

Thermodynamic and Thermophysical Properties of Organic Nitrogen Compounds. Part II. 1- and 2-Butanamine, 2-Methyl-1-Propanamine, 2-Methyl-2-Propanamine, Pyrrole, 1-,2-, and 3-Methylpyrrole, Pyridine, 2-,3-, and 4-Methylpyridine, Pyrrolidine, Piperidine, Indole, Quinoline, Isoquinoline, Acridine, Carbazole, Phenanthridine, 1- and 2-Naphthalenamine, and 9-Methylcarbazole

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Thermodynamic and Thermophysical Properties of Organic Nitrogen Compounds.

Part II. 1- and 2-Butanamine, 2-Methyl-1-Propanamine, 2-Methyl-2-Propanamine, Pyrrole, 1-, 2-, and 3-Methylpyrrole, Pyridine, 2-, 3-, and 4-Methylpyridine, Pyrrolidine, Piperidine, Indole, Quinoline, Isoquinoline, Acridine, Carbazole, Phenanthridine, 1- and 2-Naphthalenamine, and 9-Methylcarbazole

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The thermodynamic and thermophysical properties of 1- and 2-butanamine, 2-methyl-1-propanamine, 2-methyl-2-propanamine, pyrrole, 1-, 2- and 3-methylpyrrole, pyridine, 2-, 3-, and 4-methylpyridine, pyrrolidine, piperidine, indole, quinoline, isoquinoline, acridine, carbazole, phenanthridine, 1- and 2-naphthalenamine, and 9-methylcarbazole have been evaluated. Recommended values are given for the following properties: normal boiling, freezing and triple point temperatures, critical constants, thermodynamic properties in the solid and liquid phases, vapor pressure, enthalpy of vaporization, density, second virial coefficients, and enthalpy of combustion. Ideal gas thermodynamic properties have been calculated by statistical mechanical methods.

Key words: acridine; 1-butanamine; 2-butanamine; carbazole; condensed phase thermodynamic properties; critically evaluated data; density; enthalpy of combustion; enthalpy of vaporization; heat capacity; ideal gas thermodynamic properties; indole; isoquinoline; 2-methyl-1-propanamine; 2-methyl-2-propanamine; 9-methylcarbazole; 2-methylpyridine; 3-methylpyridine; 4-methylpyridine; 1-methylpyrrole; 2-methylpyrrole; 3-methylpyrrole; 1-naphthalenamine; 2-naphthalenamine; phenanthridine; piperidine; pyridine; pyrrole; pyrrolidine; quinoline; second virial coefficient; thermochemistry; thermodynamics; thermophysics; vapor pressure.

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1. Introduction

1.1. Scope and Objectives

This report, the second in a series, provides a compilation of a consistent set of evaluated physical and thermodynamic properties of a selected group of organic nitrogen compounds. The critical evaluation of the thermodynamic and physical properties of chemical substances in the crystal, liquid and gas state, including the ideal gas state has been a principal research product at the Thermodynamics Research Center (TRC) for many years. The evaluations presented in this report constitute part of a research contract entitled "Selected Values of Properties of Chemical Compounds: Organic Nitrogen Compounds" between TRC and the Office of Standard Reference Data of the National Institute for Standards and Technology.

Part II (this report) contains thermodynamic data of the following organic nitrogen compounds: 1- and 2-butanamine, 2-methyl-1-propanamine, 2-methyl-2-propanamine, pyrrole, 1-, 2-, and 3-methylpyrrole, pyridine, 2-, 3-, and 4-methylpyridine, pyrrolidine, piperidine, indole, quinoline, isoquinoline, carbazole, acridine, phenanthridine, 1- and 2-naphthalenamine, and

9-methylcarbazole. Literature measurements were evaluated for the following properties: normal boiling, freezing and triple point temperatures, critical constants, vapor pressure, enthalpy of vaporization, density, second virial coefficient, solid, liquid, and gas heat capacity and enthalpy of combustion. The ideal gas thermodynamic properties were calculated by statistical mechanical methods.

Estimates of precision were assigned to all the experimental results, and temperature dependent selected values were obtained from smoothing equations. Coefficients of the smoothing equations are listed. Where appropriate, estimates of inaccuracy limits are provided for recommended values.

1.2. Organization of the Report

The details of the smoothing equations, the recommended coefficients as well as the recommended values at selected temperatures for each compound are discussed for each property in the appropriate subsections of Sec. 2. Merits of the available experimental and spectroscopic measurements are discussed for each compound in Sec. 3. The organization is by property rather than compound.

1.3. References and Literature Coverage

Most of the selected values are based on experimental measurements of either thermophysical and thermodynamic properties or spectra. The majority of the information is from pertinent journals and periodicals. Additional information came from private and government reports, theses and other sources. The majority of the values was taken from the original documents. Chemical Abstracts, other reviews, and the TRC Source files were used to obtain references to the primary sources.

1.4. Symbols, Units, Standard States, Temperature Scale and Naming Conventions

Symbols used are those recently recommended by the International Union of Pure and Applied Chemistry (IUPAC) (1988–121) (1982–150), and the units used are either multiples or sub-multiples of the base SI units. The fundamental constants recommended by the Committee on Data for Science and Technology (CODATA) of the International Council of Scientific Union (ICSU) in 1987 (1987–158) and the relative atomic masses recommended by IUPAC in 1989 (1991–109) were used for all calculations. Some of the results are in dimensionless forms derived with the gas constant of $8.31451 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$. The relative molar masses are listed in Table 23. The standard state pressure was taken to be 0.1 MPa. The standard states of the elements used in the calculation of the enthalpy of formation were the ideal gas at 0.1 MPa for H_2 and N_2 and graphite for carbon. Where there was adequate documentation for the temperature scale used, vapor pressure and heat capacity data were converted to the International Practical Temperature Scale of 1990 (ITS-90) (1990–427). There was a slight statistical advantage in making the temperature scale corrections to vapor pressure measurements. In most cases, the corrections were less than the experimental uncertainties. Corrections due to the change of temperature scale to ITS-90 were as much as 0.1 percent for condensed phase heat capacity values at high temperatures (which is of the same order of magnitude as the experimental uncertainties). However, the corrections are negligible for the integrated thermodynamic functions.

