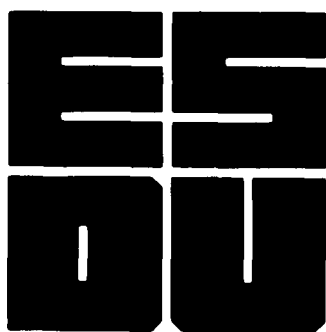




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Vapour pressures and critical points of liquids XI: Heterocyclic Nitrogen Compounds

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ENGINEERING SCIENCES DATA ITEM No. 77019

Physical Data, Chemical Engineering Sub-series

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The work of the permanent professional staff of the Engineering Sciences Data Unit on this particular Item was monitored and guided by the Physical Data and Reaction Kinetics Committee which has the following constitution:

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The work on this Item was carried out in the Fluid Mechanics and Physical Properties Group of the Engineering Sciences Data Unit under the supervision of Mr N.Thompson, Group Head. The member of staff who undertook the construction and subsequent development of the Item was

Mr J.Walton — Senior Engineer.

The Physical Data and Reaction Kinetics Committee, which first met in May 1966, has the co-operation of many engineers and scientists in industry, research establishments and universities from whom much assistance and information are being received. For this particular Item the initial assessment of the available information, the correlations and the tables calculated from them were prepared at the National Physical Laboratory. This work was supervised there by Dr D.Ambrose of the Division of Chemical Standards and was sponsored by ESDU.

In order to assist the preparation of new work, and particularly to assist the periodic review and revision of work already issued, users are encouraged to make known their experience in using the information and procedures and to notify the Unit of any additional information which they can provide or to which reference can be made. Prepaid reply service cards are available for this purpose. Whenever an Item is revised, users who are Associates of ESDU (i.e. have a standing

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(Continued on inside back cover)

VAPOUR PRESSURES AND CRITICAL POINTS OF LIQUIDS XI: HETEROCYCLIC NITROGEN COMPOUNDS

1. INTRODUCTION

This Data Item presents saturated vapour pressures of the heterocyclic nitrogen compounds listed in Table I (page 8).

The data on which the values in the Tables are based are the most reliable available and have been fitted and correlated by equations that are valid from the melting temperature (or triple point where it is known) upwards over the whole liquid range. Tabular values derived from these equations vary from just under 0.01 mmHg to the critical pressure, thus considerably extending the range of values obtainable from Antoine equations available for some of the compounds.

All quantities are expressed in SI units, in this case kN/m^2 and kelvins, but for users who require them in mmHg and $^{\circ}\text{C}$ some data are given in these units, and conversion factors to other units are provided in Section 3. Section 4 outlines the procedures used to derive the values of vapour pressure presented, Section 5 gives an explanation of the Tables, Section 6 discusses the uncertainties in the values presented and Section 7 gives a rapid interpolation procedure for use with the Tables.

In Section 8, References 1 to 19 are sources of supplementary reading matter. Derivations, the sources of systematic experimental investigations of vapour pressure data used or consulted in the preparation of the Item, are listed separately in ESDU Memorandum No.20, Reference 20.

Table I shows, for each compound, alternative names, empirical and structural formulae, molecular weight, normal boiling point and acentric factor. A foldout flap, attached to the last page, indexes each compound name against the number used to identify it in the Tables and shows the number and pages of the Table giving its vapour pressure data.

The values of vapour pressure given in the Tables were obtained by evaluating, for each compound, an equation in the form of a series of Chebyshev polynomials fitted to the data that had been selected and weighted in accordance with a critical assessment of all the data. The constants required for the evaluation of the Chebyshev equations are given in Appendix A and the constants of the approximately equivalent Wagner vapour pressure equations are given in Appendix B.

2. NOTATION AND UNITS

All temperatures are based on the International Practical Temperature Scale of 1968 (IPTS-68), which for practical purposes is interchangeable with the Thermodynamic Scale, see Reference 10.

The SI unit of pressure is the newton per square metre (N/m^2), which has now received the special name of pascal (Pa). A convenient multiple for the range of vapour pressures in this Data Item is the kilonewton per square metre (kN/m^2).

