

88012

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Vapour pressures and critical points of liquids

C_7 to C_{20} Alkanols

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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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(Continued on inside back cover)

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VAPOUR PRESSURES AND CRITICAL POINTS OF LIQUIDS

C₇ TO C₂₀ ALKANOLS

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VAPOUR PRESSURES AND CRITICAL POINTS OF LIQUIDS

C₇ TO C₂₀ ALKANOLS

1. INTRODUCTION

This Data Item presents saturated vapour pressures of the C₇ to C₂₀ alkanols listed, with alternative names if any, in Table 1 (page 4).

The values of vapour pressure given in the Tables have been obtained by evaluating, for each compound, a Wagner equation of the form

$$\ln p = \ln p_c + (T_c/T) (b_1 q + b_2 q^{3/2} + b_3 q^{5/2} + b_4 q^5), \quad (1)$$

where T is the temperature in kelvins ($T = 273.15 +$ the Celsius temperature) on the International Practical Temperature Scale of 1968 (IPTS-68), p is the vapour pressure in kPa, T_c , p_c are the critical temperature and critical pressure respectively and $q = 1 - T/T_c$.

Equation (1) was fitted to the experimental and calculated data that had been selected and weighted in accordance with a critical assessment of all the data. Note that estimated values of T_c are normally rounded to the nearest kelvin and that values in other units are obtained by exact conversion.

Table 2 is an index to Tables 5 onward. Table 3 gives T_c , p_c and the coefficients b_1 , b_2 , b_3 and b_4 for each compound to be used in Equation (1). Table 4 shows, for each compound, the normal boiling point in kelvins, degrees Celsius and degrees Fahrenheit, the value of dT/dp at the normal boiling point and the acentric factor.

Tables 5 to 8 present values of vapour pressure, in kPa, at 5 K intervals of temperature down to a temperature just above the melting point, T_m , or an arbitrary lower limit where the melting point is not known.

Tables 5(C) to 8(C) present the vapour pressures, in atm or mmHg, at intervals of 5 degrees C, the change from atm to mmHg being at approximately 2 atm. Tables 5(F) to 8(F) give the vapour pressures, in psia, at intervals of 10 degrees F.

The sources of experimental and calculated data for each compound, on which the tabulated values are based, are shown in Table A.1 and Table A.2. The uncertainties in the tabulated values of vapour pressure that the user should allow for are given in Table A.3.

The notation and units, conversion factors and additional References are given the introductory Data Item, Reference 1 (page 4).

2. 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 precise 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. Critical point data are usually of a lower degree of precision, with uncertainties in pressure of one to two per cent.

In the low pressure range direct measurements of vapour pressure have very large uncertainties because of the difficulty of making such measurements at low pressures. However, vapour pressures calculated from experimental low temperature thermal and volumetric data have much lower uncertainties. Such calculated low range vapour pressures have been reported for a small number of key compounds which includes most of the normal alkanes up to hexadecane but only two alkanols, namely ethanol and propan-1-ol.

Table A.1 lists the sources of vapour pressure data considered for the compounds included in this Item. Table A.2 shows, for each compound, the sources that were selected as giving the most reliable data in each of the four pressure ranges. The more recent sources not used are indicated in the columns headed 'Other Sources'.

For most compounds the data are restricted to the medium pressure range and values outside this range were obtained by estimation. The critical temperatures and critical pressures were initially estimated by the methods of References 1 and 2, but the critical pressures, in particular, were reestimated from a correlation developed during the preparation of the Item.

The general procedure followed to obtain the final Wagner equation for each compound is outlined in Section 3.2 of the Introductory Data Item, see Reference 4 (page 3). This procedure was, of necessity, varied from compound to compound because of the varying quality and availability of data in each case. The consequent uncertainties in the derived values of vapour pressure, therefore, also vary considerably from one compound to another.

3. DISCUSSION OF UNCERTAINTIES

For ease of interpolation, values are presented in Table A.3 according to a uniform pattern without regard to their estimated accuracy. However, except in the low pressure range, values dependent on estimated data are much less certain than values dependent upon measured data.

