

Vapour pressures and critical points of liquids: Halogenated benzenes

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THE PREPARATION OF THIS DATA ITEM

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VAPOUR PRESSURES AND CRITICAL POINTS OF LIQUIDS HALOGENATED BENZENES

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MONOHALOGENATED BENZENES

1 C_6H_5F	Fluorobenzene	Phenyl fluoride	7
2 C_6H_5Cl	Chlorobenzene	Phenyl chloride	9
3 C_6H_5Br	Bromobenzene	Phenyl bromide	11
4 C_6H_5I	Iodobenzene	Phenyl iodide	13

DIHALOGENATED BENZENES

5 1,2- $F_2C_6H_4$	1,2-Difluorobenzene	<i>o</i> -Difluorobenzene	15
6 1,3- $F_2C_6H_4$	1,3-Difluorobenzene	<i>m</i> -Difluorobenzene	17
7 1,4- $F_2C_6H_4$	1,4-Difluorobenzene	<i>p</i> -Difluorobenzene	19
8 1,2- $Cl_2C_6H_4$	1,2-Dichlorobenzene	<i>o</i> -Dichlorobenzene	21
9 1,3- $Cl_2C_6H_4$	1,3-Dichlorobenzene	<i>m</i> -Dichlorobenzene	23
10 1,4- $Cl_2C_6H_4$	1,4-Dichlorobenzene	<i>p</i> -Dichlorobenzene	25
11 1-Br-3-Cl- C_6H_4	1-Bromo-3-chlorobenzene	<i>m</i> -Bromochlorobenzene	27
12 1,2- $Br_2C_6H_4$	1,2-Dibromobenzene	<i>o</i> -Dibromobenzene	29
13 1,3- $Br_2C_6H_4$	1,3-Dibromobenzene	<i>m</i> -Dibromobenzene	31
14 1,4- $Br_2C_6H_4$	1,4-Dibromobenzene	<i>p</i> -Dibromobenzene	33

TRIHALOGENATED BENZENES

15 1,3,5- $F_3C_6H_3$	1,3,5-Trifluorobenzene	sym-Trifluorobenzene	35
16 1,2,3- $Cl_3C_6H_3$	1,2,3-Trichlorobenzene		37
17 1,2,4- $Cl_3C_6H_3$	1,2,4-Trichlorobenzene		39
18 1,3,5- $Cl_3C_6H_3$	1,3,5-Trichlorobenzene	sym-Trichlorobenzene	41

Continued overleaf

TETRAHALOGENATED BENZENES

19	$1,2,3,4\text{-F}_4\text{C}_6\text{H}_2$	1,2,3,4-Tetrafluorobenzene	43
20	$1,2,3,5\text{-F}_4\text{C}_6\text{H}_2$	1,2,3,5-Tetrafluorobenzene	45
21	$1,2,4,5\text{-F}_4\text{C}_6\text{H}_2$	1,2,4,5-Tetrafluorobenzene	47
		sym-Tetrafluorobenzene	
22	$1,2,3,4\text{-Cl}_4\text{C}_6\text{H}_2$	1,2,3,4-Tetrachlorobenzene	49
23	$1,2,3,5\text{-Cl}_4\text{C}_6\text{H}_2$	1,2,3,5-Tetrachlorobenzene	51
24	$1,2,4,5\text{-Cl}_4\text{C}_6\text{H}_2$	1,2,4,5-Tetrachlorobenzene	53
		sym-Tetrachlorobenzene	

PENTAHALOGENATED AND HEXAHALOGENATED BENZENES

25	C_6HF_5	Pentafluorobenzene	55
26	C_6HCl_5	Pentachlorobenzene	57
27	C_6F_6	Hexafluorobenzene	59
28	C_6ClF_5	Chloropentafluorobenzene	61
29	C_6BrF_5	Bromopentafluorobenzene	63
30	$1,3,5\text{-Cl}_3\text{C}_6\text{F}_3$	1,3,5-Trichlorotrifluorobenzene	65
31	C_6Cl_6	Hexachlorobenzene	67
		Perchlorobenzene	

VAPOUR PRESSURES AND CRITICAL POINTS OF LIQUIDS HALOGENATED BENZENES

1. INTRODUCTION

This Item presents saturated vapour pressures of the halogenated benzenes 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 rounded to the nearest K or °C. 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. $T_r = T/T_c$

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:

- (a) low pressure, below say 1 kPa (approximately 7.5 mmHg),
- (b) medium pressure, say 1 kPa to 200 kPa (approximately 2 atm),
- (c) high pressure, say 200 kPa to the critical point,
- (d) 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 several fluoro- and polyfluoro- compounds. On some of these compounds reliable high pressure range, and on most of them, reliable critical point measurements have also been made. For several of the chloro- and bromo- compounds medium pressure range measurements of varying reliability have been made and for remaining compounds only boiling temperatures at various pressures have been reported.

In this Item critical temperatures and critical pressures were estimated, using References 2, 3 and 8, 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 saturated vapour 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 normal 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

The vapour pressure equations of the polyfluoro- compounds with the most reliable vapour pressure and critical point data yielded values of D_3/D_5 which were consistent with the line for alkanes referred to in Section 4.1. and were constant with the criteria referred to in Section 4.2. Therefore in this Item the equations of these compounds were then used to derive a correlation which was similar to that derived for the alkanes and which is described in Items 84022, 84028 and 85002. This correlation was then used to derive the vapour pressure equations of those fluoro- compounds for which the data were not extensive or precise enough to yield reliable results when fitted by the Wagner equation in the normal way.