$a_0, a_1 \dots a_n$	constants for each compound in the Chebyshev Equation (see Appendix A)	K
b_1, b_2, b_3, b_4	non-dimensional constants for each compound in the Wagner Equation (see Appendix B)	

p	vapour pressure	kN/m ² or mmHg (torr)
T	thermodynamic temperature	K
t	Celsius temperature, $T - 273.15$	°C
ω	acentric factor, $-\log_{10} p_r - 1$ at $T_r = 0.7$	

Suffixes

b	denotes values at normal boiling point
c	denotes value at critical point
m	denotes value at melting point
r	denotes reduced quantity, e.g. $T_r = T/T_c$

3. CONVERSION FACTORS

A comprehensive set of conversion factors will be found in Appendix A of Item No. PD1 but the following are given here for convenience.

$$\begin{aligned}
 1 \text{ kN/m}^2 &= 7.500\,617 \text{ mmHg (torr)} = 1/0.133\,3224 \text{ mmHg (torr)} \\
 &= 9.869\,233 \times 10^{-3} \text{ atm} = 1/101.325 \text{ atm} \\
 &= 0.145\,0377 \text{ lbf/in}^2 = 1/6.894\,757 \text{ lbf/in}^2 \\
 &= 10.197\,16 \times 10^{-3} \text{ kgf/cm}^2 = 1/98.0665 \text{ kgf/cm}^2
 \end{aligned}$$

4. DERIVATION OF VAPOUR PRESSURES

4.1 Experimental Data

The available experimental data for each compound from the sources listed in Reference 20 were examined for consistency, compatibility and accuracy by comparing their deviations from a convenient baseline through the medium pressure range data. From this initial assessment, the data judged to be the best available for each compound were selected, extrapolated where necessary, and fitted and correlated as described in Section 4.2.

In each Derivation the experimental data reported are usually confined to one of three pressure ranges which may be considered as:—

- low pressure, below say 1 kN/m² (≈ 7.5 mmHg),
- medium pressure, say 1 kN/m² to 200 kN/m² (≈ 2 atm),
- high pressure, say 200 kN/m² to the critical point.

In the low pressure range data exist for only a few of the compounds. The bulk of the experimental data are restricted to the medium pressure range and data exist for all of the compounds. In the high pressure range reliable vapour pressure and/or critical point data exist for only fourteen of the liquids considered here, see Section 6.

4.2 Correlation and Extrapolation

The available critical point data were taken from the compilation by Ambrose and Townsend, Reference 17. The critical temperatures of the compounds and their homomorphic hydrocarbons were found to correlate well with their corresponding normal boiling points. Therefore the scheme described by Ambrose et al. in Reference 16 for the estimation of critical temperatures was extended to include all the compounds considered here.

With the critical temperatures known or estimated for each compound, the vapour pressures outside the experimental range, down to the melting temperature (or triple point where known) and up to the critical point were estimated, for the majority of the compounds, by fitting a Wagner equation¹⁴ (see Appendix B), to the most reliable experimental vapour pressure data for each compound.

The iterative procedure used to fit the Wagner equation to the data incorporated constraints that ensured that the fitted equation exhibited certain empirically established characteristics. These are:

- (i) that extrapolation to low reduced temperatures gives values of enthalpy of evaporation ΔH_e , conforming approximately to the Watson equation

$$\frac{\Delta H_{e1}}{\Delta H_{e2}} = \left(\frac{T_c - T_1}{T_c - T_2} \right)^{0.375},$$

- (ii) that a reversal of curvatures of the vapour pressure line $\log p$ plotted against $1/T$ occurs at $T_r \approx 0.85$,
(iii) that a minimum in the value of $\Delta H_e/\Delta Z$ occurs for $0.8 < T_r < 0.9$ where ΔZ is the change in the compression factor on evaporation.

For the remainder of the compounds considered the experimental data was too poor or too sparse to be treated in the above way. Using pyrrolidine and pyridine as reference compounds for the five and six membered ring compounds respectively, vapour pressures outside the experimental range were estimated by the method of Othmer and Yu⁹.