IUPAC nomenclature (1979–194) is used for the compound names. The accepted names, Chemical Abstracts registry numbers, empirical formulas, and some of the more commonly used synonyms are as follows:

- 1-butanamine, 109–73–9, $\text{C}_4\text{H}_{11}\text{N}$, 1-aminobutane, butylamine;
- 2-butanamine, 13952–84–6, $\text{C}_4\text{H}_{11}\text{N}$, 2-aminobutane, sec-butylamine;
- 2-methyl-1-propanamine, 78–81–9, $\text{C}_4\text{H}_{11}\text{N}$, 1-amino-2-methylpropanamine, isobutylamine;
- 2-methyl-2-propanamine, 75–64–9, $\text{C}_4\text{H}_{11}\text{N}$, *tert*-butylamine, 2-amino-2-methylpropane;
- pyrrole, 109–97–7, $\text{C}_4\text{H}_5\text{N}$, azole, 1 *H*-pyrrole, imidole;
- 1-methylpyrrole, 96–54–8, $\text{C}_5\text{H}_7\text{N}$, methyl-1 *H*-pyrrole, *N*-methylpyrrole;

- 2-methylpyrrole, 636–41–9, $\text{C}_5\text{H}_7\text{N}$, 2-methyl-1 *H*-pyrrole;
- 3-methylpyrrole, 616–43–3, $\text{C}_5\text{H}_7\text{N}$, 1 *H*-pyrrole, 3-methyl-;
- pyridine, 110–86–1, $\text{C}_5\text{H}_5\text{N}$, azine;
- 2-methylpyridine, 109–06–8, $\text{C}_6\text{H}_7\text{N}$, 2-picoline, α -picoline;
- 3-methylpyridine, 108–99–6, $\text{C}_6\text{H}_7\text{N}$, 3-picoline, β -picoline;
- 4-methylpyridine, 108–89–4, $\text{C}_6\text{H}_7\text{N}$, 4-picoline, γ -picoline;
- pyrrolidine, 123–75–1, $\text{C}_4\text{H}_9\text{N}$, tetrahydropyrrole, tetramethyleneimine;
- piperidine, 110–89–4, $\text{C}_5\text{H}_{11}\text{N}$, cyclopentimine, cycpenthylhexahydropyridine, azocyclohexane;
- indole, 120–72–9, $\text{C}_8\text{H}_7\text{N}$, 1-benzazole, 2,3-benzapyrrole, 1 *H*-indole;
- quinoline, 91–22–5, $\text{C}_8\text{H}_7\text{N}$, benzo[b]pyridine, 1-benzazine;
- isoquinoline, 119–65–3, $\text{C}_9\text{H}_7\text{N}$, benzo[c]pyridine, 2-benzazine;
- carbazole, 86–74–8, $\text{C}_{12}\text{H}_9\text{N}$, 9 *H*-carbazole, dibenzopyrrole, 9-azafluorene;
- acridine, 260–94–6, $\text{C}_{13}\text{H}_9\text{N}$, dibenzo[b,c]pyridine, 10-azaanthracene;
- phenanthridine, 229–87–8 $\text{C}_{13}\text{H}_9\text{N}$, 3,4-benzoquinoline, 9-azaphenanthrene, benzo[c]quinoline;
- 1-naphthalenamine, 134–32–7, $\text{C}_{10}\text{H}_9\text{N}$, 1-naphthylamine, α -naphthylamine, 1-aminonaphthalene;
- 2-naphthalenamine, 91–59–8, $\text{C}_{10}\text{H}_9\text{N}$, 2-naphthylamine, β -naphthylamine, 2-aminonaphthalene;
- 9-methylcarbazole, 1484–12–4, $\text{C}_{12}\text{H}_9\text{N}$, 9-methyl-9 *H*-carbazole;

1.5. Procedures for Evaluation, Processing and Selection of Data

The following steps were used in this compilation.

- (1) Search the scientific literature, identify the sources of data and record the pertinent numerical values in the TRC Source Database.
- (2) Rate and evaluate the available data on the basis of accuracy and reliability and sort out the “best” numerical values.
- (3) Convert the data to a uniform set of units and conditions and adjust them to the current set of fundamental constants and relative molar masses.
- (4) Make preliminary choice of “reliable” values and, where appropriate, fit them to standard functions of temperature, pressure or other variables for further testing.
- (5) Test the preliminary choices for internal thermodynamic consistency and make necessary adjustments to achieve consistency to within the experimental uncertainty.
- (6) Calculate the values of the derived properties from the final choices of the basic input data.
- (7) Estimate the uncertainties in the selected values.

The evaluation of the available data was based entirely on the judgment of the compilers, and no rigorous rules can be stated. Considerations were given to sample purity and experimental technique as described in the publications, as well as to the reputation of the authors for reliable work. Normally, more weight was given to a value obtained as the principal objective of an investigation rather than as a by-product of some other study. Often the best values were obvious. However, in many cases, after eliminating the obviously inconsistent data, several reported values of about comparable reliability were left. In such cases a properly weighted combination of the values was chosen. In some situations it was necessary to combine measurements of different reliability to obtain the final selections. For example, a series of accurate measurements of the vapor pressure of a specific compound was available over a certain range of temperature and another series of less reliable values was available outside that range. To obtain a smoothed set of selected values over the extended temperature range it was necessary to fit both sets of results to the same function of temperature. It was more common to have several sets of results of varying reliability for various temperature ranges which partially or completely overlapped. In fitting all of these results to a single function of temperature, more weight was given to the more reliable values. However, in some cases, the resulting equation did not reproduce the best results as well as desired, so the less reliable results were rejected. While there are cases in which the values of density or vapor pressure, as calculated from the selected equation, do not reproduce all results to within the imprecisions of the original results, such discrepancies are small and not much greater than the experimental uncertainty.

1.6. Fitting to Equations

Coefficients to smoothing equations were determined by weighted least squares where the weights in the squared deviation functions were the reciprocals of the variances in the deviation functions (1967–292), and the variances were determined from estimates of the imprecisions in the observed variables. Data were given zero weight either if they were obviously discordant with sets deemed most reliable, or if their inclusion would place undue weight on a particular point or region in the fit. Estimates of imprecision $\sigma(x)$ in the experimental observations x are given in the form:

$$\sigma(x) = \sigma_c(x) + x\sigma_f(x) \quad (1)$$

where the values of the constants $\sigma_c(x)$ and $\sigma_f(x)$ are tabulated in the tables that summarize sources and ranges of the measurements.

Imprecisions in the values derived from the fitting equations were determined by propagation of errors with the inverse of the normal equations for the weighted least squares process, variance-covariance matrix (1944–236),

(1986–789). The square roots from the principal diagonal of these matrices were used to calculate the standard deviations, $\sigma(A_i)$, listed with each of their associated parameters, A_i , in the appropriate tables. The off-diagonal elements were normalized by dividing the elements in each row and each column by the respective square root of the diagonal belonging to the row or column to give elements $C(A_i, A_j)$ in the correlation matrix. The diagonal elements of the correlation matrix, $C(A_i, A_i)$, are unity. Imprecision in the values for a function, $Y(A_1, A_2, \dots)$, of the parameters, $A_1, A_2, \dots$, was calculated from:

$$\sigma(Y) = \left\{ \sum_i \sum_j \left(\frac{\partial Y}{\partial A_i} \right) \sigma(A_i) C(A_i, A_j) \left(\frac{\partial Y}{\partial A_j} \right) \sigma(A_j) \right\}^{1/2}. \quad (2)$$

In many instances the parameters, A_i , are highly correlated so that the absolute values of $C(A_i, A_j)$ are close to unity and the right hand side of Eq. (2) is close to a perfect square with mixed signs on the cross product terms. The extent of these correlations required that the number of digits listed for the constants is greater than is apparently warranted by the imprecision in each of the parameters.