The correlation for the alkanes, already referred to above, was used to derive the vapour pressure equations of the remaining chloro-, bromo- and iodo- compounds. This procedure ensured that the vapour pressure equations of all the compounds presented here met the desired criteria.

For most of the compounds considered here, saturated liquid density data were available and the liquid density equations for them, see Item 98015, were derived in parallel with the vapour pressure equations presented here. Where necessary, the estimated values of critical temperature, critical pressure and critical density for some compounds 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
MONOHALOGENATED BENZENES							
1	Fluorobenzene	560.12	4551.	-7.20896	1.62034	-2.01658	-3.45473
2	Chlorobenzene	632.35	4520.	-7.30021	1.83965	-2.42930	-2.27421
3	Bromobenzene	670.	4550.	-7.26980	1.64298	-2.02250	-3.25121
4	Iodobenzene	720.	4600.	-7.31749	1.73855	-2.25888	-2.81507
DIHALOGENATED BENZENES							
5	1,2-Difluorobenzene	566.	4260.	-7.44583	1.89817	-2.57267	-2.76734
6	1,3-Difluorobenzene	550.	4280.	-7.37905	1.72145	-2.25011	-3.28484
7	1,4-Difluorobenzene	558.	4325.	-7.42313	1.69851	-2.23505	-3.48709
8	1,2-Dichlorobenzene	694.	4090.	-7.49105	1.81457	-2.50524	-3.00474
9	1,3-Dichlorobenzene	685.	4130.	-7.44057	1.79192	-2.43274	-2.95064
10	1,4-Dichlorobenzene	686.	4175.	-7.47617	1.80785	-2.48381	-2.98889
11	1-Bromo-3-chlorobenzene	721.	3950.	-7.33558	1.74623	-2.28417	-2.83533
12	1,2-Dibromobenzene	755.	4150.	-7.51748	1.82659	-2.54348	-3.03272
13	1,3-Dibromobenzene	755.	3800.	-7.26862	1.71809	-2.19101	-2.75979
14	1,4-Dibromobenzene	759.	3800.	-7.25806	1.71372	-2.17642	-2.74773
TRIHALOGENATED BENZENES							
15	1,3,5-Trifluorobenzene	534.	3930.	-7.49059	1.77326	-2.36273	-3.59907
16	1,2,3-Trichlorobenzene	745.	3700.	-7.50672	1.82168	-2.52789	-3.02136
17	1,2,4-Trichlorobenzene	736.	3700.	-7.52542	1.83023	-2.55500	-3.04108
18	1,3,5-Trichlorobenzene	730.	3700.	-7.49398	1.81589	-2.50948	-3.00786
TETRAHALOGENATED BENZENES							
19	1,2,3,4-Tetrafluorobenzene	550.79	3791.	-7.84116	2.05055	-2.91742	-3.50772
20	1,2,3,5-Tetrafluorobenzene	535.21	3747.	-7.84643	2.02418	-2.84427	-3.64899
21	1,2,4,5-Tetrafluorobenzene	543.31	3801.	-7.87236	1.99899	-2.90791	-3.71315
22	1,2,3,4-Tetrachlorobenzene	782.	3480.	-7.84628	1.98589	-3.03450	-3.36137
23	1,2,3,5-Tetrachlorobenzene	774.	3350.	-7.63440	1.88120	-2.71484	-3.15368
24	1,2,4,5-Tetrachlorobenzene	770.	3800.	-8.07914	2.10925	-3.39899	-3.57301
PENTAHALOGENATED AND HEXAHALOGENATED BENZENES							
25	Pentafluorobenzene	530.93	3531.	-7.84493	1.68085	-2.53865	-4.52214
26	Pentachlorobenzene	800.	3650.	-8.65887	2.45227	-4.36350	-4.02792
27	Hexafluorobenzene	516.69	3274.	-8.01164	1.85193	-2.82629	-4.77575
28	Chloropentafluorobenzene	570.77	3238.	-8.10343	1.96204	-2.80927	-4.19440
29	Bromopentafluorobenzene	601.	3040.	-7.84076	1.89458	-2.72609	-3.92795
30	1,3,5-Trichlorotrifluorobenzene	684.75	3240.	-8.30533	2.30806	-3.56076	-2.73167
31	Hexachlorobenzene	820.	3500.	-9.48619	3.02404	-5.87061	-4.51224

... ..

$$\text{C}_6\text{H}_5\text{F}$$

Mol. Wt. 96.1

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

$$\begin{array}{llll} \omega & = & 0.243 & \\ T_b & = & 357.855 \text{ K} & (t_b = 84.705 \text{ }^\circ\text{C}) \\ & = & 0.323 \text{ K/kPa} & (= 0.0430 \text{ }^\circ\text{C/mmHg}) \\ T_m & = & 231. \text{ K} & (t_m = -42. \text{ }^\circ\text{C}) \end{array}$$
Units: kPa v. K

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Vapour Pressure of Fluorobenzene 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	0.105	100	1.582	175	8.597	250	28.092
		30	0.132	105	1.813	180	9.417	255	30.064
-40	(0.002)	35	0.165	110	2.070	185	10.295	260	32.142
-35	(0.003)	40	0.204	115	2.354	190	11.231	265	34.333
-30	(0.004)	45	0.251	120	2.667	195	12.230	270	36.642
-25	(0.006)	50	0.306	125	3.011	200	13.292	275	39.078
-20	0.008	55	0.371	130	3.388	205	14.422	280	41.652
-15	0.011	60	0.446	135	3.800	210	15.621	285	44.382
-10	0.015	65	0.532	140	4.248	215	16.893		
-5	0.021	70	0.632	145	4.736	220	18.240		
0	0.028	75	0.746	150	5.264	225	19.666		
5	0.038	80	0.876	155	5.836	230	21.174		
10	0.049	85	1.022	160	6.452	235	22.766		
15	0.064	90	1.188	165	7.117	240	24.448		
20	0.082	95	1.374	170	7.831	245	26.222		

