

96021

Issued September 1996
Supersedes in part ESDU 80019

Vapour pressures and critical points of liquids

Esters of monobasic acids 2: Branched chain alkyl alkanoates

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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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VAPOUR PRESSURES AND CRITICAL POINTS OF LIQUIDS

ESTERS OF MONOBASIC ACIDS - 2: BRANCHED CHAIN ALKYL ALKANOATES

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1	$C_4H_8O_2$	1-Methylethyl methanoate	Isopropyl formate	7
2	$C_5H_{10}O_2$	1-Methylpropyl methanoate	<i>sec</i> -Butyl formate	9
3	$C_5H_{10}O_2$	2-Methylpropyl methanoate	Isobutyl formate	11
4	$C_5H_{10}O_2$	1,1-Dimethylethyl methanoate	<i>tert</i> -Butyl formate	13
5	$C_6H_{12}O_2$	3-Methylbutyl methanoate	Isopentyl formate	15
6	$C_5H_{10}O_2$	1-Methylethyl ethanoate	Isopropyl acetate	17
7	$C_6H_{12}O_2$	1-Methylpropyl ethanoate	<i>sec</i> -Butyl acetate	19
8	$C_6H_{12}O_2$	2-Methylpropyl ethanoate	Isobutyl acetate	21
9	$C_6H_{12}O_2$	1,1-Dimethylethyl ethanoate	<i>tert</i> -Butyl acetate	23
10	$C_7H_{14}O_2$	3-Methylbutyl ethanoate	Isopentyl acetate	25
11	$C_{12}H_{22}O_2$	4-(1,1-Dimethylethyl)cyclohexyl ethanoate	4- <i>tert</i> -Butylcyclohexyl ethanoate	27
12	$C_6H_{12}O_2$	1-Methylethyl propanoate	Isopropyl propionate	29
13	$C_7H_{14}O_2$	1-Methylpropyl propanoate	<i>sec</i> -Butyl propionate	31
14	$C_7H_{14}O_2$	2-Methylpropyl propanoate	Isobutyl propionate	33
15	$C_7H_{14}O_2$	1,1-Dimethylethyl propanoate (not issued)		
15	$C_8H_{16}O_2$	3-Methylbutyl propanoate	Isopentyl propionate	35
16	$C_7H_{14}O_2$	1-Methylethyl butanoate	Isopropyl butyrate	37
17	$C_8H_{16}O_2$	1-Methylpropyl butanoate	<i>sec</i> -Butyl butyrate	39
18	$C_8H_{16}O_2$	2-Methylpropyl butanoate	Isobutyl butyrate	41
19	$C_8H_{16}O_2$	1,1-Dimethylethyl butanoate	<i>tert</i> -Butyl butyrate	43
20	$C_9H_{18}O_2$	3-Methylbutyl butanoate	Isopentyl butyrate	45
21	$C_8H_{16}O_2$	1-Methylethyl pentanoate	Isopropyl valerate	47
22	$C_9H_{18}O_2$	1-Methylpropyl pentanoate	<i>sec</i> -Butyl valerate	49
23	$C_9H_{18}O_2$	2-Methylpropyl pentanoate	Isobutyl valerate	51
24	$C_9H_{18}O_2$	1-Methylethyl hexanoate	Isopropyl caproate	53
25	$C_{11}H_{22}O_2$	3-Methylbutyl hexanoate	Isopentyl caproate	55
26	$C_5H_{10}O_2$	Methyl 2-methylpropanoate	Methyl isobutyrate	57
27	$C_6H_{12}O_2$	Ethyl 2-methylpropanoate	Ethyl isobutyrate	59
28	$C_7H_{14}O_2$	Propyl 2-methylpropanoate	Propyl isobutyrate	61
29	$C_7H_{14}O_2$	1-Methylethyl 2-methylpropanoate	Isopropyl isobutyrate	63
30	$C_8H_{16}O_2$	Butyl 2-methylpropanoate	Butyl isobutyrate	65
31	$C_8H_{16}O_2$	2-Methylpropyl 2-methylpropanoate	Isobutyl isobutyrate	67
32	$C_8H_{16}O_2$	1,1-Dimethylethyl 2-methylpropanoate	<i>tert</i> -Butyl isobutyrate	69
33	$C_9H_{18}O_2$	3-Methylbutyl 2-methylpropanoate	Isopentyl isobutyrate	71
34	$C_6H_{12}O_2$	Methyl 2-methylbutanoate		73
35	$C_6H_{12}O_2$	Methyl 3-methylbutanoate	Methyl isovalerate	75
36	$C_7H_{14}O_2$	Ethyl 3-methylbutanoate	Ethyl isovalerate	77
37	$C_8H_{16}O_2$	Propyl 3-methylbutanoate	Propyl isovalerate	79
38	$C_8H_{16}O_2$	1-Methylethyl 3-methylbutanoate	Isopropyl isovalerate	81
39	$C_9H_{18}O_2$	Butyl 3-methylbutanoate	Butyl isovalerate	83
40	$C_9H_{18}O_2$	2-Methylpropyl 3-methylbutanoate	Isobutyl isovalerate	85
41	$C_9H_{18}O_2$	1,1-Dimethylethyl 3-methylbutanoate (not issued)		
41	$C_{10}H_{20}O_2$	3-Methylbutyl 3-methylbutanoate	Isopentyl isovalerate	87

VAPOUR PRESSURES AND CRITICAL POINTS OF LIQUIDS ESTERS OF MONOBASIC ACIDS - 2: BRANCHED CHAIN ALKYL ALKANOATES

1. INTRODUCTION

This Item presents saturated vapour pressures of the branched chain alkyl alkanoates shown in the order of arrangement on the Contents page.

Table 1, page 5, gives the constants of the Wagner vapour pressure equation for all the compounds. On the following sheets, the values of vapour pressure for each compound have been obtained by calculation from the Wagner vapour pressure equation given at the top of each sheet. Using the critical temperature and the critical pressure given, the coefficients were derived by fitting the equation to the data that had been selected and weighted in accordance with a critical assessment of all the data. Note that estimated values of critical temperature are normally rounded to the nearest kelvin and that values in other units are obtained by exact conversion. The Tables also give the acentric factor, the normal boiling point, the value of dT/dp at the normal boiling point and the approximate melting point. Brackets enclose data at temperatures outside the range of supporting experimental data.

The table of Data at Specified Pressures for each compound gives, at each pressure, the temperature and the derivative of pressure 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 pressures of 1 kPa and above the estimated uncertainties in temperature and pressure which are dependent upon the data quality are shown below each letter rounded to 1, 2, or 5 times a power of 10. Uncertainties are discussed at greater length in Section 5.

Tabulated values of vapour pressure are presented in two sets of units, namely, (i) pressures in kPa at temperatures in kelvins, (ii) pressures in bar at temperatures in degrees C. The Table providing pressures in kPa also gives the uncertainties in pressure and temperature for pressures greater than 1 kPa. In general, pressures are given from just above the melting point to just below the critical point at intervals adjusted to make maximum use of the space available, a larger interval frequently being used at low temperatures. For compounds with very high estimated critical temperatures the tables are usually truncated at a convenient lower temperature.

The sources of information which give vapour pressure and/or critical point data for the compound considered are listed on the reverse side of each sheet. Those sources that were used to derive the critical properties and the coefficients of the vapour pressure equation are shown in bold type together with the pressure ranges of their data. These arbitrary pressure ranges are described in Section 3.

2. NOTATION AND UNITS

All temperatures are based on the International Temperature Scale (ITS-90). On ITS-90 Kelvin temperatures are strictly called International Kelvin Temperatures, similarly Celsius temperatures are strictly called International Celsius Temperatures.

N_1, N_2, N_3, N_4	non-dimensional coefficients of the Wagner vapour pressure equation
p	vapour pressure
T	Kelvin temperature
t	Celsius temperature, $(T - 273.15)$
τ	$1 - T/T_c$

Note: The units of temperature and vapour pressure 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. SOURCES OF DATA

Experimental vapour pressure data are, according to the apparatus and technique applied, usually reported for different pressure regions which may loosely be defined as:

- low pressure, below say 1 kPa (approximately 7.5 mmHg),
- medium pressure, say 1 kPa to 200 kPa (approximately 2 atm),
- high pressure, say 200 kPa to the critical point,
- the critical point.

The experimental data reported for the low and high pressure ranges are usually less accurate than, and not always compatible with, data for the medium pressure range, which may be of a very high degree of precision, possibly with an uncertainty in pressure less than 0.01 per cent near the normal boiling point. In the high pressure range the uncertainties increase progressively with temperature up to the critical point where the uncertainty in pressure is seldom lower than 0.1 per cent and frequently higher than 1 per cent.

Of the compounds considered here very reliable medium pressure range measurements have been made on isopropyl acetate. Reliable critical temperatures and critical pressures of isopropyl acetate and methyl isobutanoate have also been determined. For some of the compounds considered here medium pressure range measurements of varying reliability have been made but for most of the compounds only scattered boiling temperatures at various pressures have been reported. Additional critical point measurements of low reliability have been reported for fourteen other esters.

In this Item critical temperatures and critical pressures were estimated, using References 2 and 3, for those compounds for which they were not reliably known.

4. CRITERIA TO BE MET BY VAPOUR PRESSURE EQUATIONS

4.1. Low reduced temperatures

Vapour pressures of liquids at very low temperatures are, in general, more reliably obtained by calculation than by direct measurement. In Reference 4 Ambrose and Davies show that such vapour pressures may be obtained from the difference between the heat capacities of the ideal gas and the liquid. Rigorous treatment also requires the molar volume of the liquid and the second virial coefficient of the vapour. Unfortunately, the requisite experimental data determinations have been made for comparatively few liquids and these do not include any of the compounds considered here. However, low range vapour pressures obtained in this way are available for the normal alkanes from ethane to hexadecane, and these have been used in the derivation of their vapour pressure equations, see Reference 7, which may be used as a guide to extrapolate the vapour pressure curves of other non-associated liquids as follows.

The second differential of the Wagner vapour pressure equation with respect to temperature gives the difference, D say, between the ideal gas and liquid heat capacities. Denoting the differences at reduced temperatures of 0.3 and 0.5 by, D_3 and D_5 respectively, it was noted that for the alkanes from propane to hexadecane, the variation of D_3/D_5 with D_5 could be represented by a straight line without significant error. If it is assumed that this line is approximately valid for other groups of compounds the equation of the line may be included in the program which fits the Wagner vapour pressure equation and the deviation of the extrapolation of each fit from this line may be calculated. If necessary, the ratio of the third and fourth coefficients of the equation may be slightly constrained to reduce the deviation.