In instances where parameters with known imprecisions were constrained to predetermined values, the contributions from their imprecisions were determined by perturbing each constrained parameter in question by its imprecision and then repeating the least squares process. The estimated imprecisions of the derived values of the properties are shown on the plots of deviations from the fitting equations.

2. Recommended Values

2.1. Freezing, Normal Boiling and Critical Temperatures with Critical Pressure and Volume

The selected freezing (T_m), normal boiling (T_b) (at 101.325 kPa) and critical temperatures (T_c), with the selected critical pressure (p_c) and critical volume (V_c) and the estimated uncertainties are listed in Table 1. The measurements considered in the selections are discussed in Sec. 3.1. The values for the normal boiling temperature were derived from the Cox equation used for fitting the vapor pressure results.

2.2. Vapor Pressure

The vapor pressure (p_{sat}) measurements were smoothed with the Cox equation (1936–431):

$$\ln(p_{\text{sat}}/p_{\text{ref}}) = A_x \{1 - 1/(T/T_{\text{ref}})\}, \quad (3a)$$

where

$$\ln A_x = A_0 + A_1(T/T_{\text{ref}}) + A_2(T/T_{\text{ref}})^2. \quad (3b)$$

T_{ref} and p_{ref} are a reference temperature and pressure, respectively. In this work, the boiling temperature T_b at

atmospheric pressure (101.325 kPa) was chosen as the reference temperature T_{ref} . Values of the parameters A_i and T_b with their associated imprecisions are listed in Table 2, and the correlation matrix for the Cox equation coefficients is listed in Table 2a. The values of vapor pressures at selected temperatures are listed in Table 3.

We also report constants for the Antoine equation because the equation is commonly used to fit vapor pressure measurements over a limited pressure range, and the majority of TRC tables contain values calculated from either the Antoine or extended Antoine equation (1988–1991). The coefficients of the Antoine equation were determined for the following three pressure ranges: a, triple point pressure p_{tp} to 20 kPa; b, 20 kPa to 200 kPa; and c, 130 kPa to the critical pressure p_c . For the first two pressure ranges, the three parameter Antoine equation was used.

$$\ln(p_{\text{sat}}/\text{kPa}) = A_a - B_a/(T/\text{K} + C_a) \quad (4)$$

For the higher pressure range, an extended Antoine equation was used:

$$\log_{10}(p_{\text{sat}}/\text{kPa}) = A_a - B_a/(T/\text{K} + C_a) + D_a X_a^2 + E_a X_a^3 + F_a X_a^{12} \quad (5)$$

where $X_a = (T - T_a^{\circ})/T_c$, $D_a = \log_{10}e = 0.43429$, T_c is the critical temperature and T_a° was determined from the nearest integer value of Celsius temperature at which the vapor pressure is 130 kPa. The coefficients for the medium and high pressure Antoine equation were adjusted to yield the same normal boiling temperature as the Cox equation within the uncertainty of the values. The coefficients are listed in Table 4. For solids, the vapor pressure was fitted to a three parameter Antoine equation [Eq. (4)]. Vapor pressures for the solids given in Table 3a were calculated from this equation using the coefficients given in Table 4.

2.3. Saturated Liquid and Vapor Density

The selected experimental values for the density along the saturation curve ρ_l were fitted to the equation:

$$\rho_l = \rho_c \{1 + A_1 x^{\epsilon} + x \sum_i A_i x^{(i-2)/m}\} \quad (6)$$

where $i = 2$ to 3, $m = 2$, $\epsilon = 0.35$, $x = (1 - T/T_c)$, ρ_l is the saturated liquid density, and ρ_c is the density at the critical temperature, T_c . The upper limit on the sum depended upon the extent of the data available. Various values of ϵ and m were tested; however, the available data were not sufficiently precise nor measured in sufficient detail near the critical point to provide adequate sensitivity to the choice of the values. The results indicated that there is a statistical advantage to using nonzero values of ϵ and values of m greater than 1. The value of ϵ is a commonly accepted approximation (1975–232). Equation (6) was used to reproduce the most significant terms from the complete expansion by Ley-Koo and Green (1977–

189) for the liquid density near the critical point as well as terms for classical equations of state (1970–254). The coefficients, standard errors and correlation matrix for Eq. (6) are listed in Tables 5 and 5a. The smoothed values of the densities from Eq. (6) are listed in Table 6.

For compounds for which no density measurements exit, the densities were estimated using the extended corresponding states equation of Riedel (1954–91), as formulated by Hales and Townsend (1972–87).

$$\rho_l = \rho_c \{1 + 0.85x + (1.692 + 0.986\omega)x^{1/3}\} \quad (6a)$$

where the acentric factor $\omega = -\log_{10}(p/p_c) - 1$ where p is the vapor pressure at $T_r = T/T_c = 0.7$

Experimental values of the critical density were not available for several of the substances considered here. In such cases they were estimated from extrapolations of the rectilinear density

$$(\rho_l + \rho_g)/2 = \rho_c + \alpha_m(1 - T/T_c) \quad (7)$$

where ρ_c and α_m are tabulated in Table 7 with their standard errors and correlation coefficient. The ratios α_m/ρ_c are also listed to show the approximate constancy of their values. The selected values of T_c were used in these fits. The liquid densities (ρ_l) were the experimental values selected in Sec. 3.3, and the vapor densities (ρ_g) were determined from the second virial coefficients selected in Sec. 2.4 and values of the vapor pressure derived from the Cox equation. The range of the data was limited to the region where the compressibility factor of the vapor ($p_{\text{sat}}/RT\rho_g$) was greater than 0.8. For many compounds, second virial coefficients were not available, so the range was limited to where the vapor pressure was less than 1 bar. This procedure was tested on systems where critical densities were available, see Table 15, and was shown to give reasonable agreement with experimental values of the critical density.

2.4. Second Virial Coefficients

The data available for densities below vapor saturation are limited and only second virial coefficients B_m in the equation of state

$$p/\rho RT = 1 + B_m \rho \quad (8)$$

were evaluated. For all the compounds, the second virial coefficients were first estimated using the corresponding-states equation of Pitzer and Curl (1957–639).

$$B_m = (RT_c/P_c) \{1.445 + 0.073\omega - (0.330 - 0.46\omega)T_r^{-1} - (0.1385 + 0.50\omega)T_r^{-2} - (0.0121 + 0.097\omega)T_r^{-3} - 0.0073\omega T_r^{-8}\} \quad (9)$$

For those compounds where some virial coefficients data existed, either from direct measurements or calculated from the enthalpy of vaporization, the Pitzer and Curl

equation parameters were selectively adjusted to fit these results. The selected values of the second virial coefficient were smoothed using

$$B_m = A_b + C_b e^{(D_b/T)} \quad (10)$$

The coefficients to Eq. (10) are listed in Table 8.