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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M
H C
C

C₆H₅Cl
Chlorobenzene; Phenyl chloride

C₆H₅Cl

CAS Reg. No. 108-90-7

Mol. Wt. 112.56

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

Critical Temperature $T_c = 632.35$ K ($t_c = 359.2$ °C)
 Critical Pressure $p_c = 4520$ kPa ($p_c = 44.61$ atm)

$N_1 = -7.30021$ $N_2 = 1.83965$ $N_3 = -2.42930$ $N_4 = -2.27421$

Acentric Factor $\omega = 0.249$
 Normal Boiling Point $T_b = 404.859$ K ($t_b = 131.709$ °C)
 dT/dp at T_b , t_b $= 0.365$ K/kPa ($= 0.0487$ °C/mmHg)
 Approximate Melting Point $T_m = 228$ K ($t_m = -45$ °C)

Data at Specified Pressures								
p /kPa	0.001	0.01	0.1	1	10	101.325	1000	4520.
T /K	(229.911)	255.823	289.607	335.963	404.859	516.219	632.349	
(dp/dT) /(kPa/K)	(0.001)	0.008	0.059	0.417	2.739	15.724	52.188	
Data Quality			B	B	A	B	B	
Uncert. in T (K)			0.02	0.02	0.02	0.2	5.	
Uncert. in p (kPa)			0.002	0.01	0.05	5.	200.	
Uncert. in p (%)			0.2	0.1	0.05	0.5	5.	

Vapour Pressure of Chlorobenzene

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	%
230	(0.010)			350	17.481	0.02	0.1	475	492.36	0.1	0.2
235	(0.016)			355	21.066	0.02	0.1	480	540.35	0.1	0.2
240	0.026			360	25.233	0.02	0.1	485	591.77	0.2	0.2
245	0.041			365	30.051	0.02	0.05	490	646.77	0.2	0.2
				370	35.593	0.02	0.05	495	705.51	0.2	0.5
250	0.062			375	41.936	0.02	0.05	500	768.14	0.2	0.5
255	0.094			380	49.162	0.02	0.05	505	834.81	0.2	0.5
260	0.138			385	57.358	0.02	0.05	510	905.70	0.2	0.5
265	0.200			390	66.614	0.02	0.05	515	980.97	0.2	0.5
270	0.285			395	77.025	0.02	0.05	520	1060.8	0.5	0.5
275	0.400			400	88.690	0.02	0.05	525	1145.3	0.5	0.5
280	0.555			405	101.71	0.02	0.05	530	1234.7	0.5	0.5
285	0.758			410	116.20	0.02	0.05	535	1329.2	0.5	1
290	1.023	0.02	0.2	415	132.26	0.02	0.05	540	1428.9	0.5	1
295	1.365	0.02	0.2	420	150.01	0.02	0.05	545	1534.1	0.5	1
300	1.802	0.02	0.2	425	169.56	0.05	0.1	550	1644.9	1	1
305	2.352	0.02	0.2	430	191.04	0.05	0.1	555	1761.6	1	1
310	3.040	0.02	0.1	435	214.57	0.05	0.1	560	1884.3	1	1
315	3.893	0.02	0.1	440	240.28	0.05	0.1	565	2013.3	1	1
320	4.940	0.02	0.1	445	268.29	0.05	0.1	570	2148.8	1	2
325	6.215	0.02	0.1	450	298.74	0.05	0.2	575	2291.1	1	2
330	7.756	0.02	0.1	455	331.76	0.1	0.2	580	2440.4	1	2
335	9.605	0.02	0.1	460	367.50	0.1	0.2	585	2597.0	2	2
340	11.808	0.02	0.1	465	406.08	0.1	0.2	590	2761.2	2	2
345	14.415	0.02	0.1	470	447.65	0.1	0.2	595	2933.3	2	2

Units: bar v. °C

<i>t</i> °C	<i>p</i> bar	<i>t</i> °C	<i>p</i> bar	<i>t</i> °C	<i>p</i> bar	<i>t</i> °C	<i>p</i> bar	<i>t</i> °C	<i>p</i> bar
-45	(8.E-5)	25	0.016	100	0.395	175	2.872	250	11.135
-40	(1.E-4)	30	0.021	105	0.464	180	3.192	255	12.010
-35	2.E-4	35	0.028	110	0.542	185	3.540	260	12.936
-30	3.E-4	40	0.036	115	0.631	190	3.915	265	13.914
		45	0.045	120	0.730	195	4.319	270	14.945
-25	5.E-4	50	0.057	125	0.842	200	4.754	275	16.032
-20	8.E-4	55	0.072	130	0.967	205	5.222	280	17.177
-15	0.001	60	0.089	135	1.107	210	5.723	285	18.382
-10	0.002	65	0.109	140	1.261	215	6.260	290	19.648
-5	0.003	70	0.134	145	1.432	220	6.833	295	20.979
0	0.004	75	0.163	150	1.621	225	7.445	300	22.377
5	0.005	80	0.197	155	1.829	230	8.097	305	23.843
10	0.007	85	0.236	160	2.056	235	8.790	310	25.382
15	0.009	90	0.282	165	2.305	240	9.526	315	26.995
20	0.012	95	0.335	170	2.577	245	10.307	320	28.687