4.2. High reduced temperatures

In References 5 and 6 Ambrose has examined the differences, in the high pressure range, between the shapes of well-established vapour pressure curves for a variety of compounds. He has shown that for compounds in different classes of chemical substances these differences in shape are characterised by different ranges of numerical relationships between the coefficients of their Wagner equations. In Reference 7 Ambrose and Walton have demonstrated this phenomenon for the two homologous series of normal alkanes and alkanols. Thus, for certain classes of compounds it is possible to establish criteria that should be met by vapour pressure curves based on less extensive or less reliable data.

5. EVALUATION AND CORRELATION

Section 5 of Part 1, (Item 96016) describes the evaluation and correlation of the alkyl alkanoates and the derivation of the correlation which was used to derive the vapour pressure equations of those compounds for which the data were not extensive enough or too scattered to yield reliable results when fitted by the Wagner equation in the normal way.

For the compounds considered here, those for which the data were reliable enough were fitted by the Wagner equation and found to meet the required criteria. However, for most of the compounds it was necessary to use the correlation from Part 1 to derive their vapour pressure equations. This procedure ensured the vapour equations of all the compounds presented here met all the desired criteria. In fitting the data for each compound care was taken to ensure that the values of the normal boiling points, critical temperatures and acentric factors were compatible with the values for the corresponding straight chain compounds in Part 1.

For most of the compounds considered here saturated liquid density data were available, see Item 96022, and for some compounds the critical temperature and pressure were adjusted until they were optimum values for the correlation of both properties.

6. DISCUSSION OF UNCERTAINTIES

At any temperature, the estimated uncertainties in the tabulated values of temperature and pressure are dependent upon the reliability of the experimental and estimated data on which they are based. Except in the low pressure range values dependent on estimated data are much less certain than values dependent upon measured data.

The reliability of the experimental or estimated data may vary considerably over the entire liquid range of a compound. The term 'data quality' is used here to express the assessed reliability of the fitted data and hence also the reliability of the tabulated values. In the table of Data at Specified Pressures the data quality at each pressure is denoted by one of the letters 'A', 'B' or 'C'. The uncertainties in temperature and pressure are not thought to be more than the values shown below each letter.

The majority of reliable data are considered of quality 'A' with uncertainties of about 0.01 to 0.1 K at the normal boiling point or about 0.1 to 1 K at the critical point. Similarly the letters 'B' and 'C' indicate that the vapour pressures are based on progressively less reliable data, the uncertainties increasing tenfold with each successive letter.

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. Furthermore for those compounds for which the data quality at the critical pressure is denoted by 'C' the values of critical temperature and critical pressure given in the Tables should be regarded only as correlating parameters. Since the acentric factor, ω , is dependent upon the value of critical pressure selected, the uncertainty in ω for these compounds is high, possibly greater than 0.05.

7. REFERENCES

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TABLE 1

Summary of Constants in the Wagner vapour pressure equation

$$\ln p = \ln p_c + (N_1 \tau + N_2 \tau^{1.5} + N_3 \tau^{2.5} + N_4 \tau^5)/(T/T_c) \quad \text{where } \tau = 1 - T/T_c$$

No.	Name	T_c K	p_c kPa	N_1	N_2	N_3	N_4
1	1-Methylethyl methanoate	518.	4000.	-7.5524	1.82442	-2.63241	-3.35296
2	1-Methylpropyl methanoate	545.	3500.	-7.83996	1.98695	-3.10208	-3.6231
3	2-Methylpropyl methanoate	551.	3550.	-7.84771	1.99142	-3.11481	-3.63002
4	1,1-Dimethylethyl methanoate	533.	3600.	-7.69094	1.902	-2.85803	-3.48641
5	3-Methylbutyl methanoate	576.	3150.	-8.1434	2.16468	-3.60337	-3.87992
6	1-Methylethyl ethanoate	531.00	3340.	-8.02664	2.16277	-3.46813	-3.84036
7	1-Methylpropyl ethanoate	563.	3200.	-8.00866	2.08499	-3.38007	-3.76941
8	2-Methylpropyl ethanoate	565.	3105.	-8.17285	2.18226	-3.65232	-3.90333
9	1,1-Dimethylethyl ethanoate	545.	3270.	-7.94169	2.04584	-3.2695	-3.71239
10	3-Methylbutyl ethanoate	592.	2850.	-8.28354	2.24887	-3.83681	-3.98896
11	4-(1,1-Dimethylethyl)cyclohexyl ethanoate	710.	2150.	-8.77173	2.55223	-4.65922	-4.32293
12	1-Methylethyl propanoate	557.	3100.	-8.08123	2.12776	-3.5002	-3.82963
13	1-Methylpropyl propanoate	579.	2850.	-8.31301	2.26674	-3.88605	-4.01114
14	2-Methylpropyl propanoate	586.	2780.	-8.27333	2.24269	-3.81976	-3.98122
15	1,1-Dimethylethyl propanoate (not issued)						
15	3-Methylbutyl propanoate	609.	2470.	-8.48436	2.37177	-4.1734	-4.13489
16	1-Methylethyl butanoate	577.	2800.	-8.29751	2.25733	-3.86014	-3.99951
17	1-Methylpropyl butanoate	600.	2600.	-8.48407	2.3716	-4.17291	-4.13469
18	2-Methylpropyl butanoate	606.	2560.	-8.48221	2.37045	-4.16979	-4.13339
19	1,1-Dimethylethyl butanoate	589.	2700.	-8.35288	2.291	-3.95275	-4.04072
20	3-Methylbutyl butanoate	627.	2285.	-8.66409	2.48401	-4.47668	-4.25533
21	1-Methylethyl pentanoate	600.	2500.	-8.4881	2.37409	-4.17969	-4.13749
22	1-Methylpropyl pentanoate	623.	2400.	-8.70553	2.51019	-4.54688	-4.28175
23	2-Methylpropyl pentanoate	628.	2350.	-8.7123	2.51447	-4.55836	-4.28603
24	1-Methylethyl hexanoate	620.	2300.	-8.76197	2.54601	-4.64265	-4.31694
25	3-Methylbutyl hexanoate	674.	2000.	-9.1859	2.82152	-5.36786	-4.55207
26	Methyl 2-methylpropanoate	540.70	3430.	-7.87055	2.00458	-3.15235	-3.65029
27	Ethyl 2-methylpropanoate	558.	3050.	-8.01138	2.08659	-3.38457	-3.7717
28	Propyl 2-methylpropanoate	581.	2800.	-8.31751	2.26947	-3.89357	-4.0145
29	1-Methylethyl 2-methylpropanoate	567.	2785.	-8.08716	2.13127	-3.51003	-3.83447
30	Butyl 2-methylpropanoate	606.	2540.	-8.45143	2.35144	-4.11804	-4.11179
31	Isobutyl isobutyrate	597.	2600.	-8.318	2.26977	-3.89439	-4.01486
32	1,1-Dimethylethyl 2-methylpropanoate	572.	2600.	-8.09555	2.13624	-3.52394	-3.84131
33	3-Methylbutyl 2-methylpropanoate	617.	2330.	-8.5693	2.42455	-4.31648	-4.19299
34	Methyl 2-methylbutanoate	567.	3105.	-7.95964	1.9034	-3.11964	-3.50193
35	Methyl 3-methylbutanoate	569.	3130.	-8.00513	1.96126	-3.14689	-4.41415
36	Ethyl 3-methylbutanoate	584.	2800.	-8.21679	2.2086	-3.72546	-3.93777
37	Propyl 3-methylbutanoate	604.	2550.	-8.50768	2.38622	-4.21263	-4.15105
38	1-Methylethyl 3-methylbutanoate	588.	2550.	-8.32752	2.27556	-3.91031	-4.02196
39	Butyl 3-methylbutanoate	623.	2300.	-8.67591	2.49147	-4.49669	-4.26292
40	2-Methylpropyl 3-methylbutanoate	620.	2400.	-8.4682	2.36178	-4.14621	-4.12359
	1,1-Dimethylethyl 3-methylbutanoate (not issued)						
41	3-Methylbutyl 3-methylbutanoate	640.	2150.	-8.77143	2.55204	-4.65873	-4.32275

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

CAS Reg. No. 625-55-8

Mol. Wt. 88.11

Vapour Pressure $\ln p = \ln p_c + (N_1 \tau + N_2 \tau^{1.5} + N_3 \tau^{2.5} + N_4 \tau^5)/(T/T_c)$

where T is the kelvin temperature on the International Temperature Scale of 1990 (ITS-90), p is the vapour pressure, T_c , p_c are the critical temperature and the critical pressure respectively and $\tau = 1 - T/T_c$.

Critical Temperature	$T_c = 518. \text{ K}$	$(t_c = 244.85^\circ\text{C})$
Critical Pressure	$p_c = 4000. \text{ kPa}$	$(p_c = 39.48 \text{ atm})$
$N_1 = -7.55240$	$N_2 = 1.82442$	$N_3 = -2.63241$
		$N_4 = -3.35296$
Acentric Factor	$\omega = 0.305$	
Normal Boiling Point	$T_b = 340.619 \text{ K}$	$(t_b = 67.469^\circ\text{C})$
dT/dp at T_b , t_b	$= 0.301 \text{ K/kPa}$	$(= 0.0401^\circ\text{C/mmHg})$
Melting Point	$T_m = -$	$(t_m = -)$

Data at Specified Pressures								
p/kPa	0.001	0.01	0.1	1	10	101.325	1000	4000.
T/K	(179.730)	(196.712)	(218.017)	(245.779)	283.892	340.619	(432.269)	(518.000)
$(dp/dT)/(\text{kPa/K})$	(0.000)	(0.001)	(0.010)	(0.072)	0.507	3.325	(19.157)	(58.320)
Data Quality				(C)	C	C	(C)	(C)
Uncert. in T (K)				(0.2)	0.5	0.5	(2.)	(5.)
Uncert. in p (kPa)				(0.02)	0.2	2.	(50.)	(500.)
Uncert. in p (%)				(2.)	2.	2.	(5.)	(10.)