For continuity with previous Data Items, Chebyshev equations were, for each compound, fitted to the appropriately weighted experimental data and estimated values outside the experimental range. These Chebyshev equations, see Appendix A, were then used to produce the values of vapour pressure given in Tables II to XVII. The coefficients of the Wagner equations that closely approximate to these values are given in Appendix B.

There are few previous correlations of vapour pressure data for the compounds included here. Much of the experimental work on which the present values are based has been done quite recently.

Of particular importance is the very high quality work of Herington and coworkers in the UK and Douslin and coworkers in the USA on pyridine and the picolines in the medium pressure range. Their data differ by only a few hundredths of one per cent of the pressure so that the boiling points of these compounds between 10 kN/m² (≈ 75 mmHg) and 200 kN/m² (≈ 2 atm) are established to within ± 0.01 K. The data, on these and other related compounds, see Reference 20, together with the critical temperatures determined by Ambrose and coworkers and Kobe and coworkers, enable full range vapour pressure equations of these compounds to be derived with a high degree of precision.

5. EXPLANATION OF THE TABLES

The compounds are numbered 1 to 48 in Table I and the numbers are used to identify the compounds in the subsequent Tables where space does not permit the use of the name. The compounds are identified in the first column of Table I by a systematic name and for most compounds alternative names are also given.

The names in bold type are those based on BSI Recommendations, see References 6 and 12. The molecular weights, determined from values in the Table of Atomic Weights, 1971, in Reference 11, are also given in the column headed "Name". The values of normal boiling point are those given by the Chebyshev equation for 101.325 kN/m² (1 atmosphere). Other columns give the values of dT/dp in K m²/kN (i.e. K/kPa) and dt/dp in °C/mmHg at the normal boiling point and the acentric factor ω .

Tables IIa (units: K and kN/m²) and IIb (units: °C and mmHg) present values of temperature for selected values of vapour pressure. Values of triple point temperature and pressure are given where they are known but for the majority of compounds considered only the melting point is known and this temperature is given to indicate the lower end of the liquid range. The critical pressures quoted are those given by the Chebyshev equation at the selected critical temperatures.

Tables III to XVII present values of vapour pressure at 5 K intervals of temperature over the whole pressure range. The location of the Tables giving vapour pressure data is listed on the foldout flap attached to the last page.

6. ACCURACY OF TABLES

For case of interpolation, values are presented in Tables II to XVII according to a uniform pattern without regard to their estimated accuracy. Values dependent upon estimated critical properties are much less certain than those dependent upon measurement. The suggested uncertainties that the user should allow for are shown on page 5.

In the medium pressure range, 1 to 200 kN/m² the letters "A" and "B" relate to values based on the more reliable and less reliable experimental data respectively.

In the high pressure range, 200 kN/m² to the Critical Point, the letter "A" relates to values based upon reliable experimental critical point data, while the letter "B" relates to values dependent on less reliable experimental and estimated critical properties.

7. INTERPOLATION IN THE TABLES

Given T_1, p_1, T_3, p_3 and T_2 then p_2 may be obtained by interpolation from the Tables according to

$$\log p_2 = \log p_1 + \frac{T_3}{T_2} \left(\frac{T_2 - T_1}{T_3 - T_1} \right) (\log p_3 - \log p_1) \quad (1)$$

which may be arranged as

$$\frac{1}{T_2} = \frac{1}{T_1} - \left(\frac{T_3 - T_1}{T_1 T_3} \right) \left(\frac{\log p_2 - \log p_1}{\log p_3 - \log p_1} \right) \quad (2)$$

to give T_2 when p_2 is known.

Users who frequently require a large number of values of saturation temperature or vapour pressure to be computed may wish to fit an Antoine equation* to the values given. However this equation should only be fitted over relatively short ranges of pressure. At least four equations would probably be required to fit the range of pressures given in this Data Item. For evaluation of vapour pressures over a large range of pressure, the user is advised to evaluate the Chebyshev equation for the appropriate compounds. The data required are given in Appendix A and the procedure is given in Item No. PD1.