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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C₆H₅Br
Bromobenzene; Phenyl bromide

C₆H₅Br

CAS Reg. No. 108-86-1

Mol. Wt. 157.01

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

Critical Temperature $T_c = 670. \text{ K}$ ($t_c = 396.85 \text{ }^\circ\text{C}$)
 Critical Pressure $p_c = 4550. \text{ kPa}$ ($p_c = 44.91 \text{ atm}$)

$N_1 = -7.26980$ $N_2 = 1.64298$ $N_3 = -2.02250$ $N_4 = -3.25121$

Acentric Factor $\omega = 0.252$
 Normal Boiling Point $T_b = 429.061 \text{ K}$ ($t_b = 155.911 \text{ }^\circ\text{C}$)
 dT/dp at T_b , t_b $= 0.386 \text{ K/kPa}$ ($= 0.0515 \text{ }^\circ\text{C/mmHg}$)
 Approximate Melting Point $T_m = 242. \text{ K}$ ($t_m = -31. \text{ }^\circ\text{C}$)

Data at Specified Pressures								
p/kPa	0.001	0.01	0.1	1	10	101.325	1000	4550.
T/K		(244.984)	(272.085)	307.497	356.263	429.061	(546.858)	(670.000)
$(dp/dT)/(\text{kPa/K})$		(0.001)	(0.008)	0.056	0.396	2.588	(14.895)	(49.370)
Data Quality				B	B	B	(B)	(B)
Uncert. in T (K)				0.1	0.05	0.05	(0.2)	(5.)
Uncert. in p (kPa)				0.005	0.02	0.1	(5.)	(200.)
Uncert. in p (%)				0.5	0.2	0.1	(0.5)	(5.)

Vapour Pressure of Bromobenzene

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	7.762	0.05	0.2	475	287.83	0.1	0.2
				355	9.510	0.05	0.2	480	318.10	0.1	0.2
				360	11.573	0.05	0.2	485	350.74	0.1	0.2
				365	13.995	0.05	0.2	490	385.87	0.1	0.2
245	(0.010)			370	16.820	0.05	0.2	495	423.61	0.1	0.2
250	(0.016)			375	20.098	0.05	0.2	500	464.08	0.2	0.2
255	(0.025)			380	23.883	0.05	0.2	505	507.42	0.2	0.2
260	(0.038)			385	28.231	0.05	0.1	510	553.73	0.2	0.2
265	(0.058)			390	33.202	0.05	0.1	515	603.16	0.2	0.5
270	(0.085)			395	38.859	0.05	0.1	520	655.84	0.2	0.5
275	(0.124)			400	45.271	0.05	0.1	525	711.89	0.2	0.5
280	(0.178)			405	52.507	0.05	0.1	530	771.45	0.2	0.5
285	0.251			410	60.643	0.05	0.1	535	834.67	0.2	0.5
290	0.348			415	69.755	0.05	0.1	540	901.67	0.2	0.5
295	0.478			420	79.926	0.05	0.1	545	(972.60)	0.2	0.5
300	0.648			425	91.238	0.05	0.1	550	(1047.6)	0.5	0.5
305	0.868			430	103.78	0.05	0.1	555	(1126.9)	0.5	0.5
310	1.150	0.1	0.5	435	117.64	0.05	0.1	560	(1210.5)	0.5	0.5
315	1.507	0.1	0.5	440	132.92	0.05	0.1	565	(1298.6)	0.5	0.5
320	1.955	0.1	0.5	445	149.70	0.05	0.1	570	(1391.4)	0.5	1
325	2.513	0.05	0.2	450	168.09	0.05	0.1	575	(1489.1)	0.5	1
330	3.200	0.05	0.2	455	188.19	0.05	0.2	580	(1591.8)	0.5	1
335	4.041	0.05	0.2	460	210.11	0.1	0.2	585	(1699.7)	1	1
340	5.062	0.05	0.2	465	233.95	0.1	0.2	590	(1813.0)	1	1
345	6.292	0.05	0.2	470	259.82	0.1	0.2	595	(1931.8)	1	1

Units: bar v. °C

<i>t</i> °C	<i>p</i> bar	<i>t</i> °C	<i>p</i> bar	<i>t</i> °C	<i>p</i> bar	<i>t</i> °C	<i>p</i> bar	<i>t</i> °C	<i>p</i> bar
		25	0.006	100	0.188	175	1.611	250	6.907
		30	0.008	105	0.224	180	1.806	255	7.490
		35	0.010	110	0.266	185	2.018	260	8.108
		40	0.014	115	0.313	190	2.249	265	8.764
-30	(8.E-5)	45	0.018	120	0.367	195	2.500	270	(9.459)
-25	(1.E-4)	50	0.023	125	0.428	200	2.772	275	(10.194)
-20	(2.E-4)	55	0.029	130	0.497	205	3.066	280	(10.970)
-15	(3.E-4)	60	0.037	135	0.575	210	3.384	285	(11.790)
-10	(5.E-4)	65	0.047	140	0.663	215	3.726	290	(12.655)
-5	(7.E-4)	70	0.058	145	0.760	220	4.093	295	(13.565)
0	(0.001)	75	0.072	150	0.869	225	4.488	300	(14.524)
5	(0.002)	80	0.088	155	0.990	230	4.910	305	(15.532)
10	(0.002)	85	0.108	160	1.124	235	5.362	310	(16.592)
15	0.003	90	0.131	165	1.271	240	5.845	315	(17.704)
20	0.004	95	0.157	170	1.433	245	6.360	320	(18.872)