Vapour Pressure of 1-Methylethyl methanoate

Units: kPa v. K											
Uncertainty in				Uncertainty in				Uncertainty in			
T	p	T	p	T	p	T	p	T	p	T	p
K	kPa	K	%	K	kPa	K	%	K	kPa	K	%
175	(5.E-4)			300	21.485	0.5	2	425	(867.82)	2	5
180	(0.001)			305	26.711	0.5	2	430	(957.23)	2	5
185	(0.002)			310	32.931	0.5	2	435	(1053.3)	2	5
190	(0.004)			315	40.279	0.5	2	440	(1156.5)	2	5
195	(0.008)			320	48.897	0.5	2	445	(1267.0)	2	5
200	(0.015)			325	58.939	0.5	2	450	(1385.2)	2	5
205	(0.026)			330	70.569	0.5	2	455	(1511.5)	2	5
210	(0.045)			335	83.956	0.5	2	460	(1646.3)	5	5
215	(0.075)			340	99.282	0.5	2	465	(1789.9)	5	5
220	(0.121)			345	116.74	0.5	2	470	(1942.7)	5	5
225	(0.190)			350	(136.51)	0.5	2	475	(2105.3)	5	5
230	(0.293)			355	(158.82)	1	2	480	(2278.2)	5	5
235	(0.442)			360	(183.87)	1	2	485	(2461.7)	5	10
240	(0.652)			365	(211.89)	1	2	490	(2656.7)	5	10
245	(0.945)			370	(243.09)	1	2	495	(2863.6)	5	10
250	(1.346)	0.2	2	375	(277.71)	1	2	500	(3083.4)	5	10
255	(1.884)	0.2	2	380	(315.99)	1	2	505	(3317.0)	5	10
260	(2.597)	0.2	2	385	(358.18)	1	2	510	(3565.5)	5	10
265	(3.529)	0.2	2	390	(404.53)	1	5	515	(3830.9)	5	10
270	(4.729)	0.5	2	395	(455.30)	2	5				
275	(6.257)	0.5	2	400	(510.75)	2	5				
280	8.181	0.5	2	405	(571.14)	2	5				
285	10.575	0.5	2	410	(636.76)	2	5				
290	13.526	0.5	2	415	(707.88)	2	5				
295	17.128	0.5	2	420	(784.81)	2	5				

Vapour Pressure of 1-Methylethyl methanoate continued

Units: bar v. °C									
$\frac{t}{^{\circ}\text{C}}$	$\frac{p}{\text{bar}}$	$\frac{t}{^{\circ}\text{C}}$	$\frac{p}{\text{bar}}$	$\frac{t}{^{\circ}\text{C}}$	$\frac{p}{\text{bar}}$	$\frac{t}{^{\circ}\text{C}}$	$\frac{p}{\text{bar}}$	$\frac{t}{^{\circ}\text{C}}$	$\frac{p}{\text{bar}}$
-100	(4.E-6)	-25	(0.012)	50	0.550	125	(4.897)	200	(20.440)
-95	(8.E-6)	-20	(0.017)	55	0.661	130	(5.482)	205	(22.130)
-90	(2.E-5)	-15	(0.023)	60	0.788	135	(6.119)	210	(23.925)
-85	(3.E-5)	-10	(0.032)	65	0.934	140	(6.809)	215	(25.832)
-80	(6.E-5)	-5	(0.043)	70	1.100	145	(7.557)	220	(27.856)
-75	(1.E-4)	0	(0.056)	75	1.289	150	(8.364)	225	(30.005)
-70	(2.E-4)	5	(0.074)	80	(1.503)	155	(9.234)	230	(32.289)
-65	(4.E-4)	10	0.096	85	(1.743)	160	(10.170)	235	(34.717)
-60	(6.E-4)	15	0.124	90	(2.012)	165	(11.175)	240	(37.306)
-55	(0.001)	20	0.157	95	(2.312)	170	(12.252)		
-50	(0.002)	25	0.198	100	(2.645)	175	(13.406)		
-45	(0.003)	30	0.247	105	(3.014)	180	(14.638)		
-40	(0.004)	35	0.305	110	(3.421)	185	(15.954)		
-35	(0.006)	40	0.374	115	(3.869)	190	(17.357)		
-30	(0.008)	45	0.456	120	(4.360)	195	(18.851)		

The following Sources give vapour pressure and/or critical point data for this compound. Those Sources used to derive the critical properties and coefficients of the vapour pressure equation are shown in bold type together with the pressure range (low 'L', medium 'M', normal boiling point only 'N', high 'H' or critical 'C') of the data. An asterisk (*) indicates that the Source is not a primary source of experimental data for this compound.

- 1 NELSON,O.A., *Ind.Eng.Chem.*, Vol.22, p.971, 1928.
- 2 STULL,D.R., *Ind.Eng.Chem.*, Vol.39, p.517, 1947.
- 3 VOGEL,A.I., *J.Chem.Soc.*, p.624, 1948. N
- 4 TRC Thermodynamic Tables, Texas A & M Univ., Loose leaf data sheets extant 1996.*

The following Sources were used to estimate critical point data for this compound.

- AMBROSE,D., NPL Report Chem 92, Nat.Phys.Lab., Teddington, UK, 1978.*
 AMBROSE,D., NPL Report Chem 98, Nat.Phys.Lab., Teddington, UK, 1979.*

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

CAS Reg. No. 589-40-2

Mol. Wt. 102.13

Vapour Pressure $\ln p = \ln p_c + (N_1 \tau + N_2 \tau^{1.5} + N_3 \tau^{2.5} + N_4 \tau^5)/(T/T_c)$

where T is the kelvin temperature on the International Temperature Scale of 1990 (ITS-90), p is the vapour pressure, T_c , p_c are the critical temperature and the critical pressure respectively and $\tau = 1 - T/T_c$.

Critical Temperature $T_c = 545. \text{ K}$ ($t_c = 271.85^\circ\text{C}$)
 Critical Pressure $p_c = 3500. \text{ kPa}$ ($p_c = 34.54 \text{ atm}$)

$N_1 = -7.83996$ $N_2 = 1.98695$ $N_3 = -3.10208$ $N_4 = -3.62310$

Acentric Factor $\omega = 0.357$
 Normal Boiling Point $T_b = 367.336 \text{ K}$ ($t_b = 94.186^\circ\text{C}$)
 dT/dp at T_b , t_b $= 0.320 \text{ K/kPa}$ ($= 0.0427^\circ\text{C/mmHg}$)
 Melting Point $T_m = -$ ($t_m = -$)

Data at Specified Pressures

p/kPa	0.001	0.01	0.1	1	10	101.325	1000	3500.
T/K	(195.828)	(213.991)	(236.747)	(266.359)	306.962	367.336	(464.744)	(545.000)
$(dp/dT)/(\text{kPa/K})$	(0.000)	(0.001)	(0.009)	(0.067)	0.476	3.125	(18.065)	(50.355)
Data Quality				(C)	C	C	(C)	(C)
Uncert. in T (K)				(1.)	1.	0.5	(2.)	(5.)
Uncert. in p (kPa)				(0.1)	0.5	2.	(50.)	(500.)
Uncert. in p (%)				(10.)	5.	2.	(5.)	(10.)

Vapour Pressure of 1-Methylpropyl methanoate

Units: kPa v. K

Uncertainty				Uncertainty				Uncertainty			
T	p	T in	p	T	p	T in	p	T	p	T in	p
K	kPa	K	%	K	kPa	K	%	K	kPa	K	%
175	(4.E-5)			300	(7.110)	1	5	425	(453.61)	2	5
180	(9.E-5)			305	9.101	1	5	430	(505.50)	2	5
185	(2.E-4)			310	11.538	1	5	435	(561.76)	2	5
190	(4.E-4)			315	14.494	1	5	440	(622.63)	2	5
195	(9.E-4)			320	18.050	1	5	445	(688.34)	2	5
200	(0.002)			325	22.295	1	5	450	(759.14)	2	5
205	(0.003)			330	27.325	1	2	455	(835.28)	2	5
210	(0.006)			335	33.245	1	2	460	(917.02)	2	5
215	(0.011)			340	40.166	1	2	465	(1004.6)	2	5
220	(0.019)			345	48.208	1	2	470	(1098.4)	2	5
225	(0.033)			350	57.497	0.5	2	475	(1198.6)	2	5
230	(0.053)			355	68.169	0.5	2	480	(1305.5)	2	5
235	(0.085)			360	80.363	0.5	2	485	(1419.6)	5	5
240	(0.133)			365	94.230	0.5	2	490	(1541.0)	5	5
245	(0.203)			370	109.92	0.5	2	495	(1670.1)	5	5
250	(0.304)			375	(127.60)	1	2	500	(1807.4)	5	5
255	(0.446)			380	(147.44)	1	2	505	(1953.3)	5	5
260	(0.643)			385	(169.61)	1	2	510	(2108.2)	5	5
265	(0.912)			390	(194.29)	1	2	515	(2272.5)	5	10
270	(1.273)	1	10	395	(221.67)	1	2	520	(2446.9)	5	10
275	(1.750)	1	10	400	(251.93)	1	2	525	(2632.1)	5	10
280	(2.374)	1	10	405	(285.28)	1	2	530	(2828.7)	5	10
285	(3.179)	1	5	410	(321.91)	1	2	535	(3037.7)	5	10
290	(4.205)	1	5	415	(362.03)	1	2	540	(3260.6)	5	10
295	(5.497)	1	5	420	(405.86)	2	5	545	(3500.0)	5	10

Vapour Pressure of 1-Methylpropyl methanoate continued

Units: bar v. °C									
$\frac{t}{^\circ\text{C}}$	$\frac{p}{\text{bar}}$	$\frac{t}{^\circ\text{C}}$	$\frac{p}{\text{bar}}$	$\frac{t}{^\circ\text{C}}$	$\frac{p}{\text{bar}}$	$\frac{t}{^\circ\text{C}}$	$\frac{p}{\text{bar}}$	$\frac{t}{^\circ\text{C}}$	$\frac{p}{\text{bar}}$
-100	(3.E-7)	-25	(0.003)	50	0.206	125	(2.404)	200	(11.608)
-95	(6.E-7)	-20	(0.004)	55	0.254	130	(2.726)	205	(12.652)
-90	(1.E-6)	-15	(0.006)	60	0.309	135	(3.080)	210	(13.765)
-85	(3.E-6)	-10	(0.008)	65	0.375	140	(3.468)	215	(14.952)
-80	(7.E-6)	-5	(0.011)	70	0.451	145	(3.892)	220	(16.214)
-75	(1.E-5)	0	(0.016)	75	0.539	150	(4.355)	225	(17.557)
-70	(3.E-5)	5	(0.021)	80	0.641	155	(4.858)	230	(18.983)
-65	(5.E-5)	10	(0.029)	85	0.757	160	(5.404)	235	(20.498)
-60	(9.E-5)	15	(0.038)	90	0.889	165	(5.996)	240	(22.106)
-55	(2.E-4)	20	(0.050)	95	1.039	170	(6.634)	245	(23.812)
-50	(3.E-4)	25	(0.065)	100	(1.208)	175	(7.323)	250	(25.623)
-45	(4.E-4)	30	0.083	105	(1.398)	180	(8.065)	255	(27.545)
-40	(7.E-4)	35	0.106	110	(1.611)	185	(8.861)	260	(29.589)
-35	(0.001)	40	0.133	115	(1.849)	190	(9.715)	265	(31.764)
-30	(0.002)	45	0.167	120	(2.112)	195	(10.630)	270	(34.091)

The following Sources give vapour pressure and/or critical point data for this compound. Those Sources used to derive the critical properties and coefficients of the vapour pressure equation are shown in bold type together with the pressure range (low 'L', medium 'M', normal boiling point only 'N', high 'H' or critical 'C') of the data. An asterisk (*) indicates that the Source is not a primary source of experimental data for this compound.