* $\log p = A + B/(T + C)$ where A, B and C are constants for a particular substance.

Uncertainties in Pressure and Temperature

Vapour pressure		kN/m ²	0.001	0.01	0.1	1	10	100	1 000	p_c
Vapour pressure		mmHg	0.01	0.1	1	10	100	1000	10 000	p_c
Uncertainty in pressure, per cent		$\left\{ \begin{matrix} A \\ B \end{matrix} \right\}$	50	20	10	0.5 2.0	0.2 1.0	0.02 0.1	0.2 1.0	1 10
Uncertainty in temperature, K or °C		$\left\{ \begin{matrix} A \\ B \end{matrix} \right\}$	5	2	1	0.1 0.5	0.05 0.25	0.01 0.05	0.2 1.0	0.5 5
1	Aziridine					B	B	B	B	B
2	Azetidine					B	B	B	B	B
3	Pyrrolidine					A	A	A	A	A
4	Pyrrole					A	A	A	B	B
5	1-Methylpyrrole					A	A	A	B	B
6	2,5-Dimethylpyrrole					A	A	A	B	B
7	Oxazole					B	B	B	B	B
8	Isoxazole					B	B	B	B	B
9	Piperidine					A	A	A	B	B
10	Perfluoropiperidine					A	A	A	B	B
11	2-Methylpiperidine					A	A	A	B	B
12	2-Methyl-5-ethylpiperidine					B	B	B	B	B
13	Pyridine					A	A	A	A	A
14	2-Chloropyridine					B	B	B	B	B
15	3-Bromopyridine					B	B	B	B	B
16	2-Methylpyridine					A	A	A	A	A
17	3-Methylpyridine					A	A	A	A	A
18	4-Methylpyridine					A	A	A	A	A
19	2-Ethylpyridine					B	B	B	B	B
20	3-Ethylpyridine					B	B	B	B	B
21	4-Ethylpyridine					B	B	B	B	B
22	2,3-Dimethylpyridine					A	A	A	A	A
23	2,4-Dimethylpyridine					A	A	A	A	A
24	2,5-Dimethylpyridine					A	A	A	A	A
25	2,6-Dimethylpyridine					A	A	A	A	A
26	3,4-Dimethylpyridine					A	A	A	A	A
27	3,5-Dimethylpyridine					A	A	A	A	A
28	4-Amino-2,6-dimethylpyridine					B	B	B	B	B
29	2-Methyl-5-ethylpyridine					B	B	B	B	B
30	2,4,6-Trimethylpyridine					B	B	B	B	B
31	2-Methyl-5-vinylpyridine					B	B	B	B	B
32	Piperazine					B	B	B	B	B
33	1-Methylpiperazine					B	B	B	B	B
34	cis-2,5-Dimethylpiperazine					B	B	B	B	B
35	Tetramethylpiperazine					B	B	B	B	B
36	1-Phenylpiperazine					B	B	B	B	B
37	Pyrazine					B	B	B	B	B
38	2-Methylpyrazine					A	A	A	A	A
39	Quinoline					A	A	A	B	B
40	Isoquinoline					A	A	A	B	B
41	2-Methylquinoline					A	A	A	B	B
42	4-Methylquinoline					A	A	A	B	B
43	6-Methylquinoline					A	A	A	B	B
44	7-Methylquinoline					A	A	A	B	B
45	8-Methylquinoline					A	A	A	B	B
46	3-Methylisoquinoline					A	A	A	B	B
47	2,4-Dimethylquinoline					A	A	A	B	B
48	2,6-Dimethylquinoline					A	A	A	B	B

At pressures in this range uncertainties for all compounds are as indicated above.

