

94001

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Vapour pressures and critical points of liquids

Polycyclic phenyl and cyclohexyl compounds

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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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Dr K.N.Marsh*	— Thermodynamics Research Center, USA
Mrs K.M.deReuck	— Imperial College of Science, Technology and Medicine
Mr J.T.R.Watson	— National Engineering Laboratory.

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

Mr J.Walton	— Independent.
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in consultation with Dr D.Ambrose.

The person with overall responsibility for the work in this subject area is Mr S.J.Pugh, Head of Thermofluids Group.

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)

* Corresponding Member
† Emeritus Member

VAPOUR PRESSURES AND CRITICAL POINTS OF LIQUIDS

POLYCYCLIC PHENYL AND CYCLOHEXYL COMPOUNDS

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COMPOUND TABLES in the following order

Sheet	Formula	Name	Alternative Names
1.00	C ₁₂ H ₁₀	Biphenyl	*Diphenyl
1.10	C ₁₃ H ₁₂	Diphenylmethane	Benzylbenzene
1.11a	C ₁₃ H ₁₂	2-Methylbiphenyl	2-Phenyltoluene
1.11b	C ₁₃ H ₁₂	3-Methylbiphenyl	3-Phenyltoluene
1.11c	C ₁₃ H ₁₂	4-Methylbiphenyl	4-Phenyltoluene
1.20a	C ₁₄ H ₁₄	1,1-Diphenylethane	Bibenzyl
1.20b	C ₁₄ H ₁₄	1,2-Diphenylethane	
1.30a	C ₁₅ H ₁₆	1,1-Diphenylpropane	Dibenzylmethane
1.30b	C ₁₅ H ₁₆	1,2-Diphenylpropane	
1.30c	C ₁₅ H ₁₆	1,3-Diphenylpropane	
1.30d	C ₁₅ H ₁₆	2,2-Diphenylpropane	
2.00	C ₁₂ H ₁₆	Phenylcyclohexane	Cyclohexylbenzene
2.10	C ₁₂ H ₂₂	Bicyclohexyl	*Dicyclohexyl
3.00a	C ₁₈ H ₁₄	o-Terphenyl	1,2-Diphenylbenzene
3.00b	C ₁₈ H ₁₄	m-Terphenyl	1,3-Diphenylbenzene
3.00c	C ₁₈ H ₁₄	p-Terphenyl	1,4-Diphenylbenzene
5.10	C ₁₂ H ₁₁ N	Diphenylamine	N,N-Diphenylamine
5.15	C ₁₂ H ₂₃ N	Dicyclohexylamine	
5.21	C ₁₃ H ₁₄ N ₂	4,4'-Diaminodiphenylmethane	4,4'-Methylenedianiline
6.10	C ₁₂ H ₁₀ O	Diphenyl ether	
6.15	C ₁₃ H ₁₀ O	Benzophenone	Diphenyl ketone

* These names are not in accordance with current usage.

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

VAPOUR PRESSURES AND CRITICAL POINTS OF LIQUIDS
POLYCYCLIC PHENYL AND CYCLOHEXYL COMPOUNDS

1. INTRODUCTION

This Data Item presents saturated vapour pressures of the polycyclic phenyl and cyclohexyl compounds shown in the order of arrangement on the Contents page.

Table 1, page 5, gives the constants in 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 numerical values of 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 rounded to the nearest kelvin and that values in other units are obtained by exact conversion.

The Sheets also give the acentric factor, the normal boiling point, the value of dT/dp at the normal boiling point and the approximate normal melting point. Brackets enclose data at those temperatures which are 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'. Except at very low pressures, 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 mmHg or atm at temperatures in degrees C. The table providing pressures in kPa also gives the uncertainties in pressure and temperature. Where justified, pressures are given at temperatures from just above the melting point to just below the critical point. To make maximum use of the space available, a larger temperature interval is frequently used at low temperatures. For compounds with very high estimated critical temperatures the tables are usually truncated at a convenient temperature somewhat less than the critical value. For compounds for which the available data are low in extent or quality the tabulated values are terminated at a few atmospheres pressure.

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
q	$(1-T/T_c)$
T	kelvin temperature
t	Celsius temperature ($T-273.15$)

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

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.