- 1 **NELSON, O.A.**, *Ind. Eng. Chem.*, Vol.20, p.1382, 1928. **M**
- 2 **STULL, D.R.**, *Ind. Eng. Chem.*, Vol.39, p.517, 1947.
- 3 **TRC Thermodynamic Tables**, Texas A & M Univ., Loose leaf data sheets extant 1996.*

The following Sources were used to estimate critical point data for this compound.

- AMBROSE, D.**, NPL Report Chem 92, Nat.Phys.Lab., Teddington, UK, 1978.*
AMBROSE, D., NPL Report Chem 98, Nat.Phys.Lab., Teddington, UK, 1979.*

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

CAS Reg. No. 542-55-2

Mol. Wt. 102.13

Vapour Pressure $\ln p = \ln p_c + (N_1 \tau + N_2 \tau^{1.5} + N_3 \tau^{2.5} + N_4 \tau^5)/(T/T_c)$

where T is the kelvin temperature on the International Temperature Scale of 1990 (ITS-90), p is the vapour pressure, T_c , p_c are the critical temperature and the critical pressure respectively and $\tau = 1 - T/T_c$.

Critical Temperature $T_c = 551. \text{ K}$ ($t_c = 277.85^\circ\text{C}$)
 Critical Pressure $p_c = 3550. \text{ kPa}$ ($p_c = 35.04 \text{ atm}$)

$N_1 = -7.84771$ $N_2 = 1.99142$ $N_3 = -3.11481$ $N_4 = -3.63002$

Acentric Factor $\omega = 0.358$
 Normal Boiling Point $T_b = 371.037 \text{ K}$ ($t_b = 97.887^\circ\text{C}$)
 dT/dp at T_b , t_b $= 0.322 \text{ K/kPa}$ ($= 0.0430^\circ\text{C/mmHg}$)
 Melting Point $T_m = 177. \text{ K}$ ($t_m = -96.^\circ\text{C}$)

Data at Specified Pressures

p/kPa	0.001	0.01	0.1	1	10	101.325	1000	3550.
T/K	(198.034)	(216.375)	(239.348)	(269.231)	310.184	371.037	(469.134)	(551.000)
$(dp/dT)/(\text{kPa/K})$	(0.000)	(0.001)	(0.009)	(0.067)	0.473	3.101	(17.944)	(50.568)
Data Quality				(C)	B	B	(C)	(C)
Uncert. in T (K)				(0.1)	0.1	0.05	(2.)	(5.)
Uncert. in p (kPa)				(0.01)	0.05	0.2	(50.)	(500.)
Uncert. in p (%)				(1.)	0.5	0.2	(5.)	(10.)

Vapour Pressure of 2-Methylpropyl methanoate

Units: kPa v. K

		Uncertainty		Units: kPa v. K				Uncertainty					
T	p	T	p	T	p	T	p	T	p	T	p	T	p
K	kPa	K	%	K	kPa	K	%	K	kPa	K	%	K	%
180	(6.E-5)			300	6.057	0.1	0.5	425	(414.26)	0.5	1		
185	(1.E-4)			305	7.788	0.1	0.5	430	(462.40)	1	2		
190	(3.E-4)			310	9.913	0.1	0.5	435	(514.66)	1	2		
195	(7.E-4)			315	12.502	0.1	0.5	440	(571.27)	1	2		
				320	15.629	0.1	0.5	445	(632.47)	1	2		
200	(0.001)			325	19.375	0.1	0.5	450	(698.48)	2	2		
205	(0.003)			330	23.830	0.1	0.5	455	(769.55)	2	2		
210	(0.005)			335	29.090	0.1	0.2	460	(845.92)	2	5		
215	(0.009)			340	35.261	0.1	0.2	465	(927.86)	2	5		
220	(0.015)			345	42.452	0.1	0.2	470	(1015.6)	2	5		
225	(0.025)			350	50.784	0.1	0.2	475	(1109.5)	2	5		
230	(0.042)			355	60.382	0.05	0.2	480	(1209.8)	2	5		
235	(0.067)			360	71.381	0.05	0.2	485	(1316.7)	2	5		
240	(0.106)			365	83.921	0.05	0.2	490	(1430.6)	5	5		
245	(0.163)			370	98.148	0.05	0.2	495	(1551.9)	5	5		
250	(0.245)			375	(114.22)	0.1	0.2	500	(1680.9)	5	5		
255	(0.362)			380	(132.29)	0.1	0.2	505	(1817.9)	5	5		
260	(0.526)			385	(152.52)	0.1	0.5	510	(1963.3)	5	5		
265	(0.750)			390	(175.10)	0.2	0.5	515	(2117.7)	5	5		
270	(1.053)	0.1	1	395	(200.20)	0.2	0.5	520	(2281.4)	5	10		
275	(1.456)	0.1	1	400	(227.99)	0.2	0.5	525	(2455.0)	5	10		
280	(1.985)	0.1	1	405	(258.68)	0.2	1	530	(2639.2)	5	10		
285	(2.671)	0.1	1	410	(292.45)	0.5	1	535	(2834.7)	5	10		
290	(3.550)	0.1	0.5	415	(329.50)	0.5	1	540	(3042.4)	5	10		
295	4.663	0.1	0.5	420	(370.03)	0.5	1	545	(3263.5)	5	10		

Vapour Pressure of 2-Methylpropyl methanoate continued

Units: bar v. °C									
t °C	p bar	t °C	p bar	t °C	p bar	t °C	p bar	t °C	p bar
-95	(4.E-7)	-25	(0.002)	50	0.179	125	(2.174)	200	(10.740)
-90	(1.E-6)	-20	(0.003)	55	0.221	130	(2.470)	205	(11.719)
-85	(2.E-6)	-15	(0.005)	60	0.270	135	(2.796)	210	(12.763)
-80	(5.E-6)	-10	(0.007)	65	0.329	140	(3.154)	215	(13.876)
		-5	(0.009)	70	0.397	145	(3.546)	220	(15.062)
-75	(1.E-5)	0	(0.013)	75	0.476	150	(3.975)	225	(16.322)
-70	(2.E-5)	5	(0.018)	80	0.567	155	(4.441)	230	(17.662)
-65	(4.E-5)	10	(0.024)	85	0.671	160	(4.948)	235	(19.085)
-60	(7.E-5)	15	(0.032)	90	0.791	165	(5.498)	240	(20.595)
-55	(1.E-4)	20	0.042	95	0.927	170	(6.093)	245	(22.197)
-50	(2.E-4)	25	0.055	100	1.080	175	(6.735)	250	(23.896)
-45	(3.E-4)	30	0.071	105	(1.254)	180	(7.426)	255	(25.698)
-40	(6.E-4)	35	0.091	110	(1.448)	185	(8.170)	260	(27.610)
-35	(9.E-4)	40	0.115	115	(1.665)	190	(8.969)	265	(29.640)
-30	(0.001)	45	0.144	120	(1.906)	195	(9.825)	270	(31.800)

The following Sources give vapour pressure and/or critical point data for this compound. Those Sources used to derive the critical properties and coefficients of the vapour pressure equation are shown in bold type together with the pressure range (low 'L', medium 'M', normal boiling point only 'N', high 'H' or critical 'C') of the data. An asterisk (*) indicates that the Source is not a primary source of experimental data for this compound.

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|----|--|---|---|
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| 11 | TIMMERMANS,J., | <i>Bull.Soc.Chim.Belges</i> , Vol.36, p.502, 1927. | |
| 12 | NELSON,O.A., | <i>Ind.Eng.Chem.</i> , Vol.20, p.1382, 1928. | M |
| 13 | FRIEND,J.N., HARGREAVES,W.D., | <i>Phil.Mag.</i> , Vol.34, p.643, 1943. | |
| 14 | STULL,D.R., | <i>Ind.Eng.Chem.</i> , Vol.39, p.517, 1947. | |
| 15 | VOGEL,A.I., | <i>J.Chem.Soc.</i> , p.624, 1948. | |
| 16 | BRIDSON-JONES,F.S., BUCKLEYG.D., et al., | <i>J.Chem.Soc.</i> , p.2999, 1951. | |
| 17 | SESELKIN,I.V., MIRONENKO,V.F., et al., | <i>Zh.Prkl.Khim.</i> , Vol.58, p.696, 1985. | |
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| 19 | TRC Thermodynamic Tables, | Texas A & M Univ., Loose leaf data sheets extant 1996.* | |

The following Sources were used to estimate critical point data for this compound.

- | | |
|-------------|---|
| AMBROSE,D., | NPL Report Chem 92, Nat.Phys.Lab., Teddington, UK, 1978.* |
| AMBROSE,D., | NPL Report Chem 98, Nat.Phys.Lab., Teddington, UK, 1979.* |

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

CAS Reg. No. 762-75-4

Mol. Wt. 102.13

Vapour Pressure $\ln p = \ln p_c + (N_1 \tau + N_2 \tau^{1.5} + N_3 \tau^{2.5} + N_4 \tau^5)/(T/T_c)$

where T is the kelvin temperature on the International Temperature Scale of 1990 (ITS-90), p is the vapour pressure, T_c , p_c are the critical temperature and the critical pressure respectively and $\tau = 1 - T/T_c$.

Critical Temperature $T_c = 533. \text{ K}$ ($t_c = 259.85^\circ\text{C}$)
 Critical Pressure $p_c = 3600. \text{ kPa}$ ($p_c = 35.53 \text{ atm}$)

$N_1 = -7.69094$ $N_2 = 1.90200$ $N_3 = -2.85803$ $N_4 = -3.48641$

Acentric Factor $\omega = 0.330$
 Normal Boiling Point $T_b = 356.050 \text{ K}$ ($t_b = 82.900^\circ\text{C}$)
 dT/dp at T_b , t_b $= 0.314 \text{ K/kPa}$ ($= 0.0418^\circ\text{C/mmHg}$)
 Melting Point $T_m = -$ ($t_m = -$)

Data at Specified Pressures								
p/kPa	0.001	0.01	0.1	1	10	101.325	1000	3600.
T/K	(188.438)	(206.118)	(228.298)	(257.201)	(296.900)	356.050	(451.734)	(533.000)
$(dp/dT)/(\text{kPa/K})$	(0.000)	(0.001)	(0.009)	(0.069)	(0.487)	3.186	(18.357)	(51.946)
Data Quality				(C)	(C)	B	(C)	(C)
Uncert. in T (K)				(0.2)	(0.2)	0.2	(2.)	(5.)
Uncert. in p (kPa)				(0.02)	(0.1)	0.5	(50.)	(500.)
Uncert. in p (%)				(2.)	(1.)	0.5	(5.)	(10.)