8. REFERENCES AND DERIVATION

References

1. STULL, D. Vapour pressures of pure substances. Organic compounds. *Ind. Engng Chem.*, Vol.39, pp.517-540, 1947.
2. KOBE, K.A.
LYNN, R.E. The critical properties of elements and compounds. *Chem. Rev.*, Vol.52, No.1, pp.117-236, 1953.
3. PITZER, K.S.
LIPPMAN, D.Z.
et al. The volumetric and thermodynamic properties of fluids. II: compressibility factor, vapour pressure and entropy of vaporization. *J. am. chem. Soc.*, Vol.77, pp.3430-3440, 1955.
4. — Vapour pressures of organic compounds in the range below one millimeter of mercury. NBS tech. Note 70, 1960.
5. — Landolt-Bernstein: Numerical and functional relationships in physics, chemistry, astronomy, geophysics and technology (in German). Springer-Verlag, Berlin. 6th Edition, Vol.II, Part 2a, pp.89-184, 1960.
6. — Recommended names for chemicals used in industry. British Standards Institution, B.S. 2474: 1965.
7. REID, R.C.
SHERWOOD, T.K. *The properties of liquids and gases: their correlation and estimation*. 2nd edition, McGraw-Hill Book Company, 1966.
8. KUDCHADKER, A.P.
ALANI, G.H.
ZWOLINSKI, B.J. The critical constants of organic substances. *Chem. Rev.*, Vol.68, pp.695-735, 1968.
9. OTHMER, D.F.
YU, E.S. Correlating vapour pressure and vapour volumes — use of reference substance equations. *Ind. Engng Chem.*, Vol.60, No.1, pp.22-35, 1968.
10. — The International Practical Temperature Scale of 1968. HMSO, London, 1968.
11. — Atomic weights of the elements, 1971. Engineering Sciences Data Item No. PD2, 1973.
12. — Classification of chemicals in the Brussels Nomenclature and in the United Kingdom Custom and Excise Tariff. HMSO, London, 1973.
13. AMBROSE, D. Vapour pressures. *Chemical Thermodynamics*, Vol.1 (Specialist Periodical Reports), The Chemical Society, London, 1973.
14. WAGNER, W. New vapour pressure measurements for argon and nitrogen and a new method for establishing rational vapour pressure equations. *Cryogenics*, Vol.13, pp.470-482, 1973.
15. AMBROSE, D. Vapour pressure equations. NPL Report Chem.19, National Physical Laboratory, Teddington, Middlesex, UK, November 1972, Corrected February 1974.

16. AMBROSE, D.
BRODERICK, B.E.
TOWNSEND, R. The critical temperatures and pressures of thirty organic compounds. *J. appl. Chem. Biotechnol.*, Vol.24, pp.359-372, 1974.
17. AMBROSE, D.
TOWNSEND, R. Vapour-liquid critical properties. National Physical Laboratory, Teddington, Middlesex, UK, 1975.
18. — Selected values of properties of chemical compounds, Thermodynamics Research Center Data Project. Thermodynamics Research Center, Texas A and M University, College Station, Texas, USA. (Loose leaf data sheets, extant 1977.)
19. REID, R.C.
PRAUSNITZ, J.M.
SHERWOOD, T.K. *The properties of liquids and gases*. 3rd edition, McGraw-Hill Book Company, 1977.
20. WALTON, J. Vapour pressures of liquids. Literature survey No.2: organic nitrogen compounds. ESDU Memor. No.20, 1977.

Derivation

Reference 20 lists all the sources of data which were considered in the preparation of this Item.