Low pressure range measurements have been made on two of the compounds considered here. Medium pressure range measurements have been made on eleven other compounds and for six of these critical temperatures and critical pressures have been reported. For each of the remaining compounds the available data are usually a small number of scattered points, mostly in the medium pressure range, each reported by a different author or authors.

4. EVALUATION AND CORRELATION

In References 4 and 5 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 6 Ambrose and Walton have demonstrated this phenomenon for the two homologous series of normal alkanes and alkan-1-ols. 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.

In Reference 3 Ambrose and Davies have shown how very low vapour pressures may be obtained from the differences between the ideal gas heat capacity and the liquid heat capacity at various temperatures. The procedure involves two integrations; rigorous treatment also requires the liquid molar volume and the second virial coefficient of the vapour. Low range vapour pressures obtained in this way were included in the data used to derive the vapour-pressure equations of nearly all of the alkanes in Reference 6 but, in general, were not available for the alkanols.

In Reference 7 Watson, reversing the procedure, derived the difference between the ideal gas and liquid heat capacities from the the second differential of the Wagner vapour-pressure equation. He plotted this difference against reduced temperature from the melting point to the normal boiling point for all the alkanes and alkanols in Reference 7. Although only valid up to reduced temperatures of about 0.5 these were shown to be a well ordered, uniformly varying set of curves for both series. Denoting the differences between the ideal gas and liquid heat capacities at reduced temperatures of 0.3 and 0.5 by, say, 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.

The equations for the alkanes were used to derive a correlation which was similar in form to that described in Items 84022, 84028 and 85002. As the data for the compounds considered here were either not sufficiently precise or extensive enough to be fitted without constraint their vapour pressure equations were then obtained by using this correlation to fit their data.

For most of the compounds considered here saturated liquid density data were available, see Item 94002, and for most compounds the critical temperature and pressure were adjusted until they were optimum values for the correlation of both properties.

5. 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 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.

The uncertainties in temperature and pressure are not thought to be more than the values shown below each letter. However when the data quality is 'C' it will be appreciated that the uncertainties are necessarily rather speculative and that for some compounds they may be underestimated. If the data quality is 'C' at the critical pressure the values of critical temperature and critical pressure given in the Tables should be regarded only as correlating parameters. Furthermore, 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.

6. ANTOINE EQUATION

Some users may find it more convenient to use an Antoine equation for certain applications confined to limited ranges of temperature or pressure. The coefficients of the Antoine equation given at the end of each sheet have been obtained by fitting this equation to values obtained from the Wagner equation between pressures of 2 and 200 kPa. The RMS deviation of each fit is usually less than 0.05 per cent.

WARNING. Although, for most compounds, the Antoine equation may be used in the range 5 to 500 kPa without undue error, use at pressures outside this range will give vapour pressures that get progressively lower than the values given by the Wagner equation.

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TABLE 1

Summary of Constants in the Wagner vapour pressure equation

$$\ln p = \ln p_c + (N_1q + N_2q^{1.5} + N_3q^{2.5} + N_4q^5)/(T/T_c) \quad \text{where } q = 1 - T/T_c$$

Sheet	Name	T _c K	P _c kPa	N ₁	N ₂	N ₃	N ₄
1.00	Biphenyl	770	3250	-8.12827	2.15110	-3.5004	-3.561
1.10	Diphenylmethane	770	2860	-8.32556	2.24790	-3.7700	-3.907
1.11a	2-Methylbiphenyl	755	2800	-8.37003	2.26972	-3.8307	-3.985
1.11b	3-Methylbiphenyl	767	2750	-8.66565	2.48947	-4.3841	-3.968
1.11c	4-Methylbiphenyl	764	2700	-8.69185	2.50713	-4.4286	-3.986
1.20a	1,1-Diphenylethane	768	2550	-8.50064	2.29517	-3.9630	-4.244
1.20b	1,2-Diphenylethane	781	2550	-8.47459	2.35594	-4.0518	-3.857
1.30a	1,1-Diphenylpropane	762	2250	-8.86881	2.62914	-4.7323	-4.102
1.30b	1,2-Diphenylpropane	767	2250	-8.80777	2.58652	-4.6269	-4.063
1.30c	1,3-Diphenylpropane	782	2250	-9.15850	2.83879	-5.2415	-4.276
1.30d	2,2-Diphenylpropane	762	2250	-8.95847	2.69273	-4.8884	-4.158
2.00	Phenylcyclohexane	737	2800	-8.11941	2.14592	-3.4863	-3.554
2.10	Bicyclohexyl	742	2600	-7.88551	2.01081	-3.0716	-3.354
3.00a	o-Terphenyl	834	2200	-9.10090	2.79614	-5.1391	-4.243
3.00b	m-Terphenyl	882	2250	-9.35600	2.98850	-5.5969	-4.383
3.00c	p-Terphenyl	904	2550	-9.31504	2.95701	-5.5226	-4.361
5.10	Diphenylamine	833	3150	-8.25120	2.22437	-3.6975	-3.661
5.15	Dicyclohexylamine	724	2300	-8.80964	2.58783	-4.6301	-4.064
5.21	4,4'-Diaminodiphenylmethane	890	2700	-10.22854	3.71097	-7.2402	-4.754
6.10	Diphenylether	766.8	3065	-8.29928	2.39051	-3.9706	-3.967
6.15	Benzophenone	823	2965	-8.63410	2.46834	-4.3307	-3.946