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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| 32 | TRC Thermodynamic Tables, | Texas A & M Univ., Loose leaf data sheets extant 1996.* | |



Iodobenzene; Phenyl iodide



CAS Reg. No. 591-50-4

Mol. Wt. 204.01

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

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

Critical Temperature $T_c = 720. \text{ K}$ ($t_c = 446.85 \text{ }^\circ\text{C}$)
 Critical Pressure $p_c = 4600. \text{ kPa}$ ($p_c = 45.40 \text{ atm}$)

$N_1 = -7.31749$ $N_2 = 1.73855$ $N_3 = -2.25888$ $N_4 = -2.81507$

Acentric Factor $\omega = 0.258$
 Normal Boiling Point $T_b = 461.423 \text{ K}$ ($t_b = 188.273 \text{ }^\circ\text{C}$)
 dT/dp at T_b , $t_b = 0.413 \text{ K/kPa}$ ($= 0.0551 \text{ }^\circ\text{C/mmHg}$)
 Approximate Melting Point $T_m = 242. \text{ K}$ ($t_m = -31. \text{ }^\circ\text{C}$)

Data at Specified Pressures								
p/kPa	0.001	0.01	0.1	1	10	101.325	1000	4600.
T/K		(263.541)	(292.820)	331.004	383.438	461.423	(587.286)	(720.000)
$(dp/dT)/(\text{kPa/K})$		(0.001)	(0.007)	0.052	0.369	2.420	(13.941)	(46.751)
Data Quality				C	B	B	(B)	(B)
Uncert. in T (K)				0.2	0.05	0.1	(0.5)	(5.)
Uncert. in p (kPa)				0.01	0.02	0.2	(10.)	(200.)
Uncert. in p (%)				1.	0.2	0.2	(1.)	(5.)

Vapour Pressure of Iodobenzene

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	2.531	0.1	0.5	475	138.64	0.1	0.2
				355	3.169	0.1	0.5	480	154.81	0.1	0.2
				360	3.940	0.1	0.5	485	172.42	0.1	0.2
				365	4.863	0.1	0.2	490	191.54	0.2	0.2
245	(0.002)			370	5.963	0.05	0.2	495	212.27	0.2	0.2
250	(0.003)			375	7.265	0.05	0.2	500	234.70	0.2	0.5
255	(0.005)			380	8.797	0.05	0.2	505	258.90	0.2	0.5
260	(0.007)			385	10.590	0.05	0.2	510	284.99	0.2	0.5
265	(0.011)			390	12.677	0.05	0.2	515	313.04	0.2	0.5
270	(0.017)			395	15.095	0.05	0.2	520	343.15	0.2	0.5
275	(0.026)			400	17.881	0.05	0.2	525	375.43	0.2	0.5
280	(0.039)			405	21.077	0.05	0.2	530	409.96	0.2	0.5
285	(0.057)			410	24.728	0.05	0.2	535	446.85	0.2	0.5
290	(0.082)			415	28.881	0.05	0.2	540	486.20	0.5	0.5
295	(0.116)			420	33.584	0.05	0.2	545	(528.11)	0.5	0.5
300	(0.163)			425	38.892	0.05	0.2	550	(572.69)	0.5	0.5
305	0.224			430	44.858	0.05	0.2	555	(620.04)	0.5	0.5
310	0.306			435	51.541	0.05	0.2	560	(670.28)	0.5	1
315	0.413			440	59.002	0.1	0.2	565	(723.50)	0.5	1
320	0.550			445	67.304	0.1	0.2	570	(779.82)	0.5	1
325	0.726			450	76.513	0.1	0.2	575	(839.35)	0.5	1
330	0.949			455	86.697	0.1	0.2	580	(902.21)	0.5	1
335	1.228	0.2	1	460	97.928	0.1	0.2	585	(968.51)	0.5	1
340	1.576	0.1	0.5	465	110.28	0.1	0.2	590	(1038.4)	1	1
345	2.005	0.1	0.5	470	123.82	0.1	0.2	595	(1111.9)	1	1



Vapour Pressure of Iodobenzene continued

Units: bar v. °C

<i>t</i> °C	<i>p</i> bar	<i>t</i> °C	<i>p</i> bar	<i>t</i> °C	<i>p</i> bar	<i>t</i> °C	<i>p</i> bar	<i>t</i> °C	<i>p</i> bar
		25	(0.001)	100	0.068	175	0.730	250	3.632
		30	0.002	105	0.082	180	0.828	255	3.969
		35	0.003	110	0.099	185	0.936	260	4.329
		40	0.004	115	0.119	190	1.056	265	4.713
-30	(1.E-5)	45	0.005	120	0.142	195	1.187	270	(5.123)
-25	(2.E-5)	50	0.007	125	0.168	200	1.330	275	(5.559)
-20	(4.E-5)	55	0.009	130	0.198	205	1.487	280	(6.022)
-15	(6.E-5)	60	0.011	135	0.233	210	1.657	285	(6.513)
-10	(1.E-4)	65	0.014	140	0.273	215	1.843	290	(7.035)
-5	(1.E-4)	70	0.018	145	0.318	220	2.044	295	(7.586)
0	(2.E-4)	75	0.023	150	0.369	225	2.262	300	(8.169)
5	(3.E-4)	80	0.029	155	0.426	230	2.497	305	(8.786)
10	(5.E-4)	85	0.036	160	0.490	235	2.751	310	(9.436)
15	(7.E-4)	90	0.045	165	0.561	240	3.024	315	(10.121)
20	(0.001)	95	0.055	170	0.641	245	3.318	320	(10.843)