Values of the second virial coefficient at selected temperatures are listed in Table 9.

2.5. Enthalpy of Vaporization or Sublimation

Enthalpies of vaporization from the literature were tested for consistency through the Clapeyron equation with our selections of vapor pressure, liquid density and second virial coefficient results. Values listed are the molar enthalpy of vaporization from the condensed phase, x , to the ideal gas, $\Delta_{f,m}^{\text{ig}}H$, rather than to the saturated vapor, $\Delta_{f,m}^{\text{g}}H$. Recommended values are listed in Table 10.

2.6. Enthalpy of Combustion and Formation

The enthalpy of combustion were usually available for the substances in the condensed phase (either liquid or crystal). Accepted values for the enthalpies of formation for the combustion products at 298.15 K, listed in Table 21 (1978–115), were used to derive enthalpies of formation. Enthalpies of vaporization and sublimation given in this report were used to derive enthalpies of formation for the ideal gas. Recommended values of enthalpies of formation in the condensed and ideal gas state at 298.15 K are listed in Table 11.

2.7 Condensed Phase Heat Capacities and Related Thermal Properties

Where calorimetric results for the condensed phases were available to near 10 K, the dimensionless thermodynamic functions $C_{\text{sat},m}/R$, $\Delta_f^{\text{g}}S_m^{\circ}/R$, $\Delta_f^{\text{g}}H_m^{\circ}/RT$, and $\Delta_f^{\text{g}}G_m^{\circ}/RT$ along the vapor saturation lines were evaluated. The results are listed in Table 12.

2.8 Ideal Gas Thermodynamic Properties

The thermodynamic properties for the ideal gas state for all the compounds except 9-methylcarbazole were calculated from spectroscopically derived results by standard statistical mechanical methods using the rigid rotator-harmonic oscillator model with modifications for internal rotation. Modifications were made for calculating the contributions concerned with inversion about the nitrogen atom for both 1- and 2-naphthalenamine. The ideal gas thermodynamic properties in dimensionless units include the heat capacity ($C_{p,m}^{\circ}/R$), entropy $\Delta_f^{\text{g}}S_m^{\circ}/R$, Gibbs energy $\Delta_f^{\text{g}}G_m^{\circ}/RT$, enthalpy function $\Delta_f^{\text{g}}H_m^{\circ}/RT$, enthalpy of formation $\Delta_f^{\text{g}}H_m^{\circ}/RT$, and Gibbs energy of formation $\Delta_f^{\text{g}}G_m^{\circ}/RT$. Calculations were made from 0 to 1500 K at a standard state pressure of 0.1 MPa. Wherever possible, the calculated entropies and heat capacities were compared with those derived from calorimetric measurements and with results of previous statistical mechanical calculations.

The calculated results are listed in Table 13. Details of the calculations and the selection of the spectroscopic results are given in Sec. 3.8.

TABLE 1. Selected freezing, normal boiling, and critical temperatures with critical pressure and volume

Compound	T_{fus} K	T_b K	T_c K	P_c MPa	V_c $\text{cm}^3\text{mol}^{-1}$
1-Butanamine	224.05 ± 0.02	350.15 ± 0.03	531.9 ± 1.0	4.25 ± 0.02	277 ± 2
2-Butanamine	168.7 ± 0.5	335.88 ± 0.01	514.3 ± 1.0	4.20 ± 0.02	278 ± 4
2-Methyl-1-propanamine	186.5 ± 0.5	340.90 ± 0.01	519. ± 2	4.07 ± 0.08	278 ± 4
2-Methyl-2-propanamine	206.20 ± 0.01 ^a	317.19 ± 0.02	483.9 ± 1.0	3.84 ± 0.02	292 ± 2
Pyrrole	249.75 ± 0.06 ^a	402.94 ± 0.01	639.7 ± 1.0	6.34 ± 0.02	200 ± 1
1-Methylpyrrole	216.91 ± 0.04	385.96 ± 0.02	596.0 ± 1.0	4.86 ± 0.02	271 ± 2
2-Methylpyrrole	237.6 ± 0.3	420.7 ± 0.5	654. ± 5	5.08 ± 0.10	266 ± 4
3-Methylpyrrole	224.8 ± 0.3	416.0 ± 1	647. ± 5	5.08 ± 0.10	266 ± 4
Pyridine	231.49 ± 0.05 ^a	388.38 ± 0.004	620. ± 1	5.67 ± 0.02	243 ± 1
2-Methylpyridine	206.47 ± 0.05 ^a	402.53 ± 0.02	621. ± 1	4.60 ± 0.02	292 ± 4
3-Methylpyridine	255.01 ± 0.04 ^a	417.29 ± 0.01	645. ± 1	4.65 ± 0.02	288 ± 4
4-Methylpyridine	276.81 ± 0.03 ^a	418.51 ± 0.01	646. ± 1	4.70 ± 0.02	292 ± 4
Pyrrolidine	215.31 ± 0.06 ^a	359.71 ± 0.01	568. ± 1	6.00 ± 0.05	238 ± 2
Piperidine	262.12 ± 0.02	379.37 ± 0.01	594. ± 1	4.94 ± 0.02	288 ± 4
Indole	325.7 ± 0.5	526.7 ± 0.6	794. ± 2	4.8 ± 0.1	356 ± 4
Quinoline	258.37 ± 0.03 ^a	510.31 ± 0.01	782. ± 2	4.86 ± 0.02	371 ± 2
Isoquinoline	299.62 ± 0.03 ^a	516.37 ± 0.01	803. ± 2	5.10 ± 0.05	374 ± 2
Carbazole	519.3 ± 0.5	627.84 ± 0.04	901.8 ± 1	3.13 ± 0.02	454 ± 4
Acridine	383.24 ± 0.01	618.01 ± 0.06	891.1 ± 0.5	3.21 ± 0.02	548 ± 4
Phenanthridine	379.94 ± 0.02	622.0 ± 0.5	895. ± 1	3.6 ± 0.2	548 ± 5
1-Naphthalenamine	322.4 ± 0.5	573.8 ± 0.1	850. ± 1	5.0 ± 0.1	438 ± 5
2-Naphthalenamine	386. ± 1	579.3 ± 0.1	850. ± 1	4.9 ± 0.1	438 ± 5
9-Methylcarbazole	362.49 ± 0.04 ^a	616.79 ± 0.02	890. ± 1	3.38 ± 0.05	572 ± 4

^aTriple point temperature.