In certain circumstances the user may need to allow for uncertainties in the tabulated values and an assessment of these is provided in Table A.3. For simplicity the uncertainties are given as 1, 2 or 5 times a power of 10.

In Table A.3 the letter 'X' indicates that the vapour pressures at the values at the top of the Table are derived from very high quality experimental data and that the uncertainty is considered less than the value shown. Similarly the letters 'A, B, C' indicate that the vapour pressures are based on progressively less certain data but that the uncertainties are thought to be less than the values shown. The letter 'D' indicates that the uncertainties cannot be estimated but are probably greater than the values shown. The letters 'A, B, C, D' are shown in brackets at those pressures which are above or below the range of supporting data.

For those compounds for which the uncertainties at the critical pressure are denoted by 'D' the values of critical temperature and critical pressure given in the Tables should be regarded as correlating parameters and since the acentric factor, ω , is dependent upon the value of critical pressure selected, the uncertainty in ω for these compounds is greater than 0.05.

The user should allow for uncertainties of up to 10 per cent in the values below 1 kPa. At higher pressures the uncertainties for each compound are dependent upon the quality of the experimental data and the confidence in the experimental or estimated values of critical temperature and critical pressure.

4. REFERENCES

1. AMBROSE, D. Correlation and estimation of vapour-liquid critical properties: I. Critical temperatures of organic compounds. NPL Report Chem. 92, National Physical Laboratory, Teddington, Middlesex, UK, September, 1978.
2. AMBROSE, D. Correlation and estimation of vapour-liquid critical properties: II. Critical pressures and critical volumes of organic compounds. NPL Report Chem. 98, National Physical Laboratory, Teddington, Middlesex, UK, May, 1979.
3. AMBROSE, D.
PATEL, N. C. The correlation and estimation of vapour pressures. IV: Extrapolation of vapour pressures and estimation of critical pressures by the principle of corresponding states using two reference fluids with non-spherical molecules. J. Chem. Thermodynamics, Vol. 16, pp. 459-468, 1984.
4. ESDU Vapour pressures and critical points of liquids. Introduction to Data Items issued after September 1984. Item No. 84021, ESDU International, 1984.

TABLE 1
LIST of COMPOUNDS

The empirical formula, name and alternative names, if any, of each compound considered in this Item are as follows:

No.	Emp. Form.	Name	Alternative Names
C ₇ ALKANOLS			
1	C ₇ H ₁₆ O	Heptan-1-ol	n-Heptyl Alcohol
2		Heptan-2-ol	
3		Heptan-3-ol	
4		Heptan-4-ol	
5		2-Methylhexan-2-ol	
6		2,4-Dimethylpentan-3-ol	
C ₈ ALKANOLS			
7	C ₈ H ₁₈ O	Octan-1-ol	n-Octyl Alcohol
8		Octan-2-ol	
9		2-Ethylhexan-1-ol	
10		4-Methyl-2-ethylpentan-1-ol	
C ₉ ALKANOLS			
11	C ₉ H ₂₀ O	Nonan-1-ol	Diisobutyl carbinol
12		2,6-Dimethylheptan-4-ol	
C ₁₀ to C ₂₀ ALKANOLS			
13	C ₁₀ H ₂₂ O	Decan-1-ol	
14	C ₁₁ H ₂₄ O	Undecan-1-ol	
15	C ₁₂ H ₂₆ O	Dodecan-1-ol	
16	C ₁₃ H ₂₈ O	Tridecan-1-ol	
17	C ₁₄ H ₃₀ O	Tetradecan-1-ol	
18	C ₁₅ H ₃₂ O	Pentadecan-1-ol	
19	C ₁₆ H ₃₄ O	Hexadecan-1-ol	
20	C ₁₇ H ₃₆ O	Heptadecan-1-ol	
21	C ₁₈ H ₃₈ O	Octadecan-1-ol	
22	C ₁₉ H ₄₀ O	Nonadecan-1-ol	
23	C ₂₀ H ₄₂ O	Eicosan-1-ol	