Vapour Pressure of 1,1-Dimethylethyl methanoate

Units: kPa v. K											
		Uncertainty in		Uncertainty				Uncertainty			
T	p	T	p	T	p	T	p	T	p	T	p
K	kPa	K	%	K	kPa	K	%	K	kPa	K	%
175	(1.E-4)			300	(11.607)	0.2	1	425	(592.36)	1	2
180	(3.E-4)			305	(14.648)	0.2	1	430	(656.81)	2	2
185	(6.E-4)			310	(18.319)	0.2	1	435	(726.39)	2	5
190	(0.001)			315	(22.714)	0.2	1	440	(801.37)	2	5
195	(0.002)			320	(27.937)	0.2	0.5	445	(882.00)	2	5
200	(0.005)			325	(34.099)	0.2	0.5	450	(968.55)	2	5
205	(0.009)			330	(41.318)	0.2	0.5	455	(1061.3)	2	5
210	(0.016)			335	(49.723)	0.2	0.5	460	(1160.6)	2	5
215	(0.027)			340	(59.449)	0.2	0.5	465	(1266.7)	2	5
220	(0.045)			345	(70.639)	0.2	0.5	470	(1379.9)	2	5
225	(0.073)			350	(83.444)	0.2	0.5	475	(1500.6)	5	5
230	(0.117)			355	(98.023)	0.2	0.5	480	(1629.1)	5	5
235	(0.181)			360	(114.54)	0.2	0.5	485	(1765.8)	5	5
240	(0.275)			365	(133.17)	0.2	0.5	490	(1911.1)	5	5
245	(0.410)			370	(154.09)	0.2	1	495	(2065.4)	5	5
250	(0.598)			375	(177.48)	0.2	1	500	(2229.2)	5	5
255	(0.858)			380	(203.54)	0.5	1	505	(2403.1)	5	10
260	(1.210)	0.2	2	385	(232.46)	0.5	1	510	(2587.6)	5	10
265	(1.680)	0.2	2	390	(264.45)	0.5	1	515	(2783.5)	5	10
270	(2.299)	0.2	2	395	(299.71)	0.5	2	520	(2991.6)	5	10
275	(3.102)	0.2	1	400	(338.46)	0.5	2	525	(3213.0)	5	10
280	(4.133)	0.2	1	405	(380.92)	1	2	530	(3449.4)	5	10
285	(5.439)	0.2	1	410	(427.30)	1	2				
290	(7.077)	0.2	1	415	(477.85)	1	2				
295	(9.110)	0.2	1	420	(532.79)	1	2				

Vapour Pressure of 1,1-Dimethylethyl methanoate continued

Units: bar v. °C									
$\frac{t}{^\circ\text{C}}$	$\frac{p}{\text{bar}}$	$\frac{t}{^\circ\text{C}}$	$\frac{p}{\text{bar}}$	$\frac{t}{^\circ\text{C}}$	$\frac{p}{\text{bar}}$	$\frac{t}{^\circ\text{C}}$	$\frac{p}{\text{bar}}$	$\frac{t}{^\circ\text{C}}$	$\frac{p}{\text{bar}}$
-100	(9.E-7)	-25	(0.005)	50	(0.317)	125	(3.237)	200	(14.550)
-95	(2.E-6)	-20	(0.008)	55	(0.385)	130	(3.648)	205	(15.806)
-90	(5.E-6)	-15	(0.011)	60	(0.465)	135	(4.097)	210	(17.142)
-85	(1.E-5)	-10	(0.015)	65	(0.557)	140	(4.586)	215	(18.563)
-80	(2.E-5)	-5	(0.021)	70	(0.663)	145	(5.119)	220	(20.072)
-75	(4.E-5)	0	(0.028)	75	(0.785)	150	(5.698)	225	(21.675)
-70	(7.E-5)	5	(0.037)	80	(0.924)	155	(6.324)	230	(23.376)
-65	(1.E-4)	10	(0.049)	85	(1.082)	160	(7.000)	235	(25.181)
-60	(2.E-4)	15	(0.064)	90	(1.260)	165	(7.730)	240	(27.097)
-55	(4.E-4)	20	(0.083)	95	(1.461)	170	(8.515)	245	(29.131)
-50	(6.E-4)	25	(0.106)	100	(1.685)	175	(9.358)	250	(31.295)
-45	(0.001)	30	(0.135)	105	(1.936)	180	(10.263)	255	(33.600)
-40	(0.002)	35	(0.169)	110	(2.214)	185	(11.231)		
-35	(0.002)	40	(0.210)	115	(2.522)	190	(12.266)		
-30	(0.004)	45	(0.259)	120	(2.863)	195	(13.372)		

The following Sources give vapour pressure and/or critical point data for this compound. Those Sources used to derive the critical properties and coefficients of the vapour pressure equation are shown in bold type together with the pressure range (low 'L', medium 'M', normal boiling point only 'N', high 'H' or critical 'C') of the data. An asterisk (*) indicates that the Source is not a primary source of experimental data for this compound.

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- 3 YOUNG,-., PARE,-., *J.Org.Chem.*, Vol.23, p.1772, 1958. N
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The following Sources were used to estimate critical point data for this compound.

- AMBROSE,D., NPL Report Chem 92, Nat.Phys.Lab., Teddington, UK, 1978.*
 AMBROSE,D., NPL Report Chem 98, Nat.Phys.Lab., Teddington, UK, 1979.*

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

CAS Reg. No. 110-45-2

Mol. Wt. 116.16

Vapour Pressure $\ln p = \ln p_c + (N_1 \tau + N_2 \tau^{1.5} + N_3 \tau^{2.5} + N_4 \tau^5)/(T/T_c)$

where T is the kelvin temperature on the International Temperature Scale of 1990 (ITS-90), p is the vapour pressure, T_c , p_c are the critical temperature and the critical pressure respectively and $\tau = 1 - T/T_c$.

Critical Temperature $T_c = 576. \text{ K}$ ($t_c = 302.85^\circ\text{C}$)
 Critical Pressure $p_c = 3150. \text{ kPa}$ ($p_c = 31.09 \text{ atm}$)

$N_1 = -8.14340$ $N_2 = 2.16468$ $N_3 = -3.60337$ $N_4 = -3.87992$

Acentric Factor $\omega = 0.411$
 Normal Boiling Point $T_b = 396.606 \text{ K}$ ($t_b = 123.456^\circ\text{C}$)
 dT/dp at T_b , t_b $= 0.340 \text{ K/kPa}$ ($= 0.0453^\circ\text{C/mmHg}$)
 Melting Point $T_m = 180. \text{ K}$ ($t_m = -93.^\circ\text{C}$)

Data at Specified Pressures

p/kPa	0.001	0.01	0.1	1	10	101.325	1000	3150.
T/K	(213.773)	(233.228)	(257.560)	(289.167)	332.421	396.606	(499.842)	(576.000)
$(dp/dT)/(\text{kPa/K})$	(0.000)	(0.001)	(0.008)	(0.063)	0.448	2.942	(17.104)	(44.534)
Data Quality				(C)	B	B	(C)	(C)
Uncert. in T (K)				(0.2)	0.1	0.2	(2.)	(5.)
Uncert. in p (kPa)				(0.01)	0.05	0.5	(50.)	(200.)
Uncert. in p (%)				(1.)	0.5	0.5	(5.)	(10.)

Vapour Pressure of 3-Methylbutyl methanoate

Units: kPa v. K

Uncertainty				Uncertainty				Uncertainty			
T	p	T	p	T	p	T	p	T	p	T	p
K	kPa	K	%	K	kPa	K	%	K	kPa	K	%
180	(4.E-6)	300	1.923	0.1	1	425	(216.43)	0.5	1		
185	(1.E-5)	305	2.551	0.1	1	430	(244.36)	0.5	1		
190	(3.E-5)	310	3.347	0.1	0.5	435	(274.99)	0.5	1		
195	(6.E-5)	315	4.345	0.1	0.5	440	(308.50)	0.5	2		
		320	5.583	0.1	0.5	445	(345.05)	1	2		
200	(1.E-4)	325	7.106	0.1	0.5	450	(384.82)	1	2		
205	(3.E-4)	330	8.964	0.1	0.5	455	(428.00)	1	2		
210	(6.E-4)	335	11.212	0.1	0.5	460	(474.78)	1	2		
215	(0.001)	340	13.910	0.1	0.5	465	(525.34)	1	2		
220	(0.002)	345	17.125	0.1	0.5	470	(579.89)	1	2		
225	(0.004)	350	20.930	0.1	0.5	475	(638.62)	2	2		
230	(0.007)	355	25.403	0.1	0.5	480	(701.76)	2	5		
235	(0.012)	360	30.629	0.1	0.5	485	(769.51)	2	5		
240	(0.020)	365	36.699	0.1	0.5	490	(842.09)	2	5		
245	(0.033)	370	43.710	0.1	0.5	495	(919.74)	2	5		
250	(0.052)	375	51.765	0.2	0.5	500	(1002.7)	2	5		
255	(0.080)	380	60.973	0.2	0.5	505	(1091.2)	2	5		
260	(0.122)	385	71.448	0.2	0.5	510	(1185.5)	2	5		
265	(0.183)	390	83.310	0.2	0.5	515	(1286.0)	5	5		
270	(0.268)	395	96.686	0.2	0.5	520	(1392.8)	5	5		
275	(0.386)	400	111.71	0.2	0.5	525	(1506.3)	5	5		
280	(0.547)	405	128.51	0.2	0.5	530	(1626.8)	5	5		
285	(0.765)	410	(147.23)	0.2	0.5	535	(1754.8)	5	5		
290	(1.054)	415	(168.03)	0.2	1	540	(1890.5)	5	5		
295	1.433	420	(191.04)	0.5	1	545	(2034.4)	5	5		

Vapour Pressure of 3-Methylbutyl methanoate continued

Units: bar v. °C									
t °C	p bar	t °C	p bar	t °C	p bar	t °C	p bar	t °C	p bar
		-25	(4.E-4)	50	0.065	125	1.059	200	(6.164)
		-20	(7.E-4)	55	0.082	130	1.221	205	(6.779)
-90	(8.E-8)	-15	(0.001)	60	0.103	135	(1.401)	210	(7.439)
-85	(2.E-7)	-10	(0.002)	65	0.129	140	(1.601)	215	(8.147)
-80	(5.E-7)	-5	(0.002)	70	0.159	145	(1.823)	220	(8.904)
-75	(1.E-6)	0	(0.003)	75	0.194	150	(2.068)	225	(9.714)
-70	(2.E-6)	5	(0.005)	80	0.237	155	(2.337)	230	(10.578)
-65	(5.E-6)	10	(0.007)	85	0.286	160	(2.633)	235	(11.499)
-60	(9.E-6)	15	(0.009)	90	0.343	165	(2.958)	240	(12.481)
-55	(2.E-5)	20	0.013	95	0.410	170	(3.312)	245	(13.525)
-50	(3.E-5)	25	0.017	100	0.487	175	(3.697)	250	(14.635)
-45	(6.E-5)	30	0.023	105	0.574	180	(4.116)	255	(15.814)
-40	(1.E-4)	35	0.030	110	0.674	185	(4.570)	260	(17.065)
-35	(2.E-4)	40	0.039	115	0.788	190	(5.062)	265	(18.393)
-30	(3.E-4)	45	0.051	120	0.916	195	(5.592)	270	(19.802)

The following Sources give vapour pressure and/or critical point data for this compound. Those Sources used to derive the critical properties and coefficients of the vapour pressure equation are shown in bold type together with the pressure range (low 'L', medium 'M', normal boiling point only 'N', high 'H' or critical 'C') of the data. An asterisk (*) indicates that the Source is not a primary source of experimental data for this compound.