TABLE 2. Coefficients of the Cox equation [Eq. (3)] for vapor pressure

Compound	Phase	A_0	$\sigma(A_0)^a$	A_1	$\sigma(A_1)^a$	A_2	$\sigma(A_2)^a$	T_{ref}/K	$\sigma(T_{ref})/K^a$	rmswd ^b
1-Butanamine	l	2.83162	0.03451	-0.55983	0.06389	0.17802	0.02772	350.149	0.031	0.78
2-Butanamine	l	2.89461	0.03497	-0.72541	0.06304	0.25157	0.02689	335.884	0.012	0.20
2-Methyl-1-propanamine	l	2.86131	0.02473	-0.65537	0.04391	0.22123	0.08125	340.898	0.003	2.69
2-Methyl-2-propanamine	l	2.92246	0.00363	-0.76454	0.00600	0.25785	0.00237	317.190	0.002	0.08
Pyrrole	l	2.83096	0.02569	-0.48317	0.04869	0.13878	0.02223	402.936	0.001	1.39
1-Methylpyrrole	l	2.81368	0.01194	-0.56311	0.02251	0.18959	0.01009	385.966	0.002	1.86
Pyridine	l	2.78616	0.00439	-0.54161	0.00832	0.17874	0.00372	388.385	0.004	0.57
2-Methylpyridine	l	2.81466	0.02617	-0.59817	0.04470	0.20669	0.01798	402.531	0.029	1.49
3-Methylpyridine	l	2.78574	0.00659	-0.55164	0.01178	0.18836	0.00487	417.293	0.001	0.42
4-Methylpyridine	l	2.81858	0.00454	-0.61515	0.00979	0.21835	0.00524	418.506	0.001	0.01
Pyrrolidine	l	2.98748	0.00767	-0.86004	0.01279	0.31261	0.00502	359.708	0.005	1.78
Piperidine	l	2.91085	0.00380	-0.78039	0.00799	0.27995	0.00415	379.370	0.000	0.28
Quinoline	l	2.86328	0.00273	-0.68489	0.00727	0.25411	0.00468	510.305	0.010	2.85
Isoquinoline	l	2.83900	0.00304	-0.62328	0.00790	0.21764	0.00496	516.375	0.010	2.41
Carbazole	l	2.35952	0.05274	0.31890	0.09539	-0.19072	0.04086	627.837	0.026	0.83
Acridine	l	2.88411	0.00197	-0.66939	0.00467	0.24229	0.00234	618.006	0.063	0.63
Phenanthridine	l	2.92109	0.00632	-0.74247	0.01787	0.29531	0.00982	622.467	0.238	0.20
1-Naphthalenamine	l	2.66976	0.02669	-0.23961	0.05860	0.07744	0.27835	573.786	0.264	0.23
2-Naphthalenamine	l	2.72383	0.02763	-0.36375	0.05857	0.14377	0.02744	579.282	0.206	0.31
9-Methylcarbazole	l	2.94053	0.00074	-0.73537	0.00174	0.26792	0.00100	616.966	0.001	0.88

^aSee Sec. 1.6.^brmswd = root-mean-squared-weighted deviationTABLE 2a. Correlation matrix^a for the Cox equation coefficients

Compound	Phase	$C(A_0, A_1)$	$C(A_0, A_2)$	$C(A_0, T_b)$	$C(A_1, A_2)$	$C(A_1, T_b)$	$C(A_2, T_b)$
1-Butanamine	l	-0.99839	0.99327	0.38689	-0.99804	-0.41919	0.43620
2-Butanamine	l	-0.99840	0.98969	0.63884	-0.99613	-0.64041	0.62651
2-Methyl-1-propanamine	l	-0.99869	0.99584	0.05795	-0.99909	-0.05452	0.05190
2-Methyl-2-propanamine	l	-0.99961	0.99887	-0.77995	-0.99980	0.77812	-0.77576
Pyrrole	l	-0.99782	0.98801	-0.01585	-0.99592	0.01375	-0.01172
1-Methylpyrrole	l	-0.99490	0.97265	-0.00753	-0.99053	-0.00231	0.00163
Pyridine	l	-0.99676	0.98374	-0.07541	-0.99461	0.04834	-0.02692
2-Methylpyridine	l	-0.99861	0.99616	-0.55866	-0.99935	-0.30209	0.31504
3-Methylpyridine	l	-0.99913	0.99773	-0.03469	-0.99964	0.03235	-0.03074
4-Methylpyridine	l	-0.99930	0.99688	0.49310	-0.99913	-0.50079	0.50459
Pyrrolidine	l	-0.99919	0.99785	-0.64028	-0.99968	0.63273	-0.62624
Piperidine	l	-0.99956	0.99805	-0.00001	-0.99946	0.00001	-0.00001
Quinoline	l	-0.99691	0.98726	0.52607	-0.99643	-0.54757	0.54763
Isoquinoline	l	-0.99702	0.98852	0.59174	-0.99702	-0.61445	0.61899
Carbazole	l	-0.99941	0.99843	-0.16825	-0.99976	0.15770	-0.15006
Acridine	l	-0.99423	0.98609	-0.65533	-0.99822	0.72760	-0.76565
Phenanthridine	l	-0.99887	0.99763	-0.98160	-0.99977	0.98951	-0.99235
1-Naphthalenamine	l	-0.99695	0.99254	-0.78488	-0.99896	0.82654	-0.84705
2-Naphthalenamine	l	-0.99640	0.99054	-0.59245	-0.99849	0.64906	-0.68018
9-Methylcarbazole	l	-0.99889	0.99552	0.67022	-0.99883	-0.68046	0.68299

^aSee Sec. 1.6.

TABLE 3. Values of vapor pressures of liquid calculated from the Cox equation [Eq. (3)] at selected temperatures