TABLE 2
LOCATION OF TABLES

The location of the Tables giving the vapour pressure of each compound in various units are as follows:-

Name	kPa v K		atm or mmHg v deg.C		psia v deg.F	
	Table	Pages	Table	Pages	Table	Pages
C₇ ALKANOLS						
Heptan-1-ol	5	8, 9	5(C)	16,17	5(F)	24,25
Heptan-2-ol	5	8, 9	5(C)	16,17	5(F)	24,25
Heptan-3-ol	5	8, 9	5(C)	16,17	5(F)	24,25
Heptan-4-ol	5	8, 9	5(C)	16,17	5(F)	24,25
2-Methylhexan-2-ol	5	8, 9	5(C)	16,17	5(F)	24,25
2,4-Dimethylpentan-3-ol	5	8, 9	5(C)	16,17	5(F)	24,25
C₈ ALKANOLS						
Octan-1-ol	6	10,11	6(C)	18,19	6(F)	26,27
Octan-2-ol	6	10,11	6(C)	18,19	6(F)	26,27
2-Ethylhexan-1-ol	6	10,11	6(C)	18,19	6(F)	26,27
4-Methyl-2-ethylpentan-1-ol	6	10,11	6(C)	18,19	6(F)	26,27
C₉ ALKANOLS						
Nonan-1-ol	6	10,11	6(C)	18,19	6(F)	26,27
2,6-Dimethylheptan-4-ol	6	10,11	6(C)	18,19	6(F)	26,27
C₁₀ to C₂₀ ALKANOLS						
Decan-1-ol	7	12,13	7(C)	20,21	7(F)	28,29
Undecan-1-ol	7	12,13	7(C)	20,21	7(F)	28,29
Dodecan-1-ol	7	12,13	7(C)	20,21	7(F)	28,29
Tridecan-1-ol	7	12,13	7(C)	20,21	7(F)	28,29
Tetradecan-1-ol	7	12,13	7(C)	20,21	7(F)	28,29
Pentadecan-1-ol	8	14,15	8(C)	22,23	8(F)	30,31
Hexadecan-1-ol	8	14,15	8(C)	22,23	8(F)	30,31
Heptadecan-1-ol	8	14,15	8(C)	22,23	8(F)	30,31
Octadecan-1-ol	8	14,15	8(C)	22,23	8(F)	30,31
Nonadecan-1-ol	8	14,15	8(C)	22,23	8(F)	30,31
Eicosan-1-ol	8	14,15	8(C)	22,23	8(F)	30,31

TABLE 3
CONSTANTS in EQUATION (1)

This Table lists the constants for each compound that, when used in the equation

$$\ln p = \ln p_c + (T_c/T)(b_1q + b_2q^{3/2} + b_3q^{5/2} + b_4q^5),$$

where T is in kelvins and $q = 1 - T/T_c$, give p in kilopascals when p_c is in kilopascals.