TABLE 1 (Part 1)
Heterocyclic Nitrogen Compounds

No.	Name			Alternative names	
	(Name based on BSI Recommendations in Bold Type)				
			M.W.		
1	C_2H_5N	Aziridine	43.068	Dihydroazirane	Ethyleneimine
2	C_3H_7N	Azetidine	57.095		Trimethyleneimine
3	C_4H_9N	Pyrrolidine	71.122	Tetrahydropyrrole	Tetramethyleneimine
4	C_4H_5N	Pyrrole	67.090	Azole	
5	C_5H_7N	1-Methylpyrrole	81.117	N-Methylpyrrole	
6	C_6H_9N	2,5-Dimethylpyrrole	95.144		
7	C_3H_3NO	Oxazole	69.063		
8	C_3H_3NO	Isoxazole	69.063		
9	$C_5H_{11}N$	Piperidine	85.149	Hexahydropyridine	Pentamethyleneimine
10	$C_5F_{11}N$	Perfluoropiperidine	283.044		
11	$C_6H_{13}N$	2-Methylpiperidine	99.175		
12	$C_8H_{17}N$	2-Methyl-5-ethylpiperidine	127.229		
13	C_5H_5N	Pyridine	79.101	Azine	
14	C_5H_4ClN	2-Chloropyridine	113.546		
15	C_5H_4BrN	3-Bromopyridine	157.997		
16	C_6H_7N	2-Methylpyridine	93.128	2-Picoline	
17	C_6H_7N	3-Methylpyridine	93.128	3-Picoline	
18	C_6H_7N	4-Methylpyridine	93.128	4-Picoline	
19	C_7H_9N	2-Ethylpyridine	107.155		
20	C_7H_9N	3-Ethylpyridine	107.155		
21	C_7H_9N	4-Ethylpyridine	107.155		
22	C_7H_9N	2,3-Dimethylpyridine	107.155	2,3-Lutidine	
23	C_7H_9N	2,4-Dimethylpyridine	107.155	2,4-Lutidine	
24	C_7H_9N	2,5-Dimethylpyridine	107.155	2,5-Lutidine	
25	C_7H_9N	2,6-Dimethylpyridine	107.155	2,6-Lutidine	
26	C_7H_9N	3,4-Dimethylpyridine	107.155	3,4-Lutidine	
27	C_7H_9N	3,5-Dimethylpyridine	107.155	3,5-Lutidine	
28	$C_7H_{10}N_2$	4-Amino-2,6-dimethylpyridine	122.169	4-Amino-2,6-butidine	
29	$C_8H_{11}N$	2-Methyl-5-ethylpyridine	121.182	5-Ethyl-2-picoline	
30	$C_8H_{11}N$	2,4,6-Trimethylpyridine	121.182	2,4,6-Collidine	
31	C_8H_9N	2-Methyl-5-vinylpyridine	119.166	5-Vinyl-2-picoline	
32	$C_4H_{10}N_2$	Piperazine	86.136	Hexahydropyrazine	Diethylenediamine
33	$C_5H_{12}N_2$	1-Methylpiperazine	100.163		
34	$C_6H_{14}N_2$	cis-2,5-Dimethylpiperazine	114.190		
35	$C_8H_{18}N_2$	Tetramethylpiperazine	142.244		
36	$C_{10}H_{14}N_2$	1-Phenylpiperazine	162.234		
37	$C_4H_4N_2$	Pyrazine	80.089	1,4-Diazine	Paradiazine
38	$C_5H_6N_2$	2-Methylpyrazine	94.116		
39	C_9H_7N	Quinoline	129.161		
40	C_9H_7N	Isoquinoline	129.161		
41	$C_{10}H_9N$	2-Methylquinoline	143.188	Quinaldine	
42	$C_{10}H_9N$	4-Methylquinoline	143.188	Lepidine	
43	$C_{10}H_9N$	6-Methylquinoline	143.188		
44	$C_{10}H_9N$	7-Methylquinoline	143.188		
45	$C_{10}H_9N$	8-Methylquinoline	143.188		
46	$C_{10}H_9N$	3-Methylisoquinoline	143.188		
47	$C_{11}H_{11}N$	2,4-Dimethylquinoline	157.215	4-Methylquinaldine	
48	$C_{11}H_{11}N$	2,6-Dimethylquinoline	157.215	6-Methylquinaldine	

