

Vapour pressures and critical points of liquids: Organic oxygen 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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VAPOUR PRESSURES AND CRITICAL POINTS OF LIQUIDS: ORGANIC OXYGEN COMPOUNDS

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Compound Tables are given on data sheets in the following order:-

ALICYCLIC ALCOHOLS	Sheet
1. C ₅ H ₁₀ O Cyclopentanol	M.1.5
2. C ₆ H ₁₂ O Cyclohexanol	M.1.6

AROMATIC ALCOHOLS

3. C ₇ H ₈ O Benzyl alcohol	7-Hydroxytoluene	S.1.7
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ONE OXYGEN IN RING HETEROCYCLIC OXIDES

4. C ₂ H ₄ O Ethylene oxide	1,2-Epoxyethane	Oxirane	X.1.2
5. C ₃ H ₆ O Propylene oxide	1,2-Epoxypropane		X.1.3a
6. C ₄ H ₈ O Tetrahydrofuran	1,4-Epoxybutane	Tetramethylene oxide	X.1.4a
7. C ₅ H ₁₀ O 2-Methyltetrahydrofuran			X.1.5a
8. C ₄ H ₄ O Furan	1,4-Epoxybuta-1,3-diene	Furfuran	X.3.4
9. C ₅ H ₆ O 2-Methylfuran	Sylvan		X.3.5

TWO OXYGEN IN RING HETEROCYCLIC OXIDES

10. C ₄ H ₈ O ₂ 1,4-Dioxane	Ethylene glycol ethylene ether	Diethylene dioxide	Y.1.4
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VAPOUR PRESSURES AND CRITICAL POINTS OF LIQUIDS: ORGANIC OXYGEN COMPOUNDS

1. INTRODUCTION

This Data Item presents saturated vapour pressures of organic oxygen compounds arranged by chemical category as shown on the Contents page. Table 1 is the Compound Name Index showing both the preferred and alternative names, if any, of each compound. Table 2 is the Molecular Formula Index.

The Tables giving data for each compound are identified by a simple alpha-numeric code, the first character of which is the identifying letter of the compound category and the following number distinguishes groups, *e.g.* alkyl, alkenyl *etc.*, within that category. The third character of the code is the number of carbon atoms in the molecule and subsequent lower case letters distinguish isomers.

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

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

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

Equation 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.

The Tables have been made as self explanatory as possible and need little additional comment. The form of Wagner vapour pressure equation used and an explanation of the symbols is given at the top of each Table. The six constants required for the evaluation of the equation are shown below, followed by the acentric factor, the normal boiling point and the value of dT/dp at the normal boiling point. The approximate normal melting temperature is given, where known, to indicate the lower end of the liquid range.

The short table giving data at specified vapour pressures contains an assessment of the data quality, indicated by the letters 'X', 'A', 'B' or 'C', at these pressures. The estimated uncertainties in temperature and pressure which are dependent upon the data quality are shown underneath. This subject is discussed at greater length in Section 3.

Tabulated values of vapour pressure are presented in three sets of units. Those giving pressures in kPa for temperatures in kelvin also show the uncertainties in pressure and temperature. Pressures are given down to the melting temperature and values below 0.001 are given in exponent form. It is not possible to assess uncertainties below 0.1 kPa.

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 which 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 2.

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.

For most of the compounds considered here 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 finally selected for a number of compounds were obtained by fitting and extrapolating the high pressure range data where available or from correlations developed during the analysis of the data for a group of chemically related compounds.

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 the Tables according to a uniform pattern without regard to their estimated accuracy. The uncertainties in the values 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. 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 the Tables. For simplicity the uncertainties are given as 1, 2 or 5 times a power of 10.