C₁₂H₁₀ Biphenyl (*Diphenyl)

CAS Reg. No. 92-52-4

Mol. Wt. 154.210

Vapour Pressure $\ln p = \ln p_c + (N_1q + N_2q^{1.5} + N_3q^{2.5} + N_4q^5)/(T/T_c)$

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 q = 1 - T/T_c.

Critical Temperature T_c = 770 K (t_c = 496.85 °C)
 Critical Pressure p_c = 3250 kPa (p_c = 32.08 atm)
 N₁ = -8.12827
 N₂ = 2.15110
 N₃ = -3.5004
 N₄ = -3.561

Acentric Factor = 0.406
 Normal Boiling Point = 528.150 K (= 255.000 °C)
 dT/dp at N.B.P. = 0.453 K/kPa (= 0.060 °C/mmHg)
 Normal Melting Point = 342 K (= 69 °C)

Data at Specified Pressures

p/kPa	0.001	0.01	0.1	1	10	101.325	1000	3250
T/K			342.271	384.596	442.458	528.150	665.572	770.000
(dp/dT)/(kPa/K)			0.006	0.047	0.335	2.207	12.864	34.309
Data Quality			C	C	C	B	B	C
Uncert. in T (K)			1	0.5	0.2	0.2	2	10
Uncert. in p (kPa)			0.005	0.02	0.1	0.5	20	200
Uncert. in p (%)			5	2	1	0.5	2	10

Vapour Pressure of Biphenyl

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	%
350	0.160	0.5	5	475	27.17	0.2	1	600	389.4	0.5	1
355	0.214	0.5	5	480	31.22	0.2	0.5	605	421.8	1	1
360	0.284	0.5	2	485	35.75	0.2	0.5	610	456.2	1	1
365	0.373	0.5	2	490	40.80	0.2	0.5	615	492.7	1	1
370	0.486	0.5	2	495	46.42	0.2	0.5	620	531.4	1	1
375	0.627	0.5	2	500	52.64	0.2	0.5	625	572.4	1	1
380	0.802	0.5	2	505	59.51	0.2	0.5	630	615.7	1	1
385	1.019	0.5	2	510	67.09	0.2	0.5	635	661.5	1	2
390	1.285	0.5	2	515	75.43	0.2	0.5	640	709.8	1	2
395	1.608	0.5	2	520	84.56	0.2	0.5	645	760.7	1	2
400	2.000	0.5	2	525	94.56	0.2	0.5	650	814.4	1	2
405	2.470	0.5	2	530	105.5	0.2	0.5	655	870.9	1	2
410	3.031	0.5	1	535	117.4	0.2	0.5	660	930.3	1	2
415	3.698	0.2	1	540	130.3	0.2	0.5	665	992.7	2	2
420	4.485	0.2	1	545	144.3	0.2	0.5	670	1058.	2	2
425	5.410	0.2	1	550	159.4	0.2	0.5	675	1127.	2	2
430	6.491	0.2	1	555	175.8	0.5	0.5	680	1199.	2	2
435	7.749	0.2	1	560	193.5	0.5	0.5	685	1275.	2	2
440	9.205	0.2	1	565	212.5	0.5	1	690	1354.	2	2
445	10.88	0.2	1	570	232.9	0.5	1	695	1437.	2	2
450	12.81	0.2	1	575	254.9	0.5	1	700	1524.	2	2
455	15.01	0.2	1	580	278.3	0.5	1	705	1614.	2	5
460	17.51	0.2	1	585	303.5	0.5	1	710	1709.	5	5
465	20.35	0.2	1	590	330.3	0.5	1	715	1808.	5	5
470	23.56	0.2	1	595	358.9	0.5	1	720	1912.	5	5