TABLE 1 (Part 2)
General Information

No.	Name	Structural formula Also see page 28	Normal Boiling Point				Acentric factor ω
			$p = 101.325 \text{ kN/m}^2$		$p = 760 \text{ mmHg}$		
			T K	dT/dp K m ² /kN	t °C	dt/dp °C/mmHg	
1	Aziridine	$\text{C}_2\text{H}_4\text{NH}$	328.55	0.2605	55.40	0.03473	0.432
2	Azetidine	$\text{C}_3\text{H}_6\text{NH}$	333.25	0.2726	60.10	0.03634	0.275
3	Pyrrolidine	$\text{C}_4\text{H}_8\text{NH}$	359.70	0.3094	86.55	0.04125	0.273
4	Pyrrole	$\text{C}_4\text{H}_4\text{NH}$	402.93	0.3304	129.78	0.04405	0.340
5	1-Methylpyrrole	$\text{C}_4\text{H}_4\text{NCH}_3$	385.90	0.3320	112.75	0.04427	0.311
6	2,5-Dimethylpyrrole	$(\text{CH}_3)_2\text{C}_4\text{H}_2\text{NH}$	440.67	0.3461	167.52	0.04614	0.446
7	Oxazole	$\text{C}_3\text{H}_3\text{NO}$	342.65	0.2997	69.50	0.03996	0.352
8	Isoxazole	$\text{C}_3\text{H}_3\text{NO}$	368.40	0.3215	95.25	0.04287	0.353
9	Piperidine	$\text{C}_5\text{H}_{10}\text{NH}$	379.37	0.3362	106.22	0.04483	0.241
10	Perfluoropiperidine	$\text{C}_5\text{F}_{10}\text{NF}$	322.75	0.2880	49.60	0.03839	0.410
11	2-Methylpiperidine	$(\text{CH}_3)\text{C}_5\text{H}_9\text{NH}$	391.44	0.3526	118.29	0.04701	0.269
12	2-Methyl-5-ethylpiperidine	$(\text{CH}_3)(\text{C}_2\text{H}_5)\text{C}_5\text{H}_8\text{NH}$	436.55	0.3842	163.40	0.05122	0.373
13	Pyridine	$\text{C}_5\text{H}_5\text{N}$	388.40	0.3404	115.25	0.04539	0.242
14	2-Chloropyridine	$\text{ClC}_5\text{H}_4\text{N}$	443.58	0.3844	170.43	0.05125	0.287
15	3-Bromopyridine	$\text{BrC}_5\text{H}_4\text{N}$	446.74	0.3901	173.59	0.05201	0.277
16	2-Methylpyridine	$(\text{CH}_3)\text{C}_5\text{H}_4\text{N}$	402.56	0.3522	129.41	0.04696	0.300
17	3-Methylpyridine	$(\text{CH}_3)\text{C}_5\text{H}_4\text{N}$	417.31	0.3656	144.16	0.04874	0.296
18	4-Methylpyridine	$(\text{CH}_3)\text{C}_5\text{H}_4\text{N}$	418.52	0.3667	145.38	0.04890	0.297
19	2-Ethylpyridine	$(\text{C}_2\text{H}_5)\text{C}_5\text{H}_4\text{N}$	421.76	0.3641	148.61	0.04855	0.363
20	3-Ethylpyridine	$(\text{C}_2\text{H}_5)\text{C}_5\text{H}_4\text{N}$	438.49	0.3830	165.34	0.05106	0.342
21	4-Ethylpyridine	$(\text{C}_2\text{H}_5)\text{C}_5\text{H}_4\text{N}$	440.05	0.3815	166.90	0.05086	0.353
22	2,3-Dimethylpyridine	$(\text{CH}_3)_2\text{C}_5\text{H}_3\text{N}$	434.33	0.3769	161.18	0.05025	0.347
23	2,4-Dimethylpyridine	$(\text{CH}_3)_2\text{C}_5\text{H}_3\text{N}$	431.58	0.3741	158.43	0.04987	0.360
24	2,5-Dimethylpyridine	$(\text{CH}_3)_2\text{C}_5\text{H}_3\text{N}$	430.18	0.3743	157.03	0.04990	0.357