Name	T_c K	p_c kPa	b_1	b_2	b_3	b_4
C₇ ALKANOLS						
Heptan-1-ol	632.5	3135	-9.68778	5.35716	-10.1672	-8.010
Heptan-2-ol	607	3000	-8.67822	2.54430	-5.9028	-9.931
Heptan-3-ol	604	2990	-8.80284	2.94810	-6.8986	-7.771
Heptan-4-ol	602	2980	-8.90303	4.05202	-9.5628	-2.916
2-Methylhexan-2-ol	584	2890	-8.63507	2.93283	-7.3027	-9.624
2,4-Dimethylpentan-3-ol	583	2890	-8.31782	2.01603	-5.1006	-4.024
C₈ ALKANOLS						
Octan-1-ol	652.5	2860	-10.01437	5.90629	-10.4026	-9.048
Octan-2-ol	638	2790	-8.74183	3.41871	-7.2425	-12.494
2-Ethylhexan-1-ol	641	2800	-9.54163	5.06004	-9.0455	-11.006
4-Methyl-2-ethylpentan-1-ol	633	2760	-9.20340	5.16064	-10.8373	-4.283
C₉ ALKANOLS						
Nonan-1-ol	671.5	2630	-9.91542	5.13670	-8.8073	-12.497
2,6-Dimethylheptan-4-ol	630	2450	-8.79031	3.37390	-6.2417	-15.414
C₁₀ to C₂₀ ALKANOLS						
Decan-1-ol	689	2410	-9.75478	4.18634	-7.0572	-15.980
Undecan-1-ol	705	2240	-9.85733	3.97841	-6.6002	-16.691
Dodecan-1-ol	720	2080	-9.91901	3.61884	-5.8537	-18.204
Tridecan-1-ol	734	1935	-9.99402	3.36986	-5.4865	-18.592
Tetradecan-1-ol	747	1810	-10.13519	3.27661	-5.3447	-18.711
Pentadecan-1-ol	759	1700	-10.32431	3.32013	-5.4785	-18.263
Hexadecan-1-ol	770	1610	-10.54087	3.47260	-6.0771	-15.939
Heptadecan-1-ol	780	1505	-10.73125	3.55515	-6.3591	-15.696
Octadecan-1-ol	790	1440	-10.91637	3.57835	-6.6199	-15.060
Nonadecan-1-ol	799	1380	-11.22657	4.03454	-7.0775	-11.970
Eicosan-1-ol	809	1300	-11.23154	3.66900	-7.0775	-14.321

TABLE 4

NORMAL BOILING POINTS and ACENTRIC FACTORS

	Normal Boiling Point						Acentric
	p= 101.325 kPa		760 mmHg		14.69595 psia		Factor
Name	$\frac{T}{K}$	$\frac{dT/dp}{K/kPa}$	$\frac{T}{deg.C}$	$\frac{dT/dp}{deg.C}$ per mmHg	$\frac{T}{deg.F}$	$\frac{dT/dp}{deg.F}$ per psia	
C ₇ ALKANOLS							
Heptan-1-ol	449.70	0.3407	176.55	0.04542	349.80	4.228	0.580
Heptan-2-ol	431.04	0.3359	157.89	0.04478	316.21	4.169	0.551
Heptan-3-ol	429.68	0.3324	156.53	0.04432	313.75	4.126	0.561
Heptan-4-ol	426.83	0.3275	153.68	0.04366	308.62	4.064	0.541
2-Methylhexan-2-ol	415.45	0.3206	142.30	0.04275	288.13	3.979	0.546
2,4-Dimethylpentan-3-ol	411.90	0.3330	138.75	0.04440	281.75	4.133	0.505
C ₈ ALKANOLS							
Octan-1-ol	468.33	0.3601	195.18	0.04801	383.32	4.469	0.594
Octan-2-ol	453.03	0.3559	179.88	0.04744	355.78	4.416	0.519
2-Ethylhexan-1-ol	457.77	0.3578	184.62	0.04771	364.32	4.441	0.553
4-Methyl-2-ethylpentan-1-ol	450.24	0.3499	177.09	0.04665	350.77	4.342	0.525
C ₉ ALKANOLS							
Nonan-1-ol	486.52	0.3789	213.37	0.05052	416.07	4.703	0.610
2,6-Dimethylheptan-4-ol	451.17	0.3668	178.02	0.04890	352.44	4.552	0.506
C ₁₀ to C ₂₀ ALKANOLS							
Decan-1-ol	504.25	0.3970	231.10	0.05293	447.98	4.927	0.629
Undecan-1-ol	521.24	0.4119	248.09	0.05492	478.56	5.113	0.656
Dodecan-1-ol	537.78	0.4264	264.63	0.05685	508.34	5.292	0.684
Tridecan-1-ol	553.72	0.4391	280.57	0.05854	537.03	5.449	0.712
Tetradecan-1-ol	569.04	0.4502	295.89	0.06002	564.60	5.587	0.744
Pentadecan-1-ol	583.68	0.4597	310.53	0.06129	590.96	5.705	0.778
Hexadecan-1-ol	597.53	0.4661	324.38	0.06214	615.88	5.784	0.818
Heptadecan-1-ol	610.96	0.4739	337.81	0.06318	640.06	5.881	0.853
Octadecan-1-ol	623.57	0.4787	350.42	0.06382	662.75	5.941	0.892
Nonadecan-1-ol	634.57	0.4873	361.42	0.06497	682.56	6.048	0.913
Eicosan-1-ol	647.69	0.4912	374.54	0.06548	706.17	6.096	0.954