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| 9 | TRC Thermodynamic Tables, | Texas A & M Univ., Loose leaf data sheets extant 1996.* | |

The following Sources were used to estimate critical point data for this compound.

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| AMBROSE,D., | NPL Report Chem 92, Nat.Phys.Lab., Teddington, UK,1978.* |
| AMBROSE,D., | NPL Report Chem 98, Nat.Phys.Lab., Teddington, UK,1979.* |

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

CAS Reg. No. 108-21-4

Mol. Wt. 102.13

Vapour Pressure $\ln p = \ln p_c + (N_1 \tau + N_2 \tau^{1.5} + N_3 \tau^{2.5} + N_4 \tau^5)/(T/T_c)$

where T is the kelvin temperature on the International Temperature Scale of 1990 (ITS-90), p is the vapour pressure, T_c , p_c are the critical temperature and the critical pressure respectively and $\tau = 1 - T/T_c$.

Critical Temperature $T_c = 531.00 \text{ K}$ ($t_c = 257.85^\circ\text{C}$)
 Critical Pressure $p_c = 3340. \text{ kPa}$ ($p_c = 32.96 \text{ atm}$)

$N_1 = -8.02664$ $N_2 = 2.16277$ $N_3 = -3.46813$ $N_4 = -3.84036$

Acentric Factor $\omega = 0.385$
 Normal Boiling Point $T_b = 361.726 \text{ K}$ ($t_b = 88.576^\circ\text{C}$)
 dT/dp at T_b , t_b $= 0.312 \text{ K/kPa}$ ($= 0.0416^\circ\text{C/mmHg}$)
 Melting Point $T_m = 200. \text{ K}$ ($t_m = -73.^\circ\text{C}$)

Data at Specified Pressures								
p/kPa	0.001	0.01	0.1	1	10	101.325	1000	3340.
T/K		(212.164)	(234.400)	(263.302)	302.893	361.726	456.594	531.000
$(dp/dT)/(\text{kPa/K})$		(0.001)	(0.009)	(0.069)	0.489	3.207	18.573	50.488
Data Quality				(B)	A	A	A	B
Uncert. in T (K)				(0.01)	0.01	0.005	0.1	1.
Uncert. in p (kPa)				(0.0010)	0.005	0.02	2.	50.
Uncert. in p (%)				(0.1)	0.05	0.02	0.2	2.

Vapour Pressure of 1-Methylethyl ethanoate

Units: kPa v. K

Uncertainty				Units: kPa v. K				Uncertainty			
in				in				in			
T	p	T	p	T	p	T	p	T	p	T	p
K	kPa	K	%	K	kPa	K	%	K	kPa	K	%
200	(0.002)			325	26.940	0.01	0.02	450	883.08	0.1	0.2
205	(0.004)			330	32.959	0.01	0.02	455	970.73	0.1	0.2
210	(0.008)			335	40.028	0.01	0.02	460	1064.8	0.1	0.2
215	(0.014)			340	48.275	0.005	0.02	465	1165.6	0.1	0.2
220	(0.024)			345	57.837	0.005	0.02	470	1273.5	0.2	0.2
225	(0.040)			350	68.859	0.005	0.02	475	1388.8	0.2	0.5
230	(0.066)			355	81.496	0.005	0.02	480	1511.9	0.2	0.5
235	(0.106)			360	95.907	0.005	0.02	485	1643.2	0.2	0.5
240	(0.165)			365	112.26	0.005	0.02	490	1783.2	0.5	0.5
245	(0.251)			370	130.74	0.01	0.02	495	1932.3	0.5	0.5
250	(0.376)			375	151.51	0.01	0.02	500	2091.1	0.5	1
255	(0.551)			380	174.78	0.01	0.02	505	2260.1	0.5	1
260	(0.793)			385	200.73	0.01	0.05	510	2440.1	0.5	1
265	(1.123)	0.01	0.1	390	229.58	0.02	0.05	515	2631.9	1	1
270	(1.566)	0.01	0.1	395	261.52	0.02	0.05	520	2836.4	1	1
275	2.151	0.01	0.1	400	296.78	0.02	0.05	525	3055.1	1	2
280	2.913	0.01	0.05	405	335.56	0.02	0.05	530	3290.4	1	2
285	3.894	0.01	0.05	410	378.11	0.02	0.1				
290	5.142	0.01	0.05	415	424.65	0.05	0.1				
295	6.712	0.01	0.05	420	475.42	0.05	0.1				
300	8.667	0.01	0.05	425	530.66	0.05	0.1				
305	11.075	0.01	0.05	430	590.63	0.05	0.1				
310	14.016	0.01	0.05	435	655.59	0.05	0.1				
315	17.576	0.01	0.05	440	725.80	0.05	0.1				
320	21.849	0.01	0.05	445	801.53	0.1	0.2				

Vapour Pressure of 1-Methylethyl ethanoate continued

Units: bar v. °C									
$\frac{t}{^\circ\text{C}}$	$\frac{p}{\text{bar}}$	$\frac{t}{^\circ\text{C}}$	$\frac{p}{\text{bar}}$	$\frac{t}{^\circ\text{C}}$	$\frac{p}{\text{bar}}$	$\frac{t}{^\circ\text{C}}$	$\frac{p}{\text{bar}}$	$\frac{t}{^\circ\text{C}}$	$\frac{p}{\text{bar}}$
-70	(3.E-5)	0	0.019	75	0.646	150	5.097	225	20.312
-65	(6.E-5)	5	0.026	80	0.766	155	5.679	230	21.963
-60	(1.E-4)	10	0.035	85	0.904	160	6.310	235	23.722
-55	(2.E-4)	15	0.046	90	1.060	165	6.992	240	25.595
		20	0.061	95	1.236	170	7.728	245	27.592
-50	(3.E-4)	25	0.079	100	1.435	175	8.522	250	29.724
-45	(6.E-4)	30	0.101	105	1.659	180	9.376	255	32.011
-40	(9.E-4)	35	0.129	110	1.908	185	10.292		
-35	(0.001)	40	0.162	115	2.186	190	11.275		
-30	(0.002)	45	0.202	120	2.493	195	12.327		
-25	(0.003)	50	0.250	125	2.833	200	13.452		
-20	(0.005)	55	0.306	130	3.208	205	14.654		
-15	(0.007)	60	0.373	135	3.619	210	15.936		
-10	(0.010)	65	0.451	140	4.069	215	17.304		
-5	(0.014)	70	0.541	145	4.561	220	18.760		

The following Sources give vapour pressure and/or critical point data for this compound. Those Sources used to derive the critical properties and coefficients of the vapour pressure equation are shown in bold type together with the pressure range (low 'L', medium 'M', normal boiling point only 'N', high 'H' or critical 'C') of the data. An asterisk (*) indicates that the Source is not a primary source of experimental data for this compound.

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

CAS Reg. No. 105-46-4

Mol. Wt. 116.16

Vapour Pressure $\ln p = \ln p_c + (N_1 \tau + N_2 \tau^{1.5} + N_3 \tau^{2.5} + N_4 \tau^5)/(T/T_c)$

where T is the kelvin temperature on the International Temperature Scale of 1990 (ITS-90), p is the vapour pressure, T_c , p_c are the critical temperature and the critical pressure respectively and $\tau = 1 - T/T_c$.

Critical Temperature $T_c = 563. \text{ K}$ ($t_c = 289.85^\circ\text{C}$)
 Critical Pressure $p_c = 3200. \text{ kPa}$ ($p_c = 31.58 \text{ atm}$)

$N_1 = -8.00866$ $N_2 = 2.08499$ $N_3 = -3.38007$ $N_4 = -3.76941$

Acentric Factor $\omega = 0.387$
 Normal Boiling Point $T_b = 385.113 \text{ K}$ ($t_b = 111.963^\circ\text{C}$)
 dT/dp at T_b , t_b $= 0.334 \text{ K/kPa}$ ($= 0.0445^\circ\text{C/mmHg}$)
 Melting Point $T_m = -$ ($t_m = -$)

Data at Specified Pressures

p/kPa	0.001	0.01	0.1	1	10	101.325	1000	3200.
T/K	(206.274)	(225.232)	(248.971)	(279.849)	(322.175)	385.113	(486.624)	(563.000)
$(dp/dT)/(\text{kPa/K})$	(0.000)	(0.001)	(0.009)	(0.065)	(0.457)	2.997	(17.361)	(45.526)
Data Quality				(C)	(C)	B	(C)	(C)
Uncert. in T (K)				(0.2)	(0.2)	0.2	(2.)	(5.)
Uncert. in p (kPa)				(0.02)	(0.1)	0.5	(50.)	(200.)
Uncert. in p (%)				(2.)	(1.)	0.5	(5.)	(10.)

Vapour Pressure of 1-Methylpropyl ethanoate

Units: kPa v. K

Uncertainty in				Uncertainty in				Uncertainty in			
T	p	T	p	T	p	T	p	T	p	T	p
K	kPa	K	%	K	kPa	K	%	K	kPa	K	%
175	(6.E-6)			300	(3.306)	0.2	1	425	(289.46)	0.5	1
180	(2.E-5)			305	(4.318)	0.2	1	430	(324.92)	0.5	2
185	(4.E-5)			310	(5.579)	0.2	1	435	(363.61)	1	2
190	(9.E-5)			315	(7.138)	0.2	1	440	(405.72)	1	2
195	(2.E-4)			320	(9.046)	0.2	1	445	(451.44)	1	2
200	(4.E-4)			325	(11.363)	0.2	1	450	(500.97)	1	2
205	(8.E-4)			330	(14.152)	0.2	1	455	(554.51)	1	2
210	(0.002)			335	(17.486)	0.2	1	460	(612.27)	2	2
215	(0.003)			340	(21.441)	0.2	1	465	(674.47)	2	2
220	(0.006)			345	(26.102)	0.2	1	470	(741.32)	2	5
225	(0.010)			350	(31.559)	0.2	0.5	475	(813.05)	2	5
230	(0.017)			355	(37.908)	0.2	0.5	480	(889.90)	2	5
235	(0.028)			360	(45.254)	0.2	0.5	485	(972.11)	2	5
240	(0.045)			365	(53.706)	0.2	0.5	490	(1059.9)	2	5
245	(0.071)			370	(63.380)	0.2	0.5	495	(1153.6)	2	5
250	(0.109)			375	(74.399)	0.2	0.5	500	(1253.5)	2	5
255	(0.165)			380	(86.890)	0.2	0.5	505	(1359.8)	5	5
260	(0.246)			385	100.99	0.2	0.5	510	(1472.8)	5	5
265	(0.359)			390	(116.83)	0.2	0.5	515	(1593.0)	5	5
270	(0.514)			395	(134.57)	0.2	0.5	520	(1720.5)	5	5
275	(0.726)			400	(154.34)	0.2	1	525	(1855.9)	5	5
280	(1.010)	0.2	2	405	(176.32)	0.2	1	530	(1999.6)	5	5
285	(1.385)	0.2	2	410	(200.65)	0.5	1	535	(2152.0)	5	10
290	(1.874)	0.2	2	415	(227.50)	0.5	1	540	(2313.6)	5	10
295	(2.504)	0.2	2	420	(257.05)	0.5	1	545	(2485.1)	5	10