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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|----|--|---|----------|----------|
| 1 | FEITLER, -; | <i>Z.Phys.Chem.</i> , Vol.4, p.71, 1889. | | |
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| 3 | PERKIN, W.H.; | <i>J.Chem.Soc.</i> , Vol.69, p.1025, 1896. | | |
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| 8 | SUGDEN, S.; | <i>J.Chem.Soc.</i> , Vol.125, p.1167, 1924. | | |
| 9 | STULL, D.R.; | <i>J.Am.Chem.Soc.</i> , Vol.59, p.2726, 1937. | | |
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| 11 | LECAT, M.; | <i>C.R.Hebd.Sean.Acad.Sci.</i> , Vol.217, p.242, 1943. | | |
| 12 | BERINGER, F.M.; BRIERLEY, A.; et al.; | <i>J.Am.Chem.Soc.</i> , Vol.75, p.2708, 1953. | | |
| 13 | AMBROSE, D.; | in <i>Hndbk.Chem.Phys.</i> , CRC Press, 72nd.ed., pp.6-49 to 6-63, 1991.* | | |
| 14 | TRC Thermodynamic Tables, | Texas A & M Univ., Loose leaf data sheets extant 1996.* | | |

1,2-F₂C₆H₄
1,2-Difluorobenzene; o-Difluorobenzene



CAS Reg. No. 367-11-3

Mol. Wt. 114.09

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

Critical Temperature $T_c = 566. \text{ K}$ ($t_c = 292.85 \text{ }^\circ\text{C}$)
 Critical Pressure $p_c = 4260. \text{ kPa}$ ($p_c = 42.04 \text{ atm}$)

$N_1 = -7.44583$ $N_2 = 1.89817$ $N_3 = -2.57267$ $N_4 = -2.76734$

Acentric Factor $\omega = 0.275$
 Normal Boiling Point $T_b = 367.071 \text{ K}$ ($t_b = 93.921 \text{ }^\circ\text{C}$)
 dT/dp at T_b , t_b $= 0.328 \text{ K/kPa}$ ($= 0.0437 \text{ }^\circ\text{C/mmHg}$)
 Approximate Melting Point $T_m = 239. \text{ K}$ ($t_m = -34. \text{ }^\circ\text{C}$)

Data at Specified Pressures

p/kPa	0.001	0.01	0.1	1	10	101.325	1000	4260.
T/K				(263.666)	305.229	367.071	(467.076)	(566.000)
$(dp/dT)/(\text{kPa/K})$				(0.066)	0.465	3.050	(17.530)	(56.034)
Data Quality				(A)	A	A	(A)	(B)
Uncert. in T (K)				(0.01)	0.002	0.002	(0.02)	(2.)
Uncert. in p (kPa)				(0.0005)	0.0010	0.01	(0.5)	(100.)
Uncert. in p (%)				(0.05)	0.01	0.01	(0.05)	(2.)

Vapour Pressure of 1,2-Difluorobenzene

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	58.852	0.002	0.01	475	(1146.2)	0.05	0.05
				355	69.443	0.002	0.01	480	(1246.4)	0.05	0.1
				360	81.500	0.002	0.01	485	(1352.8)	0.05	0.1
240	(0.175)			365	95.162	0.002	0.01	490	(1466.0)	0.1	0.1
245	(0.262)			370	110.57	0.005	0.01	495	(1586.0)	0.1	0.2
250	(0.384)			375	127.88	0.005	0.01	500	(1713.2)	0.1	0.2
255	(0.552)			380	147.24	0.005	0.01	505	(1848.0)	0.2	0.2
260	(0.782)			385	168.82	0.005	0.01	510	(1990.6)	0.2	0.2
265	(1.091)	0.005	0.05	390	192.78	0.005	0.02	515	(2141.3)	0.2	0.2
270	(1.500)	0.005	0.05	395	219.29	0.005	0.02	520	(2300.6)	0.2	0.5
275	(2.034)	0.005	0.02	400	248.52	0.01	0.02	525	(2468.9)	0.2	0.5
280	(2.723)	0.005	0.02	405	(280.67)	0.01	0.02	530	(2646.5)	0.5	0.5
285	(3.601)	0.005	0.02	410	(315.90)	0.01	0.02	535	(2833.9)	0.5	0.5
290	(4.709)	0.002	0.02	415	(354.41)	0.01	0.02	540	(3031.7)	0.5	1
295	(6.092)	0.002	0.01	420	(396.40)	0.01	0.02	545	(3240.6)	0.5	1
300	(7.801)	0.002	0.01	425	(442.05)	0.01	0.02	550	(3461.1)	1	1
305	9.894	0.002	0.01	430	(491.56)	0.01	0.02	555	(3694.3)	1	1
310	12.435	0.002	0.01	435	(545.15)	0.02	0.02	560	(3941.5)	1	2
315	15.496	0.002	0.01	440	(603.02)	0.02	0.05	565	(4204.8)	1	2
320	19.153	0.002	0.01	445	(665.38)	0.02	0.05				
325	23.491	0.002	0.01	450	(732.44)	0.02	0.05				
330	28.603	0.002	0.01	455	(804.43)	0.02	0.05				
335	34.586	0.002	0.01	460	(881.57)	0.02	0.05				
340	41.545	0.002	0.01	465	(964.09)	0.02	0.05				
345	49.594	0.002	0.01	470	(1052.2)	0.02	0.05				