$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$
1-Butanamine											
224.05	0.077	280	4.82	330	49.50	390	323.0	450	1187.	510	3141.
230	0.133	290	8.30	340	71.54	400	414.	460	1421.	520	3616.
240	0.315	298.15	12.52	350	100.8	410	523.	470	1688.	530	4144.
250	0.688	300	13.69	360	138.8	420	653.	480	1991.	531.9	4251.
260	1.39	310	21.72	370	187.3	430	805.	490	2331.		
270	2.66	320	33.31	380	248.1	440	982.	500	2714.		
2-Butanamine											
168.65	0.00018	240	0.762	300	25.42	370	280.2	440	1293.	510	3952.
180	0.00112	250	1.580	310	38.89	380	362.4	450	1544.	512	4200.
190	0.00469	260	3.06	320	57.59	390	461.7	460	1832.	514.3	4160.
200	0.0165	270	5.59	330	82.83	400	580.	470	2158.		
210	0.0508	280	9.69	340	116.1	410	720.	480	2529.		
220	0.138	290	16.02	350	158.9	420	883.	490	2947.		
230	0.339	298.15	23.41	360	213.0	430	1073.	500	3419.		
2-Methyl-1-propanamine											
186.45	0.00204	250	1.209	300	20.68	360	183.5	420	790.	480	2299.
200	0.0119	260	2.37	310	31.98	370	243.3	430	965.	490	2681.
210	0.0369	270	4.39	320	47.85	380	317.0	440	1166.	500	3111.
220	0.1019	280	7.69	330	69.52	390	406.5	450	1397.	510	3592.
230	0.253	290	12.88	340	98.34	400	513.9	460	1661.	519.	4074.
240	0.575	298.15	19.00	350	135.81	410	641.	470	1960.		
2-Methyl-2-propanamine											
206.20	0.1143	260	7.54	300	52.85	350	282.7	400	925.	450	2285.
220	0.4267	270	13.14	310	78.03	360	369.5	410	1128.	460	2679.
230	0.9833	280	21.79	320	111.8	370	474.8	420	1362.	470	3125.
240	2.0812	290	34.60	330	155.8	380	600.8	430	1630.	480	3627.
250	4.091	298.15	49.00	340	212.1	390	749.9	440	1937.	483.9	3840.
Pyrrole											
249.75	0.0297	310	2.252	380	48.61	450	346.5	520	1335.	590	3596.
260	0.0731	320	3.85	390	67.82	460	432.9	530	1566.	600	4060.
270	0.163	330	6.34	400	92.76	470	534.9	540	1824.	610	4566.
280	0.341	340	10.10	410	124.54	480	654.	550	2112.	620	5116.
290	0.673	350	15.58	420	164.44	490	791.	560	2431.	630	5712.
298.15	1.127	360	23.35	430	213.7	500	950.	570	2783.	635	6033.
300	1.261	370	34.09	440	273.9	510	1131.	580	3171.	639.7	6338.
1-Methylpyrrole											
216.912	0.00436	290	1.815	350	30.47	420	253.2	490	1063.	560	3070.
230	0.0178	298.15	2.884	360	43.80	430	321.1	500	1259.	570	3503.
240	0.0464	300	3.190	370	61.51	440	402.1	510	1481.	580	3983.
250	0.1109	310	5.37	380	84.57	450	497.8	520	1732.	590	4513.
260	0.245	320	8.70	390	114.06	460	610.0	530	2013.	596.	4857.
270	0.506	330	13.62	400	151.16	470	740.	540	2328.		
280	0.985	340	20.66	410	197.1	480	890.	550	2679.		
Pyridine											
231.49	0.0210	298.15	2.772	360	41.09	430	296.2	500	1144.	570	3128.
240	0.0467	300	3.063	370	57.54	440	370.1	510	1343.	580	3543.
250	0.1103	310	5.133	380	78.91	450	457.3	520	1567.	590	4005.
260	0.2418	320	8.279	390	106.16	460	559.2	530	1817.	600	4509.
270	0.4955	330	12.91	400	140.35	470	677.3	540	2096.	610	5063.
280	0.957	340	19.51	410	182.62	480	813.1	550	2406.	615	5359.
290	1.753	350	28.67	420	234.15	490	968.3	560	2749.	620.0	5669.

TABLE 3. Values of vapor pressures of liquid calculated from the Cox equation [Eq. (3)] at selected temperatures — Continued

$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$
2-Methylpyridine											
206.47	0.000456	290	0.935	360	25.94	440	260.9	520	1183.	600	3577.
220	0.00247	298.15	1.517	370	36.97	450	325.7	530	1381.	610	4038.
230	0.00747	300	1.685	380	51.52	460	402.1	540	1604.	620	4546.
240	0.0203	310	2.90	390	70.36	470	491.5	550	1853.	621.	4600.
250	0.0504	320	4.80	400	94.33	480	595.	560	2130.		
260	0.1155	330	7.67	410	124.3	490	714.	570	2439.		
270	0.246	340	11.85	420	161.4	500	851.	580	2781.		
280	0.493	350	17.77	430	206.5	510	1007.	590	3159.		
3-Methylpyridine											
255.01	0.0375	320	2.749	390	45.58	460	283.6	530	1029.	600	2738.
270	0.1250	330	4.479	400	62.00	470	350.2	540	1201.	610	3096.
280	0.2573	340	7.056	410	82.86	480	427.9	550	1395.	620	3490.
290	0.500	350	10.78	420	108.95	490	518.1	560	1611.	630	3922.
298.15	0.826	360	16.02	430	141.14	500	622.0	570	1851.	640	4396.
300	0.922	370	23.21	440	180.35	510	740.9	580	2117.	645.	4649.
310	1.625	380	32.87	450	227.58	520	876.2	590	2412.		
4-Methylpyridine											
276.81	0.1896	340	6.74	410	80.14	480	416.	550	1367.	620	3473.
290	0.465	350	10.32	420	105.47	490	504.	560	1581.	630	3914.
298.15	0.774	360	15.38	430	136.7	500	605.	570	1820.	640	4401.
300	0.865	370	22.33	440	174.9	510	722.	580	2086.	645.7	4700.
310	1.53	380	31.68	450	220.8	520	855.	590	2382.		
320	2.61	390	43.99	460	275.6	530	1006.	600	2709.		
330	4.26	400	59.90	470	340.3	540	1176.	610	3072.		
Pyrrolidine											
215.31	0.0139	290	5.46	350	73.55	420	500.5	490	1877.	560	5353.
230	0.0661	298.15	8.41	360	102.27	430	620.9	500	2206.	568.2	5999.
240	0.1673	300	9.24	370	139.13	440	762.2	510	2579.		
250	0.3867	310	14.98	380	185.59	450	927.	520	3004.		
260	0.8254	320	23.37	390	243.22	460	1118.	530	3485.		
270	1.643	330	35.26	400	313.7	470	1337.	540	4031.		
280	3.078	340	51.62	410	398.8	480	1589.	550	4650.		
Piperidine											
262.12	0.566	310	7.381	370	76.30	430	364.4	490	1134.	550	2779.
270	0.739	320	11.76	380	103.21	440	451.	500	1333.	560	3180.
280	1.418	330	18.09	390	137.02	450	551.	510	1559.	570	3630.
290	2.576	340	26.97	400	178.83	460	668.	520	1814.	580	4132.
298.15	4.040	350	39.09	410	229.81	470	803.	530	2099.	590	4692.
300	4.456	360	55.25	420	291.2	480	958.	540	2420.	594.	4940.
Quinoline											
258.37	0.00026	350	0.3552	450	21.21	550	228.2	650	1091.	750	3501.
270	0.00088	360	0.6055	460	28.44	560	274.2	660	1242.	760	3885.
280	0.00232	370	0.997	470	37.58	570	327.1	670	1410.	770	4304.
290	0.00568	380	1.592	480	48.96	580	387.7	680	1594.	780	4761.
298.15	0.01118	390	2.469	490	62.98	590	456.6	690	1797.	782.	4858.
300	0.01296	400	3.732	500	80.05	600	534.6	700	2020.		
310	0.02779	410	5.504	510	100.63	610	622.5	710	2265.		
320	0.0564	420	7.940	520	125.20	620	721.1	720	2534.		
330	0.1088	430	11.222	530	154.27	630	831.4	730	2828.		
340	0.2007	440	15.564	540	188.41	640	954.4	740	3150.		