Vapour Pressure of 1-Methylpropyl ethanoate continued

Units: bar v. °C									
t °C	p bar	t °C	p bar	t °C	p bar	t °C	p bar	t °C	p bar
-95	(1.E-7)	-25	(9.E-4)	50	(0.105)	125	(1.468)	200	(7.859)
-90	(3.E-7)	-20	(0.001)	55	(0.131)	130	(1.679)	205	(8.609)
-85	(7.E-7)	-15	(0.002)	60	(0.162)	135	(1.914)	210	(9.411)
-80	(1.E-6)	-10	(0.003)	65	(0.199)	140	(2.173)	215	(10.268)
		-5	(0.005)	70	(0.243)	145	(2.458)	220	(11.183)
-75	(3.E-6)	0	(0.006)	75	(0.294)	150	(2.771)	225	(12.158)
-70	(7.E-6)	5	(0.009)	80	(0.354)	155	(3.114)	230	(13.197)
-65	(1.E-5)	10	(0.012)	85	(0.424)	160	(3.489)	235	(14.302)
-60	(2.E-5)	15	(0.017)	90	(0.504)	165	(3.897)	240	(15.477)
-55	(4.E-5)	20	(0.023)	95	(0.597)	170	(4.341)	245	(16.724)
-50	(8.E-5)	25	(0.030)	100	(0.702)	175	(4.822)	250	(18.049)
-45	(1.E-4)	30	(0.039)	105	(0.821)	180	(5.342)	255	(19.454)
-40	(2.E-4)	35	(0.051)	110	(0.956)	185	(5.904)	260	(20.945)
-35	(4.E-4)	40	(0.065)	115	(1.108)	190	(6.509)	265	(22.527)
-30	(6.E-4)	45	(0.083)	120	(1.278)	195	(7.160)	270	(24.205)

The following Sources give vapour pressure and/or critical point data for this compound. Those Sources used to derive the critical properties and coefficients of the vapour pressure equation are shown in bold type together with the pressure range (low 'L', medium 'M', normal boiling point only 'N', high 'H' or critical 'C') of the data. An asterisk (*) indicates that the Source is not a primary source of experimental data for this compound.

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The following Sources were used to estimate critical point data for this compound.

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

CAS Reg. No. 110-19-0

Mol. Wt. 116.16

Vapour Pressure $\ln p = \ln p_c + (N_1 \tau + N_2 \tau^{1.5} + N_3 \tau^{2.5} + N_4 \tau^5)/(T/T_c)$

where T is the kelvin temperature on the International Temperature Scale of 1990 (ITS-90), p is the vapour pressure, T_c , p_c are the critical temperature and the critical pressure respectively and $\tau = 1 - T/T_c$.

Critical Temperature $T_c = 565. \text{ K}$ ($t_c = 291.85^\circ\text{C}$)
 Critical Pressure $p_c = 3105. \text{ kPa}$ ($p_c = 30.64 \text{ atm}$)

$N_1 = -8.17285$ $N_2 = 2.18226$ $N_3 = -3.65232$ $N_4 = -3.90333$

Acentric Factor $\omega = 0.416$
 Normal Boiling Point $T_b = 389.950 \text{ K}$ ($t_b = 116.800^\circ\text{C}$)
 dT/dp at T_b , t_b $= 0.334 \text{ K/kPa}$ ($= 0.0445^\circ\text{C/mmHg}$)
 Melting Point $T_m = 174. \text{ K}$ ($t_m = -99.^\circ\text{C}$)

Data at Specified Pressures

p/kPa	0.001	0.01	0.1	1	10	101.325	1000	3105.
T/K	(210.349)	(229.463)	(253.368)	(284.416)	326.903	389.950	(491.343)	(565.000)
$(dp/dT)/(\text{kPa/K})$	(0.000)	(0.001)	(0.009)	(0.064)	0.456	2.995	(17.420)	(44.908)
Data Quality				(B)	B	B	(B)	(C)
Uncert. in T (K)				(0.1)	0.1	0.2	(1.)	(5.)
Uncert. in p (kPa)				(0.005)	0.05	0.5	(20.)	(200.)
Uncert. in p (%)				(0.5)	0.5	0.5	(2.)	(10.)

Vapour Pressure of 2-Methylpropyl ethanoate

Units: kPa v. K

Uncertainty				Uncertainty				Uncertainty			
T	p	T in	p	T	p	T in	p	T	p	T in	p
K	kPa	K	%	K	kPa	K	%	K	kPa	K	%
175	(3.E-6)			300	2.556	0.1	0.5	425	(258.04)	0.5	1
180	(8.E-6)			305	3.369	0.1	0.5	430	(290.57)	0.5	1
185	(2.E-5)			310	4.392	0.1	0.5	435	(326.16)	0.5	1
190	(5.E-5)			315	5.666	0.1	0.5	440	(365.00)	0.5	1
195	(1.E-4)			320	7.239	0.1	0.5	445	(407.28)	0.5	1
200	(2.E-4)			325	9.163	0.1	0.5	450	(453.20)	0.5	1
205	(5.E-4)			330	11.497	0.1	0.5	455	(502.95)	0.5	1
210	(0.001)			335	14.305	0.1	0.5	460	(556.75)	0.5	1
215	(0.002)			340	17.659	0.1	0.5	465	(614.80)	1	1
220	(0.003)			345	21.636	0.1	0.5	470	(677.33)	1	2
225	(0.006)			350	26.320	0.1	0.5	475	(744.55)	1	2
230	(0.011)			355	31.801	0.1	0.5	480	(816.71)	1	2
235	(0.018)			360	38.178	0.1	0.5	485	(894.05)	1	2
240	(0.030)			365	45.552	0.1	0.5	490	(976.81)	1	2
245	(0.048)			370	54.036	0.2	0.5	495	(1065.3)	1	2
250	(0.075)			375	63.744	0.2	0.5	500	(1159.7)	1	2
255	(0.115)			380	74.800	0.2	0.5	505	(1260.4)	2	2
260	(0.173)			385	87.332	0.2	0.5	510	(1367.6)	2	2
265	(0.256)			390	101.47	0.2	0.5	515	(1481.7)	2	2
270	(0.372)			395	(117.37)	0.2	0.5	520	(1603.1)	2	5
275	(0.532)			400	(135.16)	0.2	0.5	525	(1732.1)	2	5
280	(0.749)			405	(155.00)	0.2	0.5	530	(1869.1)	2	5
285	(1.038)	0.1	0.5	410	(177.04)	0.2	0.5	535	(2014.6)	2	5
290	1.420	0.1	0.5	415	(201.45)	0.2	1	540	(2169.1)	5	5
295	1.917	0.1	0.5	420	(228.40)	0.2	1	545	(2333.3)	5	5

Vapour Pressure of 2-Methylpropyl ethanoate continued

Units: bar v. °C									
t °C	p bar	t °C	p bar	t °C	p bar	t °C	p bar	t °C	p bar
-95	(5.E-8)	-25	(6.E-4)	50	0.084	125	(1.283)	200	(7.191)
-90	(1.E-7)	-20	(0.001)	55	0.106	130	(1.474)	205	(7.894)
-85	(3.E-7)	-15	(0.001)	60	0.132	135	(1.686)	210	(8.648)
-80	(8.E-7)	-10	(0.002)	65	0.163	140	(1.921)	215	(9.455)
		-5	(0.003)	70	0.201	145	(2.181)	220	(10.319)
-75	(2.E-6)	0	(0.005)	75	0.245	150	(2.467)	225	(11.240)
-70	(4.E-6)	5	(0.007)	80	0.297	155	(2.782)	230	(12.224)
-65	(7.E-6)	10	(0.009)	85	0.357	160	(3.126)	235	(13.271)
-60	(1.E-5)	15	0.013	90	0.427	165	(3.502)	240	(14.387)
-55	(3.E-5)	20	0.017	95	0.508	170	(3.912)	245	(15.573)
-50	(5.E-5)	25	0.023	100	0.600	175	(4.358)	250	(16.834)
-45	(9.E-5)	30	0.030	105	0.705	180	(4.841)	255	(18.174)
-40	(1.E-4)	35	0.040	110	0.825	185	(5.364)	260	(19.597)
-35	(2.E-4)	40	0.052	115	0.960	190	(5.928)	265	(21.109)
-30	(4.E-4)	45	0.066	120	(1.113)	195	(6.537)	270	(22.714)

The following Sources give vapour pressure and/or critical point data for this compound. Those Sources used to derive the critical properties and coefficients of the vapour pressure equation are shown in bold type together with the pressure range (low 'L', medium 'M', normal boiling point only 'N', high 'H' or critical 'C') of the data. An asterisk (*) indicates that the Source is not a primary source of experimental data for this compound.

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The following Sources were used to estimate critical point data for this compound.

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 AMBROSE, D., NPL Report Chem 98, Nat.Phys.Lab., Teddington, UK, 1979.*

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

CAS Reg. No. 540-88-5

Mol. Wt. 116.16

Vapour Pressure $\ln p = \ln p_c + (N_1 \tau + N_2 \tau^{1.5} + N_3 \tau^{2.5} + N_4 \tau^5)/(T/T_c)$

where T is the kelvin temperature on the International Temperature Scale of 1990 (ITS-90), p is the vapour pressure, T_c , p_c are the critical temperature and the critical pressure respectively and $\tau = 1 - T/T_c$.

