1.77286 \quad N_2 = -0.62056 \quad N_3 = 0.00000 \quad N_4 = 0.20876$$

Density at 298.15 K (25 °C)	ρ_{25}	= 861.34 kg/m ³	(V_{25}	= 134.86 cm ³ /mol)
Normal Boiling Point	T_b	= 369.629 K	(t_b	= 96.479 °C)
Melting Point	T_m	= -	(t_m	= -)

Data at Specified Temperatures

$t/^\circ\text{C}$	-100	0	25	50	96.48	200	271.85
T/K	173.15	273.15	298.15	323.15	369.63	473.15	545.00
$\rho/(\text{kg/m}^3)$	(987.87)	(887.70)	861.34	834.13	(780.44)	(630.13)	(296.00)
$(d\rho/dT)/(\text{kg/m}^3 \text{ K})$	(-0.97)	(-1.04)	-1.07	-1.11	(-1.21)	(-1.86)	$-\infty$
$V/(\text{cm}^3/\text{mol})$	(117.59)	(130.85)	134.86	139.26	(148.84)	(184.34)	(392.43)
$(dV/dT)/(\text{cm}^3/\text{mol K})$	(0.12)	(0.15)	0.17	0.18	(0.23)	(0.54)	∞
Data Quality	(B)	(B)	B	B	(C)	(C)	(C)
Uncertainty in ρ (kg/m ³)	(5.)	(2.)	2.	5.	(5.)	(10.)	(10.)
Uncertainty in V (cm ³ /mol)	(0.5)	(0.2)	0.2	0.5	(1.)	(2.)	(10.)

Orthobaric Liquid Density of 1,1-Dimethylethyl ethanoateUnits: kg/m³ v. °C

t	ρ	Uncert.	t	ρ	Uncert.	t	ρ	Uncert.	t	ρ	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
-100	(988.)	5.	0	(888.)	2.	100	(776.)	5.	200	(630.)	10.
-95	(983.)	5.	5	(882.)	2.	105	(770.)	5.	205	(621.)	10.
-90	(978.)	5.	10	(877.)	2.	110	(764.)	5.	210	(611.)	10.
-85	(973.)	5.	15	(872.)	2.	115	(757.)	5.	215	(600.)	10.
-80	(968.)	2.	20	867.	2.	120	(751.)	5.	220	(590.)	10.
-75	(963.)	2.	25	861.	2.	125	(745.)	5.	225	(578.)	10.
-70	(958.)	2.	30	856.	2.	130	(738.)	5.	230	(566.)	10.
-65	(954.)	2.	35	851.	2.	135	(731.)	5.	235	(553.)	10.
-60	(949.)	2.	40	845.	2.	140	(725.)	5.	240	(539.)	10.
-55	(944.)	2.	45	840.	2.	145	(718.)	5.	245	(524.)	10.
-50	(939.)	2.	50	834.	5.	150	(711.)	5.	250	(506.)	10.
-45	(934.)	2.	55	829.	5.	155	(703.)	5.	255	(487.)	10.
-40	(929.)	2.	60	823.	5.	160	(696.)	5.	260	(463.)	10.
-35	(924.)	2.	65	(817.)	5.	165	(689.)	5.	265	(433.)	10.
-30	(918.)	2.	70	(812.)	5.	170	(681.)	5.	270	(381.)	10.
-25	(913.)	2.	75	(806.)	5.	175	(673.)	5.			
-20	(908.)	2.	80	(800.)	5.	180	(665.)	10.			
-15	(903.)	2.	85	(794.)	5.	185	(657.)	10.			
-10	(898.)	2.	90	(788.)	5.	190	(648.)	10.			
-5	(893.)	2.	95	(782.)	5.	195	(639.)	10.			

Orthobaric Liquid Molar Volume of 1,1-Dimethylethyl ethanoate

Units: cm ³ /mol v. K											
T	V	Uncert.	T	V	Uncert.	T	V	Uncert.	T	V	Uncert.
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
175	(117.8)	0.5	275	(131.1)	0.2	375	(150.)	1.	475	(185.)	2.
180	(118.4)	0.5	280	(131.9)	0.2	380	(151.)	1.	480	(188.)	2.
185	(119.0)	0.5	285	(132.7)	0.2	385	(153.)	1.	485	(191.)	2.
190	(119.6)	0.5	290	(133.5)	0.2	390	(154.)	1.	490	(195.)	2.
195	(120.2)	0.5	295	134.3	0.2	395	(155.)	1.	495	(198.)	2.
200	(120.8)	0.5	300	135.2	0.2	400	(157.)	1.	500	(202.)	2.
205	(121.4)	0.5	305	136.0	0.5	405	(158.)	1.	505	(207.)	2.
210	(122.1)	0.5	310	136.9	0.5	410	(159.)	1.	510	(212.)	5.
215	(122.7)	0.5	315	137.8	0.5	415	(161.)	2.	515	(218.)	5.
220	(123.3)	0.5	320	138.7	0.5	420	(162.)	2.	520	(224.)	5.
225	(124.0)	0.5	325	139.6	0.5	425	(164.)	2.	525	(233.)	5.
230	(124.7)	0.5	330	140.5	0.5	430	(166.)	2.	530	(243.)	5.
235	(125.3)	0.5	335	(141.5)	1.	435	(168.)	2.	535	(256.)	5.
240	(126.0)	0.2	340	(142.5)	1.	440	(169.)	2.	540	(278.)	5.
245	(126.7)	0.2	345	(143.5)	1.	445	(171.)	2.	545	(392.)	10.
250	(127.4)	0.2	350	(144.5)	1.	450	(173.)	2.			
255	(128.2)	0.2	355	(145.6)	1.	455	(175.)	2.			
260	(128.9)	0.2	360	(147.)	1.	460	(178.)	2.			
265	(129.6)	0.2	365	(148.)	1.	465	(180.)	2.			
270	(130.4)	0.2	370	(149.)	1.	470	(183.)	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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|---|---------------------------|--|---|
| 1 | HENRY, L. | <i>Rec.Trav.Chim.</i> , Vol.26, p.444, 1907. | |
| 2 | SMITH, -.; OLSSON, -. | <i>Z.Phys.Chem.Stoech.Verw.</i> , Vol.118, p.99, 1925. | |
| 3 | NORRIS, -.; RIGBY, -. | <i>J.Am.Chem.Soc.</i> , Vol.54, p.2088, 1932. | |
| 4 | VOGEL, A. I. | <i>J.Chem.Soc.</i> , p.616, 1948. | |
| 5 | MARONI-BARNAUD, -. | <i>Bull.Soc.Chim.France</i> , p.583, 1959. | |
| 6 | SHRETS, -. et al. | <i>Izv.Vys.Uch.Zav.Khim.Khim.Tekh.</i> , Vol.13, p.1535, 1970. | |
| 7 | TRC Thermodynamic Tables, | Texas A & M Univ., Loose leaf data sheets extant 1996.* | A |