TABLE 3. Values of vapor pressures of liquid calculated from the Cox equation [Eq. (3)] at selected temperatures — Continued

T K	p_{sat} kPa	T K	p_{sat} kPa	T K	p_{sat} kPa	T K	p_{sat} kPa	T K	p_{sat} kPa	T K	p_{sat} kPa
Isoquinoline											
299.62	0.00953	390	2.015	480	42.19	570	290.7	660	1109.9	750	3064.
310	0.02127	400	3.066	490	54.52	580	345.1	670	1258.2	760	3386.
320	0.04353	410	4.554	500	69.60	590	407.1	680	1421.1	770	3735.
330	0.0847	420	6.613	510	87.84	600	477.2	690	1599.7	780	4113.
340	0.1575	430	9.406	520	109.69	610	556.1	700	1794.	790	4521.
350	0.2810	440	13.125	530	135.62	620	644.7	710	2007.	800	4963.
360	0.4829	450	17.992	540	166.15	630	743.5	720	2240.	803.	5102.
370	0.8016	460	24.262	550	201.79	640	853.5	730	2492.		
380	1.289	470	32.22	560	243.12	650	975.3	740	2766.		
Carbazole											
519.3	8.08	590	46.72	660	181.7	730	532.	800	1246.	870	2432.
530	10.86	600	57.89	670	215.2	740	608.	810	1385.	880	2641.
540	14.16	610	71.22	680	253.5	750	692.	820	1534.	890	2860.
550	18.30	620	87.01	690	297.0	760	785.	830	1693.	900	3088.
560	23.42	630	105.59	700	346.1	770	886.	840	1863.	901.3	3130.
570	29.73	640	127.32	710	401.4	780	997.	850	2042.		
580	37.41	650	152.5	720	463.	790	1116.	860	2232.		
Acridine											
383.24	0.0360	480	2.942	580	46.72	680	288.6	780	1060.	880	2904.
390	0.0534	490	4.127	590	57.94	690	334.9	790	1184.	890.	3178.
400	0.0927	500	5.696	600	71.24	700	386.7	800	1320.	891.1	3209.
410	0.1560	510	7.743	610	86.9	710	444.6	810	1468.		
420	0.2551	520	10.377	620	105.2	720	508.9	820	1628.		
430	0.4059	530	13.723	630	126.4	730	580.3	830	1802.		
440	0.6299	540	17.922	640	150.9	740	659.1	840	1990.		
450	0.9551	550	23.14	650	179.0	750	745.9	850	2193.		
460	1.4173	560	29.54	660	211.1	760	841.2	860	2412.		
470	2.061	570	37.33	670	247.5	770	945.8	870	2649.		
Phenanthridine											
379.94	0.0226	470	1.73	560	26.3	650	167.	740	645.	830	1869.
390	0.0414	480	2.49	570	33.4	660	198.	750	734.	840	2080.
400	0.0729	490	3.52	580	42.0	670	233.	760	833.	850	2309.
410	0.1242	500	4.89	590	52.4	680	273.	770	942.	860	2560.
420	0.2052	510	6.69	600	64.7	690	318.	780	1063.	870	2833.
430	0.3298	520	9.03	610	79.4	700	370.	790	1196.	880	3131.
440	0.5168	530	12.0	620	97.	710	427.	800	1342.	890	3456.
450	0.790	540	15.8	630	117.	720	492.	810	1502.	895.	3629.
460	1.18	550	20.5	640	140.	730	564.	820	1677.		
1-Naphthalenamine											
322.35	0.0042	420	0.994	520	28.2	620	251.	720	1176.	820	3727.
330	0.0073	430	1.499	530	36.4	630	300.	730	1339.	830	4120.
340	0.0145	440	2.215	540	46.8	640	356.	740	1519.	840	4543.
350	0.0275	450	3.212	550	59.4	650	421.	750	1718.	845	4767.
360	0.0504	460	4.576	560	74.8	660	494.	760	1936.	850.	5000.
370	0.0891	470	6.41	570	93.3	670	578.	770	2174.		
380	0.152	480	8.85	580	115.5	680	672.	780	2435.		
390	0.253	490	12.05	590	141.8	690	778.	790	2719.		
400	0.409	500	16.19	600	172.	700	896.	800	3029.		
410	0.645	510	21.47	610	209.	710	1029.	810	3364.		

TABLE 3. Values of vapor pressures of liquid calculated from the Cox equation [Eq. (3)] at selected temperatures — Continued

$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$
2-Naphthalenamine											
386	0.171	470	5.57	550	52.6	630	269.	710	941.	790	2571.
400	0.342	480	7.72	560	66.4	640	320.	720	1079.	800	2878.
410	0.544	490	10.54	570	83.0	650	379.	730	1233.	810	3215.
420	0.843	500	14.20	580	102.8	660	446.	740	1405.	820	3583.
430	1.280	510	18.88	590	126.4	670	523.	750	1594.	830	3984.
440	1.901	520	24.80	600	154.4	680	610.	760	1804.	840	4422.
450	2.77	530	32.22	610	187.	690	708.	770	2036.	845	4656.
460	3.96	540	41.4	620	225.	700	818.	780	2291.	850.	4900.
9-Methylcarbazole											
362.49	0.0079	450	0.8887	540	17.782	630	129.37	720	530.	810	1547.
370	0.0131	460	1.3317	550	23.060	640	154.80	730	605.	820	1718.
380	0.0250	470	1.9542	560	29.568	650	184.02	740	688.	830	1904.
390	0.0458	480	2.8126	570	37.512	660	217.43	750	779.	840	2106.
400	0.0809	490	3.9754	580	47.118	670	255.42	760	880.	850	2324.
410	0.1383	500	5.5250	590	58.631	680	298.4	770	991.	860	2560.
420	0.2292	510	7.5585	600	72.318	690	346.8	780	1112.	870	2816.
430	0.3694	520	10.1892	610	88.463	700	401.2	790	1245.	880	3092.
440	0.5799	530	13.548	620	107.372	710	461.9	800	1389.	890.	3389.

TABLE 3a. Values of vapor pressures of crystal calculated from the Antoine equation [Eq. (4)] at selected temperatures

$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$	$\frac{T}{K}$	$\frac{p_{sat}}{kPa}$
Indole											
270	0.000079	290	0.000719	310	0.0045	325.65	0.0152				
280	0.000252	298.15	0.001575	320	0.0100						
Carbazole											
340	0.000075	380	0.00167	420	0.018	460	0.116	500	0.525		
350	0.000177	390	0.00319	430	0.030	470	0.174	510	0.733		
360	0.000394	400	0.0059	440	0.048	480	0.256	519.3	0.987		
370	0.00083	410	0.0104	450	0.075	490	0.370				
Acridine											
280	0.000001	310	0.000026	340	0.00053	370	0.0060				
290	0.000002	320	0.000078	350	0.00126	380	0.0120				
298.15	0.000006	330	0.000211	360	0.00282	383.24	0.0149				
Phenanthridine											
290	0.000001	310	0.000012	330	0.00011	350	0.0007	370	0.0033		
298.15	0.000003	320	0.000040	340	0.00029	360	0.0016	379.94	0.0065		
2-Naphthalenamine											
260	0.0000017	290	0.000134	320	0.00269	350	0.0241	380	0.1284		
270	0.0000096	298.15	0.000336	330	0.00602	360	0.0442	386	0.171		
280	0.0000379	310	0.00111	340	0.0125	370	0.0770				
9-Methylcarbazole											
300	0.0000108	320	0.000118	340	0.00095	360	0.0060				
310	0.0000371	330	0.000346	350	0.00246	362.04	0.0075				

TABLE 4. Coefficients^a of the Antoine equation [Eqs. (4) and (5)] over the following ranges: a, below 20 kPa; b, 20 kPa to 200 kPa; c, 100 kPa to critical pressure.