TABLE 5
VAPOUR PRESSURE of C₇ ALKANOLS

Units: kPa v. K

1	C ₇ H ₁₆ O	Heptan-1-ol			n-Heptyl Alcohol		
2		Heptan-2-ol					
3		Heptan-3-ol					
4		Heptan-4-ol					
5		2-Methylhexan-2-ol					
6		2,4-Dimethylpentan-3-ol					
No.		1	2	3	4	5	6
T _C /K		632.5	607	604	602	584	583
p _C /kPa		3135	3000	2990	2980	2890	2890
T		p					
K		kPa					
630		3020.8					
625		2810.1					
620		2616.7					
615		2437.5					
610		2270.6					
605		2114.6	2916.6				
600		1968.4	2719.6	2824.0	2895.1		
595		1831.3	2535.7	2631.0	2697.1		
590		1702.4	2363.2	2450.9	2514.1		
585		1581.2	2201.1	2282.1	2343.6		
580		1467.2	2048.3	2123.5	2183.8	2727.4	2770.3
575		1360.0	1904.4	1974.3	2033.8	2538.5	2582.4
570		1259.0	1768.8	1833.8	1892.6	2362.3	2406.2
565		1164.0	1640.9	1701.5	1759.7	2197.3	2240.4
560		1074.6	1520.4	1576.9	1634.4	2042.3	2084.3
555		990.59	1406.9	1459.5	1516.2	1896.4	1937.1
550		911.64	1300.0	1349.0	1404.7	1759.2	1798.3
545		837.52	1199.4	1245.1	1299.6	1629.9	1667.4
540		768.01	1104.9	1147.3	1200.5	1508.2	1544.0
535		702.89	1016.0	1055.4	1107.1	1393.6	1427.7
530		641.97	932.72	969.21	1019.2	1285.7	1318.2
525		585.04	854.64	888.38	936.52	1184.3	1215.1
520		531.94	781.57	812.70	858.85	1088.9	1118.3
515		482.49	713.28	741.94	785.98	999.40	1027.3
510		436.53	649.56	675.87	717.69	915.44	942.04
505		393.89	590.21	614.29	653.82	836.80	862.15
500		354.42	535.01	556.99	594.17	763.24	787.43
495		317.96	483.78	503.78	538.58	694.54	717.65
490		284.38	436.33	454.46	486.87	630.49	652.61
485		253.52	392.47	408.84	438.87	570.90	592.08
480		225.25	352.02	366.76	394.44	515.55	535.85
475		199.42	314.80	328.02	353.40	464.26	483.74
470		175.89	280.65	292.45	315.61	416.83	435.54
465		154.54	249.39	259.88	280.89	373.09	391.05
460		135.23	220.86	230.15	249.11	332.86	350.10
455		117.82	194.89	203.09	220.10	295.95	312.48
450		102.20	171.34	178.53	193.71	262.19	278.04
445		88.229	150.05	156.33	169.79	231.41	246.57
440		75.797	130.87	136.32	148.20	203.43	217.92
435		64.782	113.65	118.36	128.77	178.10	191.90
430		55.070	98.255	102.31	111.37	155.24	168.36
425		46.550	84.544	88.008	95.857	134.71	147.13