Vapour Pressure of 1,2-Difluorobenzene 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	(0.071)	100	1.212	175	(7.071)	250	(24.056)
		30	(0.091)	105	1.398	180	(7.772)	255	(25.796)
		35	0.114	110	1.606	185	(8.524)	260	(27.634)
		40	0.143	115	1.836	190	(9.329)	265	(29.573)
-30	(0.002)	45	0.177	120	2.092	195	(10.190)	270	(31.620)
-25	(0.003)	50	0.218	125	2.374	200	(11.108)	275	(33.781)
-20	(0.005)	55	0.266	130	(2.684)	205	(12.086)	280	(36.065)
-15	(0.007)	60	0.323	135	(3.025)	210	(13.127)	285	(38.483)
-10	(0.010)	65	0.388	140	(3.398)	215	(14.233)	290	(41.052)
-5	(0.013)	70	0.465	145	(3.804)	220	(15.408)		
0	(0.018)	75	0.553	150	(4.247)	225	(16.653)		
5	(0.024)	80	0.654	155	(4.728)	230	(17.972)		
10	(0.033)	85	0.769	160	(5.248)	235	(19.369)		
15	(0.043)	90	0.899	165	(5.811)	240	(20.846)		
20	(0.055)	95	1.047	170	(6.418)	245	(22.407)		

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 SCOTT, D.W.; MESSERLY, J.F.; et al.; *J.Chem.Phys.*, Vol.38, p.532, 1963. M

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.*
 SOMAYAJULU G.,R.; *J.Chem.Eng.Data*, Vol.34, p.106, 1989.*

1,3-F₂C₆H₄C₆H₄F₂1,3-Difluorobenzene; *m*-Difluorobenzene

CAS Reg. No. 372-18-9

Mol. Wt. 114.09

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

Critical Temperature

 $T_c = 550. \text{ K}$ ($t_c = 276.85 \text{ }^\circ\text{C}$)

Critical Pressure

 $p_c = 4280. \text{ kPa}$ ($p_c = 42.24 \text{ atm}$) $N_1 = -7.37905$ $N_2 = 1.72145$ $N_3 = -2.25011$ $N_4 = -3.28484$

Acentric Factor

 $\omega = 0.272$

Normal Boiling Point

 $T_b = 356.169 \text{ K}$ ($t_b = 83.019 \text{ }^\circ\text{C}$) dT/dp at T_b , t_b $= 0.319 \text{ K/kPa}$ ($= 0.0425 \text{ }^\circ\text{C/mmHg}$)

Approximate Melting Point

 $T_m = -$ ($t_m = -$)

Data at Specified Pressures

p/kPa	0.001	0.01	0.1	1	10	101.325	1000	4280.
T/K	(186.242)	(204.083)	(226.505)	(255.782)	(296.067)	356.169	(453.425)	(550.000)
$(dp/dT)/(\text{kPa/K})$	(0.000)	(0.001)	(0.009)	(0.068)	(0.479)	3.135	(18.042)	(57.415)
Data Quality				(A)	(A)	A	(A)	(B)
Uncert. in T (K)				(0.005)	(0.002)	0.002	(0.02)	(1.)
Uncert. in p (kPa)				(0.0005)	(0.0010)	0.01	(0.5)	(100.)
Uncert. in p (%)				(0.05)	(0.01)	0.01	(0.05)	(2.)

Vapour Pressure of 1,3-Difluorobenzene

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	%
250	(0.668)			375	175.41	0.005	0.01	500	(2142.0)	0.2	0.2
255	(0.948)			380	200.80	0.005	0.02	505	(2306.2)	0.2	0.5
260	(1.325)	0.005	0.05	385	228.95	0.005	0.02	510	(2479.7)	0.2	0.5
265	(1.824)	0.005	0.02	390	260.04	0.01	0.02	515	(2663.2)	0.5	0.5
270	(2.476)	0.005	0.02	395	(294.27)	0.01	0.02	520	(2857.0)	0.5	0.5
275	(3.317)	0.005	0.02	400	(331.85)	0.01	0.02	525	(3061.8)	0.5	1
280	(4.389)	0.002	0.02	405	(372.99)	0.01	0.02	530	(3278.2)	0.5	1
285	(5.739)	0.002	0.01	410	(417.89)	0.01	0.02	535	(3507.0)	1	1
290	(7.422)	0.002	0.01	415	(466.77)	0.01	0.02	540	(3749.0)	1	1
295	(9.499)	0.002	0.01	420	(519.86)	0.01	0.02	545	(4005.8)	1	2
300	(12.039)	0.002	0.01	425	(577.37)	0.02	0.02	550	(4280.0)	1	2
305	(15.119)	0.002	0.01	430	(639.55)	0.02	0.05				
310	(18.820)	0.002	0.01	435	(706.62)	0.02	0.05				
315	23.235	0.002	0.01	440	(778.82)	0.02	0.05				
320	28.462	0.002	0.01	445	(856.40)	0.02	0.05				
325	34.609	0.002	0.01	450	(939.62)	0.02	0.05				
330	41.788	0.002	0.01	455	(1028.7)	0.02	0.05				
335	50.123	0.002	0.01	460	(1124.0)	0.05	0.05				
340	59.743	0.002	0.01	465	(1225.6)	0.05	0.1				
345	70.784	0.002	0.01	470	(1334.0)	0.05	0.1				
350	83.390	0.002	0.01	475	(1449.4)	0.1	0.1				
355	97.712	0.002	0.01	480	(1572.0)	0.1	0.2				
360	113.91	0.005	0.01	485	(1702.3)	0.1	0.2				
365	132.14	0.005	0.01	490	(1840.5)	0.1	0.2				
370	152.58	0.005	0.01	495	(1987.0)	0.2	0.2				