25	2,6-Dimethylpyridine	$(\text{CH}_3)_2\text{C}_5\text{H}_3\text{N}$	417.21	0.3614	144.06	0.04818	0.367
26	3,4-Dimethylpyridine	$(\text{CH}_3)_2\text{C}_5\text{H}_3\text{N}$	452.32	0.3931	179.17	0.05240	0.341
27	3,5-Dimethylpyridine	$(\text{CH}_3)_2\text{C}_5\text{H}_3\text{N}$	445.09	0.3862	171.94	0.05149	0.360
28	4-Amino-2,6-dimethylpyridine	$(\text{NH}_2)(\text{CH}_3)_2\text{C}_5\text{H}_2\text{N}$	519.15	0.4176	246.00	0.05567	0.544
29	2-Methyl-5-ethylpyridine	$(\text{CH}_3)(\text{C}_2\text{H}_5)\text{C}_5\text{H}_3\text{N}$	451.45	0.3939	178.30	0.05252	0.393
30	2,4,6-Trimethylpyridine	$(\text{CH}_3)_3\text{C}_5\text{H}_2\text{N}$	443.55	0.3859	170.40	0.05144	0.413
31	2-Methyl-5-vinylpyridine	$(\text{CH}_3)(\text{C}_2\text{H}_3)\text{C}_5\text{H}_3\text{N}$	455.38	0.3958	182.23	0.05277	0.379
32	Piperazine	$\text{C}_4\text{H}_8\text{N}_2\text{H}_2$	419.20	0.3749	146.05	0.04998	0.244
33	1-Methylpiperazine	$\text{C}_4\text{H}_8\text{NHNCH}_3$	411.15	0.3567	138.00	0.04756	0.322
34	cis-2,5-Dimethylpiperazine	$(\text{CH}_3)_2\text{C}_4\text{H}_6\text{N}_2\text{H}_2$	438.38	0.3856	165.23	0.05141	0.404
35	Tetramethylpiperazine	$(\text{CH}_3)_4\text{C}_4\text{H}_4\text{N}_2\text{H}_2$	455.53	0.4041	182.38	0.05387	0.429
36	1-Phenylpiperazine	$\text{C}_4\text{H}_8\text{NHNHC}_6\text{H}_5$	559.65	0.4593	286.50	0.06123	0.443
37	Pyrazine	$\text{C}_4\text{H}_4\text{N}_2$	388.69	0.3390	115.54	0.04520	0.240
38	2-Methylpyrazine	$(\text{CH}_3)\text{C}_4\text{H}_3\text{N}_2$	407.26	0.3537	134.11	0.04716	0.292
39	Quinoline	$\text{C}_9\text{H}_7\text{N}$	510.84	0.4618	237.69	0.06156	0.262
40	Isoquinoline	$\text{C}_9\text{H}_7\text{N}$	516.45	0.4547	243.30	0.06062	0.268
41	2-Methylquinoline	$(\text{CH}_3)\text{C}_9\text{H}_6\text{N}$	520.95	0.4312	247.80	0.05748	0.406
42	4-Methylquinoline	$(\text{CH}_3)\text{C}_9\text{H}_6\text{N}$	538.84	0.4325	265.69	0.05766	0.481
43	6-Methylquinoline	$(\text{CH}_3)\text{C}_9\text{H}_6\text{N}$	538.27	0.4571	265.12	0.06094	0.386
44	7-Methylquinoline	$(\text{CH}_3)\text{C}_9\text{H}_6\text{N}$	530.92	0.4310	257.77	0.05746	0.448
45	8-Methylquinoline	$(\text{CH}_3)\text{C}_9\text{H}_6\text{N}$	521.11	0.4300	247.96	0.05733	0.391
46	3-Methylisoquinoline	$(\text{CH}_3)\text{C}_9\text{H}_6\text{N}$	526.36	0.4396	253.21	0.05861	0.351
47	2,4-Dimethylquinoline	$(\text{CH}_3)_2\text{C}_9\text{H}_5\text{N}$	540.43	0.4587	267.28	0.06116	0.369
48	2,6-Dimethylquinoline	$(\text{CH}_3)_2\text{C}_9\text{H}_5\text{N}$	538.60	0.4570	265.45	0.06093	0.370