Vapour Pressure of Biphenyl continued

Units: atm or mmHg v. °C

t °C	p mmHg	t °C	p mmHg	t °C	p atm	t °C	p atm	t °C	p atm
75	1.076	175	90.49	275	1.517	375	7.838	475	25.55
80	1.445	180	106.2	280	1.674	380	8.385	480	26.93
85	1.923	185	124.1	285	1.844	385	8.961	485	28.36
90	2.534	190	144.5	290	2.026	390	9.565	490	29.87
95	3.308	195	167.5	295	2.223	395	10.20	495	31.46
100	4.283	200	193.4	300	2.433	400	10.87		
105	5.499	205	222.5	305	2.659	405	11.57		
110	7.004	210	255.1	310	2.901	410	12.30		
115	8.854	215	291.5	315	3.160	415	13.07		
120	11.11	220	332.1	320	3.435	420	13.87		
125	13.85	225	377.0	325	3.729	425	14.72		
130	17.14	230	426.7	330	4.042	430	15.60		
135	21.09	235	481.6	335	4.374	435	16.52		
140	25.79	240	541.9	340	4.727	440	17.48		
145	31.34	245	608.2	345	5.101	445	18.49		
150	37.88	250	680.7	350	5.497	450	19.54		
155	45.54	255	760.0	355	5.916	455	20.64		
160	54.47	260	846.4	360	6.358	460	21.79		
165	64.82	265	940.4	365	6.826	465	22.99		
170	76.76	270	1042.	370	7.319	470	24.24		

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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Antoine equation: $\ln(p/\text{kPa}) = 14.24768 - 4256.771/(T/K - 86.087)$ for $2 < p/\text{kPa} < 200$.

C₁₃H₁₂ Diphenylmethane (Benzylbenzene)

CAS Reg. No. 101-81-5

Mol. Wt. 168.240

Vapour Pressure $\ln p = \ln p_c + (N_1q + N_2q^{1.5} + N_3q^{2.5} + N_4q^5)/(T/T_c)$

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 $q = 1 - T/T_c$.

Critical Temperature	T = 770 K	(t _c = 496.85 °C)
Critical Pressure	p _c = 2860 kPa	(p _c = 28.23 atm)
	N ₁ = -8.32556	
	N ₂ = 2.24790	
	N ₃ = -3.7700	
	N ₄ = -3.907	

Acentric Factor	= 0.442	
Normal Boiling Point	= 538.029 K	(= 264.879 °C)
dT/dp at N.B.P.	= 0.460 K/kPa	(= 0.061 °C/mmHg)
Normal Melting Point	= 298 K	(= 25 °C)

Data at Specified Pressures

p/kPa	0.001	0.01	0.1	1	10	101.325	1000	2860
T/K		316.614	349.592	392.431	451.057	538.029	677.582	770.000
(dp/dT)/(kPa/K)		8.E-4	0.006	0.047	0.330	2.172	12.698	30.927
Data Quality		C	C	C	C	C	C	C
Uncert. in T (K)		1	1	0.5	0.2	0.5	5	10
Uncert. in p (kPa)		0.001	0.005	0.02	0.1	1	50	200
Uncert. in p (%)		10	5	2	1	1	5	10