Critical Temperature $T_c = 545. \text{ K}$ ($t_c = 271.85^\circ\text{C}$)
 Critical Pressure $p_c = 3270. \text{ kPa}$ ($p_c = 32.27 \text{ atm}$)

$N_1 = -7.94169$ $N_2 = 2.04584$ $N_3 = -3.26950$ $N_4 = -3.71239$

Acentric Factor $\omega = 0.375$
 Normal Boiling Point $T_b = 371.099 \text{ K}$ ($t_b = 97.949^\circ\text{C}$)
 dT/dp at T_b , t_b $= 0.323 \text{ K/kPa}$ ($= 0.0430^\circ\text{C/mmHg}$)
 Melting Point $T_m = -$ ($t_m = -$)

Data at Specified Pressures

p/kPa	0.001	0.01	0.1	1	10	101.325	1000	3270.
T/K	(198.265)	(216.565)	(239.490)	(269.321)	310.233	371.099	(469.343)	(545.000)
$(dp/dT)/(\text{kPa/K})$	(0.000)	(0.001)	(0.009)	(0.067)	0.473	3.098	(17.925)	(47.650)
Data Quality				(B)	B	B	(B)	(C)
Uncert. in T (K)				(0.05)	0.1	0.2	(1.)	(5.)
Uncert. in p (kPa)				(0.005)	0.05	0.5	(20.)	(200.)
Uncert. in p (%)				(0.5)	0.5	0.5	(2.)	(10.)

Vapour Pressure of 1,1-Dimethylethyl ethanoate

Units: kPa v. K

		Uncertainty		Units: kPa v. K				Uncertainty					
T	p	T	p	T	p	T	p	T	p	T	p	T	p
K	kPa	K	%	K	kPa	K	%	K	kPa	K	%	K	%
175	(2.E-5)			300	6.040	0.1	0.5	425	(412.98)	0.5	1		
180	(6.E-5)			305	7.768	0.1	0.5	430	(460.92)	0.5	1		
185	(1.E-4)			310	9.890	0.1	0.5	435	(512.96)	0.5	1		
190	(3.E-4)			315	12.476	0.1	0.5	440	(569.33)	0.5	1		
195	(6.E-4)			320	15.598	0.1	0.5	445	(630.26)	1	2		
200	(0.001)			325	19.340	0.1	0.5	450	(695.99)	1	2		
205	(0.002)			330	23.789	0.1	0.5	455	(766.75)	1	2		
210	(0.005)			335	29.042	0.1	0.5	460	(842.81)	1	2		
215	(0.008)			340	35.203	0.1	0.5	465	(924.41)	1	2		
220	(0.015)			345	42.383	0.1	0.5	470	(1011.8)	1	2		
225	(0.025)			350	50.701	0.1	0.5	475	(1105.3)	1	2		
230	(0.041)			355	60.281	0.1	0.5	480	(1205.3)	1	2		
235	(0.066)			360	71.259	0.2	0.5	485	(1311.9)	2	2		
240	(0.105)			365	83.771	0.2	0.5	490	(1425.5)	2	2		
245	(0.161)			370	97.966	0.2	0.5	495	(1546.5)	2	5		
250	(0.243)			375	(113.99)	0.2	0.5	500	(1675.2)	2	5		
255	(0.359)			380	(132.02)	0.2	0.5	505	(1812.1)	2	5		
260	(0.522)			385	(152.20)	0.2	0.5	510	(1957.6)	2	5		
265	(0.745)			390	(174.71)	0.2	0.5	515	(2112.1)	5	5		
270	(1.046)	0.1	0.5	395	(199.72)	0.2	1	520	(2276.2)	5	5		
275	1.448	0.1	0.5	400	(227.43)	0.2	1	525	(2450.5)	5	5		
280	1.976	0.1	0.5	405	(258.00)	0.5	1	530	(2635.9)	5	5		
285	2.660	0.1	0.5	410	(291.65)	0.5	1	535	(2833.1)	5	10		
290	3.537	0.1	0.5	415	(328.55)	0.5	1	540	(3043.6)	5	10		
295	4.648	0.1	0.5	420	(368.93)	0.5	1	545	(3270.0)	5	10		

Vapour Pressure of 1,1-Dimethylethyl ethanoate continued

Units: bar v. °C					
t °C	p bar	t °C	p bar	t °C	p bar
-95	(4.E-7)	-25	(0.002)	50	0.179
-90	(1.E-6)	-20	(0.003)	55	0.221
-85	(2.E-6)	-15	(0.005)	60	0.270
-80	(5.E-6)	-10	(0.007)	65	0.328
		-5	(0.009)	70	0.396
-75	(1.E-5)	0	0.013	75	0.475
-70	(2.E-5)	5	0.018	80	0.566
-65	(4.E-5)	10	0.024	85	0.670
-60	(7.E-5)	15	0.032	90	0.790
-55	(1.E-4)	20	0.042	95	0.925
-50	(2.E-4)	25	0.055	100	(1.078)
-45	(3.E-4)	30	0.071	105	(1.251)
-40	(6.E-4)	35	0.091	110	(1.445)
-35	(9.E-4)	40	0.115	115	(1.661)
-30	(0.001)	45	0.144	120	(1.902)
				125	(2.169)
				130	(2.463)
				135	(2.788)
				140	(3.145)
				145	(3.536)
				150	(3.962)
				155	(4.427)
				160	(4.932)
				165	(5.480)
				170	(6.072)
				200	(10.700)
				205	(11.675)
				210	(12.716)
				215	(13.826)
				220	(15.008)
				225	(16.267)
				230	(17.605)
				235	(19.027)
				240	(20.538)
				245	(22.143)
				250	(23.848)
				255	(25.660)
				260	(27.587)
				265	(29.641)
				270	(31.840)

The following Sources give vapour pressure and/or critical point data for this compound. Those Sources used to derive the critical properties and coefficients of the vapour pressure equation are shown in bold type together with the pressure range (low 'L', medium 'M', normal boiling point only 'N', high 'H' or critical 'C') of the data. An asterisk (*) indicates that the Source is not a primary source of experimental data for this compound.

- 1 KAILAN,-., RAFF,-., *Monatsh.Chem.*, Vol.61, p.116, 1932.
- 2 HOUTMAN,-., STEENIS,-., et al., *Rec.Trav.Chim.*, Vol.65, p.781, 1946.
- 3 VOGEL,A.I., *J.Chem.Soc.*, p.624, 1948.
- 4 MOSHER,-., KEHR,-., *J.Am.Chem.Soc.*, Vol.75, p.3172, 1953.
- 5 WOLL,W., **Unpublished work at BASF AG, Ludwigshafen, Germany. Priv.Com. 1996. M**
- 6 TRC Thermodynamic Tables, Texas A & M Univ., Loose leaf data sheets extant 1996.*

The following Sources were used to estimate critical point data for this compound.

- AMBROSE,D., NPL Report Chem 92, Nat.Phys.Lab., Teddington, UK, 1978.*
 AMBROSE,D., NPL Report Chem 98, Nat.Phys.Lab., Teddington, UK, 1979.*

**C₇H₁₄O₂ 3-Methylbutyl ethanoate; Isopentyl acetate**

CAS Reg. No. 123-92-2

Mol. Wt. 130.19

Vapour Pressure $\ln p = \ln p_c + (N_1 \tau + N_2 \tau^{1.5} + N_3 \tau^{2.5} + N_4 \tau^5)/(T/T_c)$

where T is the kelvin temperature on the International Temperature Scale of 1990 (ITS-90), p is the vapour pressure, T_c , p_c are the critical temperature and the critical pressure respectively and $\tau = 1 - T/T_c$.

Critical Temperature $T_c = 592. \text{ K}$ ($t_c = 318.85^\circ\text{C}$)
 Critical Pressure $p_c = 2850. \text{ kPa}$ ($p_c = 28.13 \text{ atm}$)

$N_1 = -8.28354$ $N_2 = 2.24887$ $N_3 = -3.83681$ $N_4 = -3.98896$

Acentric Factor $\omega = 0.436$
 Normal Boiling Point $T_b = 413.302 \text{ K}$ ($t_b = 140.152^\circ\text{C}$)
 dT/dp at T_b , t_b $= 0.354 \text{ K/kPa}$ ($= 0.0472^\circ\text{C/mmHg}$)
 Melting Point $T_m = 195. \text{ K}$ ($t_m = -78.^\circ\text{C}$)

Data at Specified Pressures								
p/kPa	0.001	0.01	0.1	1	10	101.325	1000	2850.
T/K	(223.211)	(243.418)	(268.694)	(301.533)	346.500	413.302	(520.831)	(592.000)
$(dp/dT)/(\text{kPa/K})$	(0.000)	(0.001)	(0.008)	(0.061)	0.430	2.825	(16.445)	(39.884)
Data Quality				(C)	C	C	(C)	(C)
Uncert. in T (K)				(0.2)	0.2	0.5	(2.)	(5.)
Uncert. in p (kPa)				(0.02)	0.1	2.	(50.)	(200.)
Uncert. in p (%)				(2.)	1.	2.	(5.)	(10.)

Vapour Pressure of 3-Methylbutyl ethanoate

Units: kPa v. K

		Uncertainty		Units: kPa v. K				Uncertainty					
		in		Uncertainty				in					
T	p	T	p	T	p	T	p	T	p	T	p	T	p
K	kPa	K	%	K	kPa	K	%	K	kPa	K	%	K	%
200	(4.E-5)			325	3.670	0.2	1	450	(255.27)	1	2		
205	(8.E-5)			330	4.701	0.2	1	455	(285.60)	1	2		
210	(2.E-4)			335	5.968	0.2	1	460	(318.63)	1	2		
215	(3.E-4)			340	7.509	0.2	1	465	(354.51)	2	2		
220	(7.E-4)			345	9.372	0.2	1	470	(393.40)	2	2		
225	(0.001)			350	11.604	0.2	1	475	(435.47)	2	5		
230	(0.002)			355	14.263	0.2	1	480	(480.88)	2	5		
235	(0.004)			360	17.406	0.2	1	485	(529.81)	2	5		
240	(0.007)			365	21.099	0.2	1	490	(582.43)	2	5		
245	(0.012)			370	25.413	0.5	1	495	(638.93)	2	5		
250	(0.019)			375	30.422	0.5	1	500	(699.49)	2	5		
255	(0.031)			380	36.206	0.5	1	505	(764.31)	2	5		
260	(0.048)			385	42.851	0.5	2	510	(833.59)	2	5		
265	(0.074)			390	50.447	0.5	2	515	(907.55)	2	5		
270	(0.111)			395	59.090	0.5	2	520	(986.40)	2	5		
275	(0.164)			400	68.881	0.5	2	525	(1070.4)	2	5		
280	(0.238)			405	79.924	0.5	2	530	(1159.7)	2	5		
285	(0.340)			410	92.329	0.5	2	535	(1254.7)	5	5		
290	(0.479)			415	(106.21)	0.5	2	540	(1355.5)	5	5		
295	(0.665)			420	(121.69)	1	2	545	(1462.6)	5	5		
300	(0.911)			425	(138.89)	1	2	550	(1576.1)	5	5		
305	(1.231)	0.2	2	430	(157.93)	1	2	555	(1696.5)	5	5		
310	(1.644)	0.2	2	435	(178.95)	1	2	560	(1824.1)	5	5		
315	2.172	0.2	2	440	(202.09)	1	2	565	(1959.4)	5	5		
320	2.838	0.2	1	445	(227.48)	1	2	570	(2102.8)	5	10		