In the Table giving temperatures at specified vapour pressures the letter 'X' indicates that the vapour pressures at the values above are derived from very high quality experimental data and that the uncertainty is considered less than the value shown. Such data are available for relatively few compounds. The majority of reliable data are considered quality 'A' with uncertainties up to 10 times those of quality 'X'. Similarly the letters 'B' and 'C' indicate that the vapour pressures are based on progressively less reliable data, the uncertainties increasing tenfold with each change of letter. Brackets enclose the letters 'A, B, C' 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 'C' 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.

4. ANTOINE EQUATION

Some Users may require 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 Table have been obtained by fitting this equation to values obtained from the Wagner equation between pressures of 5 and 200 kPa.

5. 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

Summary of constants in the Wagner vapour pressure equation

$$\ln p = \ln p_c + (T_c/T) (n_1q + n_2q^{3/2} + n_3q^{5/3} + n_4q^5)$$

Sheet	Name	T _c K	p _c kPa	n ₁	n ₂	n ₃	n ₄
M.1.5	Cyclopentanol	619.5	4900	-7.40989	1.71865	-6.8746	-4.360
M.1.6	Cyclohexanol	650	4260	-7.12855	1.40132	-5.6053	-9.576
S.1.7	Benzyl alcohol	715	4300	-7.29533	1.18307	-4.7323	-5.510
X.1.2	Ethylene oxide	469	7190	-6.80434	1.03715	-1.1972	-2.915
X.1.3a	Propylene oxide	482.3	4950	-7.21336	1.54999	-2.3414	-2.321
X.1.4a	Tetrahydrofuran	540	5130	-7.12293	1.76110	-2.3335	-2.444
X.1.5a	2-Methyltetrahydrofuran	537	3780	-7.44134	1.76039	-2.4293	-2.991
X.3.4	Furan	490	5615	-7.02682	1.54243	-1.8972	-3.467
X.3.5	2-Methylfuran	528	4810	-7.36263	1.69083	-2.2826	-2.934
Y.1.4	1,4-Dioxane	587	5265	-7.42978	1.71729	-2.3080	-3.601

TABLE 2
EMPIRICAL FORMULA INDEX

Formula	Table	Name	Alternative Names	
C_2H_4O	X.1.2	Ethylene oxide	1,2-Epoxyethane	Oxirane
C_3H_6O	X.1.3a	Propylene oxide	1,2-Epoxypropane	
$C_3H_8O_2$	E.1.3	2-Methoxyethanol	Ethylene glycol methyl ether	Methyl cellosolve
C_4H_4O	X.3.4	Furan	1,4-Epoxybuta-1,3-diene	Furfuran
C_4H_8O	X.1.4a	Tetrahydrofuran	1,4-Epoxybutane	Tetramethylene oxide
$C_4H_8O_2$	Y.1.4	1,4-Dioxane	Ethylene glycol ethylene ether	Diethylene dioxide
$C_4H_{10}O_2$	E.1.4	2-Ethoxyethanol	Ethylene glycol ethyl ether	Ethyl cellosolve
C_5H_6O	X.3.5	2-Methylfuran	Sylvan	
C_5H_8O	L.1.5	Cyclopentanone		
$C_5H_{10}O$	M.1.5	Cyclopentanol		
$C_5H_{10}O$	X.1.5a	2-Methyltetrahydrofuran		
$C_5H_{12}O_2$	E.1.5a	2-Propoxyethanol	Ethylene glycol propyl ether	Propyl cellosolve
$C_5H_{12}O_2$	E.1.5b	2-Isopropoxyethanol	Ethylene glycol isopropyl ether	Isopropyl cellosolve
$C_6H_{10}O$	L.1.6	Cyclohexanone		
$C_6H_{12}O$	M.1.6	Cyclohexanol		
$C_6H_{14}O_2$	E.1.6a	2-Butoxyethanol	Ethylene glycol butyl ether	Butyl cellosolve
$C_6H_{14}O_2$	E.1.6c	2-Isobutoxyethanol	Ethylene glycol isobutyl ether	Isobutyl cellosolve
C_7H_8O	S.1.7	Benzyl Alcohol	7-Hydroxytoluene	

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