Vapour Pressure of Diphenylmethane

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	%
300	0.002			525	75.99	0.5	1	650	693.8	2	5
310	0.006			530	85.03	0.5	1	655	743.1	2	5
320	0.013	1	10	535	94.91	0.5	1	660	795.0	2	5
330	0.027	1	5	540	105.7	0.5	1	665	849.7	2	5
340	0.054	1	5	545	117.4	0.5	1	670	907.2	5	5
350	0.103	1	5	550	130.1	0.5	1	675	967.6	5	5
360	0.186	0.5	5	555	143.9	0.5	1	680	1031.	5	5
370	0.325	0.5	2	560	158.7	0.5	1	685	1098.	5	5
380	0.547	0.5	2	565	174.8	1	1	690	1167.	5	5
390	0.892	0.5	2	570	192.1	1	2	695	1241.	5	5
400	1.411	0.5	2	575	210.7	1	2	700	1317.	5	5
410	2.172	0.5	2	580	230.7	1	2	705	1398.	5	5
420	3.260	0.5	1	585	252.1	1	2	710	1482.	5	5
430	4.781	0.2	1	590	275.0	1	2	715	1570.	5	5
440	6.862	0.2	1	595	299.4	1	2	720	1662.	5	5
450	9.656	0.2	1	600	325.5	1	2	725	1759.	5	5
460	13.34	0.2	1	605	353.4	1	2	730	1859.	5	5
470	18.13	0.2	1	610	383.0	2	2	735	1965.	5	5
480	24.24	0.5	1	615	414.5	2	2	740	2075.	5	10
490	31.95	0.5	1	620	447.9	2	2	745	2191.	5	10
Interval change											
500	41.55	0.5	1	625	483.4	2	2	750	2312.	10	10
505	47.16	0.5	1	630	520.9	2	2	755	2439.	10	10
510	53.36	0.5	1	635	560.6	2	2	760	2572.	10	10
515	60.20	0.5	1	640	602.6	2	5	765	2712.	10	10
520	67.73	0.5	1	645	647.0	2	5	770	2860.	10	10

Vapour Pressure of Diphenylmethane continued

Units: atm or mmHg v. °C

t °C	p mmHg	t °C	p mmHg	t °C	p mmHg	t °C	p atm	t °C	p atm
25	0.016	125	9.745	200	149.2	300	2.010	400	9.326
30	0.025	130	12.16	205	172.5	305	2.202	405	9.941
35	0.038	135	15.07	210	198.7	310	2.408	410	10.59
40	0.057	140	18.57	215	228.0	315	2.628	415	11.26
45	0.085	145	22.73	220	260.7	320	2.864	420	11.97
50	0.124	150	27.65	225	297.2	325	3.116	425	12.72
55	0.179	155	33.46	230	337.7	330	3.384	430	13.50
60	0.255	160	40.27	235	382.5	335	3.670	435	14.31
65	0.359	165	48.21	240	432.0	340	3.973	440	15.17
70	0.499	170	57.43	245	486.5	345	4.296	445	16.06
75	0.686	175	68.09	250	546.4	350	4.638	450	17.00
80	0.932	180	80.34	255	612.0	355	5.001	455	17.98
85	1.254	185	94.38	260	683.7	360	5.385	460	19.00
90	1.671	190	110.4	265	762.0	365	5.791	465	20.07
95	2.205	195	128.6	270	847.1	370	6.220	470	21.19
100	2.883			275	939.6	375	6.673	475	22.37
105	3.737			280	1040.	380	7.151	480	23.60
110	4.804			285	1148.	385	7.654	485	24.89
115	6.127			290	1265.	390	8.183	490	26.24
120	7.756			295	1392.	395	8.740	495	27.67

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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Antoine equation: $\ln(p/\text{kPa}) = 14.21947 - 4297.566/(T/K - 90.419)$ for $2 < p/\text{kPa} < 200$.

C₁₃H₁₂ 2-Methylbiphenyl (2-Phenyltoluene)

CAS Reg. No. 643-58-3

Mol. Wt. 168.240

Vapour Pressure $\ln p = \ln p_c + (N_1q + N_2q^{1.5} + N_3q^{2.5} + N_4q^5)/(T/T_c)$

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 q = 1 - T/T_c.

Critical Temperature	T _c = 755 K	(t _c = 481.85 °C)
Critical Pressure	p _c = 2800 kPa	(p _c = 27.63 atm)
	N ₁ = -8.37003	
	N ₂ = 2.26972	
	N ₃ = -3.8307	
	N ₄ = -3.985	

Acentric Factor	= 0.450	
Normal Boiling Point	= 529.366 K	(= 256.216 °C)
dT/dp at N.B.P.	= 0.452 K/kPa	(= 0.060 °C/mmHg)
Normal Melting Point	= 273 K	(= 0 °C)

