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Vapour pressures and critical points of liquids

Alkyl Amides

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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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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 G.H.Walter, Head of Heat Transfer, Internal Flow and Physical Data.

KEEPING UP TO DATE

We are constantly striving to develop new work and review data already issued. Any comments arising out of your use of our data, or any suggestions for new topics or information that might lead to improvements, will help us to provide a better service.

(Continued on inside back cover)

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VAPOUR PRESSURES AND CRITICAL POINTS OF LIQUIDS
ALKYL AMIDES

CONTENTS

1.	INTRODUCTION	page 1
2.	NOTATION AND UNITS	page 2
3.	SOURCES OF DATA	page 2
4.	EVALUATION AND CORRELATION	page 2
5.	DISCUSSION OF UNCERTAINTIES	page 3
6.	ANTOINE EQUATION	page 3
7.	REFERENCES	page 4
	COMPOUND NAME INDEX	page 5
	COMPOUND TABLES in the following order	

Sheet No.	Formula	Name	Alternative Name
1.0	CH ₃ NO	Formamide	Methanamide
1.1	C ₂ H ₅ NO	N-Methylformamide	Formylmethanamine
1.2	C ₃ H ₇ NO	N,N-Dimethylformamide	Formyldimethanamine
1.3	C ₅ H ₁₁ NO	N,N-Diethylformamide	Formyldiethanamine
2.0	C ₂ H ₅ NO	Acetamide	Ethanamide
2.1	C ₃ H ₇ NO	N-Methylacetamide	Acetylmethanamine
2.2	C ₄ H ₉ NO	N,N-Dimethylacetamide	Acetyldimethanamine

VAPOUR PRESSURES AND CRITICAL POINTS OF LIQUIDS
ALKYL AMIDES

1. INTRODUCTION

This Data Item presents saturated vapour pressures of the alkyl amides arranged in the order shown on the Contents page. Table 1 is the Compound Name Index which lists alternative names of the compounds with, in bold, the first name used for each compound on the Contents page and at the head of each Table.

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 Table. 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 the 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 normal melting point.

In certain circumstances the user may need to allow for uncertainties in the tabulated values and estimates of these are provided in the Tables. For simplicity the uncertainties are rounded to 1, 2 or 5 times a power of 10.

The short table giving data at specified vapour pressures contains an assessment of the data quality, indicated by the letters '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 5.

Tabulated values of vapour pressure are presented in three sets of units, namely, (i) pressures in kPa at temperatures in kelvins, (ii) pressures in mmHg or atm at temperatures in degrees C, (iii) pressures in psia at temperatures in degrees F. The Table providing pressures in kPa also gives the uncertainties in pressure and temperature. Pressures are given from just above the melting point to a convenient temperature well above the normal boiling point.

Brackets enclose values above or below the range of supporting experimental data and values below 0.001 are given in exponent form. It is not feasible to assess uncertainties at pressures below 0.1 kPa or at the critical temperature when the data quality is denoted by 'C'.

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 Practical Temperature Scale (IPTS-68), the errors incurred by changing to ITS-90 are less than the uncertainties in the data. On IPTS-68 kelvin temperatures are strictly called International Practical Kelvin Temperatures, similarly Celsius temperatures are strictly called International Practical Celsius Temperatures.

b_1, b_2, b_3, b_4	non-dimensional coefficients of the Wagner vapour-pressure equation
p	vapour pressure
q	$(1-T/T_c)$
T	kelvin temperature
t	Celsius temperature ($T-273.15$) or Fahrenheit temperature ($9T/5-459.67$)

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.

For the alkyl amides considered here the data are restricted to the medium pressure range and values outside this range were obtained by estimation.

4. EVALUATION AND CORRELATION

Because of the difficulties in the experimental study of alkyl amides the data for these compounds are limited and often of low quality. The critical temperatures and critical pressures were estimated by the methods of References 1 and 2 respectively but it was not possible to develop a specific correlation for them. The equations given have been derived from the correlation for the alkanes described in Reference 3. Since this is likely to have limited applicability the Tables extend over a shorter range of temperature than is usually given in other Items.

5. 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 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 giving data at specified vapour pressures the data quality at each pressure is denoted by one of the letters 'A', 'B' or 'C'. Brackets enclose the letters at those pressures which are outside the range of supporting experimental data. 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 in temperature of 0.01 K at the normal boiling point or about 0.1 K at the critical point. 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. 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.

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.

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 between 0.05 and 0.1 per cent.

WARNING. Although, for most compounds, the Antoine equation may be used up to about 500 kPa without undue additional error, use at pressures outside the range 2 to 500 kPa will give vapour pressures that get progressively lower than the values given by the Wagner equation.

7. 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. Vapour pressures up to their critical temperatures of normal alkanes and alkan-1-ols. Pure & Appl.Chem., Vol.61, pp.1395-1403, 1989.
WALTON, J.