Vapour Pressure of 1,3-Difluorobenzene 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	(0.006)	50	0.322	125	(3.175)	200	(14.059)	275	(41.761)
-20	(0.008)	55	0.390	130	(3.573)	205	(15.258)		
-15	(0.012)	60	0.469	135	(4.008)	210	(16.532)		
-10	(0.016)	65	0.560	140	(4.482)	215	(17.884)		
-5	(0.022)	70	0.665	145	(4.997)	220	(19.318)		
0	(0.030)	75	0.785	150	(5.556)	225	(20.836)		
5	(0.040)	80	0.922	155	(6.160)	230	(22.444)		
10	(0.052)	85	1.077	160	(6.812)	235	(24.144)		
15	(0.068)	90	1.251	165	(7.515)	240	(25.941)		
20	(0.087)	95	1.448	170	(8.271)	245	(27.841)		
25	(0.110)	100	1.667	175	(9.082)	250	(29.847)		
30	(0.139)	105	1.911	180	(9.950)	255	(31.967)		
35	(0.174)	110	2.182	185	(10.880)	260	(34.208)		
40	0.215	115	2.482	190	(11.873)	265	(36.579)		
45	0.264	120	(2.812)	195	(12.931)	270	(39.090)		

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 OSBORN, D.W.; SCOTT, D.W.; *J.Chem.Thermodynamics*, Vol.12, p.429, 1980. M

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.*
 SOMAYAJULU G.,R.; *J.Chem.Eng.Data*, Vol.34, p.106, 1989.*

1,4-Difluorobenzene; *p*-Difluorobenzene

CAS Reg. No. 540-36-3

Mol. Wt. 114.09

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

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

Critical Temperature

$$T_c = 558. \text{ K} \quad (t_c = 284.85 \text{ }^\circ\text{C})$$

Critical Pressure

$$p_c = 4325. \text{ kPa} \quad (p_c = 42.68 \text{ atm})$$

$$N_1 = -7.42313$$

$$N_2 = 1.69851$$

$$N_3 = -2.23505$$

$$N_4 = -3.48709$$

Acentric Factor

$$\omega = 0.282$$

Normal Boiling Point

$$T_b = 362.031 \text{ K} \quad (t_b = 88.881 \text{ }^\circ\text{C})$$

 dT/dp at T_b , t_b

$$= 0.322 \text{ K/kPa} \quad (= 0.0429 \text{ }^\circ\text{C/mmHg})$$

Approximate Melting Point

$$T_m = 260. \text{ K} \quad (t_m = -13. \text{ }^\circ\text{C})$$

Data at Specified Pressures

p/kPa	0.001	0.01	0.1	1	10	101.325	1000	4325.
T/K				(260.565)	301.310	362.031	(460.064)	(558.000)
$(dp/dT)/(\text{kPa/K})$				(0.067)	0.474	3.105	(17.927)	(57.529)
Data Quality				(A)	A	A	(A)	(B)
Uncert. in T (K)				(0.005)	0.002	0.002	(0.02)	(2.)
Uncert. in p (kPa)				(0.0005)	0.0010	0.01	(0.5)	(100.)
Uncert. in p (%)				(0.05)	0.01	0.01	(0.05)	(2.)

Vapour Pressure of 1,4-Difluorobenzene

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	%
				375	148.39	0.005	0.01	500	(1931.1)	0.2	0.2
				380	170.52	0.005	0.01	505	(2082.1)	0.2	0.2
260	(0.963)			385	195.14	0.005	0.02	510	(2241.9)	0.2	0.5
265	(1.339)	0.005	0.05	390	222.42	0.005	0.02	515	(2410.9)	0.2	0.5
270	(1.836)	0.005	0.02	395	252.57	0.01	0.02	520	(2589.4)	0.5	0.5
275	(2.484)	0.005	0.02	400	(285.76)	0.01	0.02	525	(2778.1)	0.5	0.5
280	(3.316)	0.005	0.02	405	(322.21)	0.01	0.02	530	(2977.3)	0.5	0.5
285	(4.374)	0.002	0.02	410	(362.10)	0.01	0.02	535	(3187.7)	0.5	1
290	(5.703)	0.002	0.01	415	(405.66)	0.01	0.02	540	(3410.0)	1	1
295	(7.357)	0.002	0.01	420	(453.08)	0.01	0.02	545	(3644.9)	1	1
300	(9.395)	0.002	0.01	425	(504.59)	0.01	0.02	550	(3893.6)	1	1
305	11.882	0.002	0.01	430	(560.42)	0.02	0.02	555	(4157.7)	1	2
310	14.893	0.002	0.01	435	(620.77)	0.02	0.05				
315	18.507	0.002	0.01	440	(685.90)	0.02	0.05				
320	22.814	0.002	0.01	445	(756.03)	0.02	0.05				
325	27.907	0.002	0.01	450	(831.40)	0.02	0.05				
330	33.890	0.002	0.01	455	(912.25)	0.02	0.05				
335	40.873	0.002	0.01	460	(998.86)	0.02	0.05				
340	48.975	0.002	0.01	465	(1091.5)	0.05	0.05				
345	58.319	0.002	0.01	470	(1190.3)	0.05	0.1				
350	69.040	0.002	0.01	475	(1295.7)	0.05	0.1				
355	81.275	0.002	0.01	480	(1408.0)	0.05	0.1				
360	95.172	0.002	0.01	485	(1527.3)	0.1	0.1				
365	110.88	0.005	0.01	490	(1654.1)	0.1	0.2				
370	128.57	0.005	0.01	495	(1788.6)	0.1	0.2				