Data at Specified Pressures

p/kPa	0.001	0.01	0.1	1	10	101.325	1000	2800
T/K	(285.957)	(311.858)	344.252	386.332	(443.922)	(529.366)	(666.431)	(755.000)
(dp/dT)/(kPa/K)	(1.E-4)	(8.E-4)	0.006	0.047	(0.336)	(2.211)	(12.938)	(31.045)
Data Quality			C	C	(C)	(C)	(C)	(C)
Uncert. in T (K)			2	1	(0.5)	(1)	(5)	(10)
Uncert. in p (kPa)			0.01	0.05	(0.2)	(2)	(50)	(200)
Uncert. in p (%)			10	5	(2)	(2)	(5)	(10)

Vapour Pressure of 2-Methylbiphenyl

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	%
				500	(50.98)	1	2	650	(804.1)	2	5
				510	(65.12)	1	2	655	(860.3)	5	5
				520	(82.23)	1	2	660	(919.4)	5	5
280	(5.E-4)			530	(102.7)	1	2	665	(981.6)	5	5
290	(0.001)			540	(127.1)	1	2	670	(1047.)	5	5
				Interval change							
300	(0.004)			550	(155.8)	1	2	675	(1116.)	5	5
310	(0.009)			555	(171.9)	1	2	680	(1188.)	5	5
320	(0.019)			560	(189.3)	1	2	685	(1263.)	5	5
330	0.039			565	(208.0)	1	2	690	(1343.)	5	5
340	0.076			570	(228.1)	2	2	695	(1426.)	5	5
350	0.143	1	10	575	(249.8)	2	2	700	(1513.)	5	5
360	0.256	1	10	580	(272.9)	2	2	705	(1604.)	5	5
370	0.442	1	5	585	(297.7)	2	2	710	(1700.)	5	5
380	0.736	1	5	590	(324.2)	2	2	715	(1800.)	5	5
390	1.188	1	5	595	(352.5)	2	2	720	(1905.)	5	5
400	(1.861)	1	5	600	(382.6)	2	2	725	(2015.)	5	10
410	(2.839)	1	2	605	(414.6)	2	5	730	(2130.)	5	10
420	(4.225)	0.5	2	610	(448.7)	2	5	735	(2251.)	10	10
430	(6.145)	0.5	2	615	(484.8)	2	5	740	(2378.)	10	10
440	(8.752)	0.5	2	620	(523.2)	2	5	745	(2511.)	10	10
450	(12.23)	0.5	2	625	(563.8)	2	5	750	(2651.)	10	10
460	(16.78)	0.5	2	630	(606.7)	2	5	755	(2800.)	10	10
470	(22.64)	0.5	2	635	(652.2)	2	5				
480	(30.09)	0.5	2	640	(700.1)	2	5				
490	(39.43)	1	2	645	(750.7)	2	5				

Vapour Pressure of 2-Methylbiphenyl continued

Units: atm or mmHg v. °C

t °C	p mmHg	t °C	p mmHg	t °C	p mmHg	t °C	p atm	t °C	p atm
0	(0.002)	100	3.905	200	(186.0)	300	(2.384)	400	(10.76)
5	(0.003)	105	5.035	205	(214.4)	305	(2.607)	405	(11.46)
10	(0.006)	110	6.440	210	(246.1)	310	(2.846)	410	(12.19)
15	(0.009)	115	8.172	215	(281.6)	315	(3.101)	415	(12.96)
20	(0.015)	120	10.29	220	(321.1)	320	(3.373)	420	(13.76)
25	(0.024)	125	(12.87)	225	(365.0)	325	(3.664)	425	(14.61)
30	(0.036)	130	(15.99)	230	(413.6)	330	(3.973)	430	(15.50)
35	(0.055)	135	(19.73)	235	(467.2)	335	(4.301)	435	(16.42)
40	(0.083)	140	(24.20)	240	(526.3)	340	(4.650)	440	(17.40)
45	(0.123)	145	(29.49)	245	(591.2)	345	(5.021)	445	(18.41)
50	0.178	150	(35.74)	250	(662.3)	350	(5.413)	450	(19.48)
55	0.256	155	(43.07)	255	(740.1)	355	(5.828)	455	(20.60)
60	0.362	160	(51.63)	260	(824.8)	360	(6.268)	460	(21.77)
65	0.506	165	(61.58)	265	(917.1)	365	(6.732)	465	(23.00)
70	0.700	170	(73.08)	270	(1017.)	370	(7.221)	470	(24.29)
75	0.956	175	(86.32)	275	(1126.)	375	(7.738)	475	(25.65)
80	1.291	180	(101.5)	280	(1243.)	380	(8.282)	480	(27.08)
85	1.727	185	(118.8)	285	(1370.)	385	(8.854)		
90	2.288	190	(138.5)	290	(1507.)	390	(9.457)		
95	3.002	195	(160.8)	295	(1654.)	395	(10.09)		

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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Antoine equation: $\ln(p/\text{kPa}) = 14.21956 - 4222.143/(T/\text{K} - 89.615)$ for $2 < p/\text{kPa} < 200$.

C₁₃H₁₂ 3-Methylbiphenyl (3-Phenyltoluene)

CAS Reg. No. 643-93-6

Mol. Wt. 168.240

Vapour Pressure $\ln p = \ln p_c + (N_1q + N_2q^{1.5} + N_3q^{2.5} + N_4q^5)/(T/T_c)$

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 q = 1 - T/T_c.

Critical Temperature	T _c = 767 K	(t _c = 493.85 °C)
Critical Pressure	p _c = 2750 kPa	(p _c = 27.14 atm)
	N ₁ = -8.66565	
	N ₂ = 2.48947	
	N ₃ = -4.3841	
	N ₄ = -3.968	
Acentric Factor	= 0.499	
Normal Boiling Point	= 543.740 K	(= 270.590 °C)
dT/dp at N.B.P.	= 0.454 K/kPa	(= 0.061 °C/mmHg)
Normal Melting Point	= 278 K	(= 5 °C)

Data at Specified Pressures

p/kPa	0.001	0.01	0.1	1	10	101.325	1000	2750
T/K	(297.162)	(323.642)	(356.672)	(399.434)	457.715	543.740	(680.872)	(767.000)
(dp/dT)/(kPa/K)	(1.E-4)	(8.E-4)	(0.006)	(0.047)	0.333	2.202	(12.986)	(31.070)
Data Quality				(C)	C	C	(C)	(C)
Uncert. in T (K)				(1)	0.5	2	(10)	(20)
Uncert. in p (kPa)				(0.05)	0.2	5	(100)	(500)
Uncert. in p (%)				(5)	2	5	(10)	(20)

Vapour Pressure of 3-Methylbiphenyl

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	%
				500	35.31	1	2	650	(656.7)	5	10
				510	45.83	1	5	655	(704.9)	5	10
				520	58.76	2	5	660	(755.9)	5	10
280	(2.E-4)			530	74.46	2	5	665	(809.7)	5	10
290	(5.E-4)			540	93.35	2	5	670	(866.3)	5	10
Interval change											
300	(0.001)			550	(115.9)	2	5	675	(926.0)	5	10
310	(0.003)			555	(128.6)	2	5	680	(988.7)	10	10
320	(0.007)			560	(142.5)	2	5	685	(1055.)	10	10
330	(0.016)			565	(157.5)	2	5	690	(1124.)	10	10
340	(0.033)			570	(173.7)	2	5	695	(1197.)	10	10
350	(0.066)			575	(191.2)	2	5	700	(1273.)	10	10
360	(0.123)			580	(210.0)	2	5	705	(1354.)	10	10
370	(0.220)			585	(230.2)	5	5	710	(1438.)	10	10
380	(0.380)			590	(252.0)	5	5	715	(1526.)	10	10
390	(0.635)			595	(275.2)	5	5	720	(1619.)	10	10
400	(1.027)	1	5	600	(300.1)	5	5	725	(1716.)	10	10
410	(1.613)	1	5	605	(326.8)	5	5	730	(1818.)	10	10
420	(2.469)	1	5	610	(355.2)	5	5	735	(1925.)	10	20
430	3.686	1	2	615	(385.4)	5	10	740	(2037.)	10	20
440	5.381	0.5	2	620	(417.7)	5	10	745	(2154.)	10	20
450	7.692	0.5	2	625	(451.9)	5	10	750	(2278.)	20	20
460	10.79	0.5	2	630	(488.3)	5	10	755	(2408.)	20	20
470	14.86	1	2	635	(526.8)	5	10	760	(2545.)	20	20
480	20.13	1	2	640	(567.7)	5	10	765	(2689.)	20	20
490	26.85	1	2	645	(610.9)	5	10				