Compound	Range	A_s	B_s	C_s	T_s^*/K	n	E_s	F_s	T_c/K
1-Butanamine	b	6.0335	1139.32	-67.37	350	1.7439	746.9	-64397.	531.9
	c	6.0335	1139.32	-67.37					
2-Butanamine	b	5.9843	1088.84	-62.22					
2-Methyl-1-propanamine	a	7.579	1708.7	-23.5					
	b	5.9799	1094.48	-65.32					
2-Methyl-2-propanamine	b	5.9062	992.361	-62.77					
Pyrrole	a	7.578	1982.2	-30.	420.15	2.5692	985.4	-87777.	639.7
	b	6.4267	1506.33	-62.20					
	c	6.4267	1506.33	-62.20					
1-Methylpyrrole	a	5.533	1124.4	-76.9					
	b	6.2136	1370.97	-60.09					
Pyridine	a	6.009	1282.3	-68.0	400.15	2.8467	-36.98	3621.2	620.0
	b	6.1853	1384.77	-57.09					
	c	6.1853	1384.77	-57.09					
2-Methylpyridine	b	6.1756	1427.97	-60.10					
3-Methylpyridine	b	6.1921	1493.72	-60.49					
4-Methylpyridine	b	6.1703	1483.15	-62.37					
Pyrrolidine (Liquid)	b	6.0330	1170.97	-68.95	380	1.7344	5.662	-4088.8	568.2
	c	6.0330	1170.97	-68.95					
Piperidine (Liquid)	b	5.9823	1239.80	-67.60					
Indole (Crystal)	a	6.0670	1953.27	-77.93					
Quinoline (Liquid)	a	6.5441	2044.06	-57.68	520	2.5640	5996.0	-914620.	782.0
	b	6.1960	1811.50	-77.99					
	c	6.1960	1811.50	-77.99					
Isoquinoline (Liquid)	a	6.5781	2090.06	-56.83					
	b	6.2009	1835.64	-78.84					
Carbazole (Crystal) (Liquid)	a	5.9414	2605.21	-81.23					
	b	7.0858	3098.85	-17.85					
Acridine (Crystal) (Liquid)	a	7.2884	2875.70	-67.71					
	a	6.5979	2493.62	-73.18					
	b	6.2653	2217.00	-97.58					
Phenanthridine (Crystal) (Liquid)	a	5.6401	2123.69	-108.55					
	a	6.4598	2406.19	-83.31					
1-Naphthalenamine (Liquid)	b	6.5715	2299.03	-71.20					
2-Naphthalenamine (Crystal) (Liquid)	a	4.4950	1360.41	-127.43					
	b	6.6401	2392.46	-64.01					
9-Methylcarbazole (Crystal) (Liquid) (Liquid)	a	10.5610	4333.69	-20.93					
	a	6.6823	2515.35	-76.41					
	b	6.0973	2048.59	-117.32					

^aIn Eq. (5), $D_s = \log_{10} e = 0.43429$

TABLE 5. Coefficients^a and their standard deviations^b for Eq. (6) representing densities of the liquids

Compound	A_1	$\sigma(A_1)$	A_2	$\sigma(A_2)$	A_3	$\sigma(A_3)$	rmswd ^c
1-Butanamine	2.26401	0.02029	-0.26241	0.08934	0.75811	0.08227	1.77
2-Butanamine	2.03447	0.06467	0.56635	0.11274			1.27
2-Methyl-1-propanamine	2.22424	0.01942	-0.11770	0.08726	0.62276	0.08106	1.53
2-Methyl-2-propanamine	2.04443	0.07198	0.77552	0.13304			1.38
Pyrrole	1.89559	0.02717	0.66646	0.04039			2.79
1-Methylpyrrole	2.11648	0.00407	0.72005	0.00676			2.89
Pyridine	2.29807	0.06843	-0.39016	0.25162	1.00456	0.20379	1.27
2-Methylpyridine	1.96644	0.00379	0.74341	0.00599			0.84
3-Methylpyridine	1.94310	0.02768	0.71321	0.04146			1.39
4-Methylpyridine	1.93973	0.01678	0.77039	0.02520			1.93
Pyrrolidine	1.97615	0.00057	0.70678	0.00093			1.48
Piperidine	1.94106	0.02044	0.76342	0.03169			0.32
Quinoline	2.70629	0.27610	-1.88961	0.93450	2.09401	0.70955	2.89
Isoquinoline	2.22340	0.03865	-0.22074	0.13336	0.83498	0.10278	5.24
Carbazole	2.09926	0.01343	0.43435	0.02486			2.34
Acridine	1.94869	0.03438	2.38558	0.19172	-1.51823	0.20529	5.47
Phenanthridine	2.37296	0.00347	0.41201	0.01865	0.30526	0.01947	1.59
1-Naphthalenamine	1.52939	0.15919	1.70572	0.22951			1.33
2-Naphthalenamine	2.41268	0.00507	0.32107	0.02880	0.40011	0.03141	1.89
9-Methylcarbazole	2.33411	0.00464	0.37455	0.02468	0.34165	0.02559	1.85

^aSee Table 7 for values of ρ_c and Table 1 for T_c .^bSee Sec. 1.6.^crmswd = root-mean-squared-weighted deviation.TABLE 5a. Correlation matrix^a for coefficients in Eq. (6) representing densities of the liquids

Compound	$C(A_1, A_2)$	$C(A_1, A_3)$	$C(A_2, A_3)$
1-Butanamine	-0.99080	0.97509	-0.99595
2-Butanamine	-0.99964		
2-Methyl-1-propanamine	-0.99020	0.97432	-0.99598
2-Methyl-2-propanamine	-0.99964		
Pyrrole	-0.99982		
1-Methylpyrrole	-0.97706		
Pyridine	-0.99962	0.99886	-0.99979
2-Methylpyridine	-0.99908		
3-Methylpyridine	-0.99989		
4-Methylpyridine	-0.99980		
Pyrrolidine	-0.99995		
Piperidine	-0.99962		
Quinoline	-0.99929	0.99784	-0.99960
Isoquinoline	-0.99895	0.99696	-0.99948
Carbazole	-0.99913		
Acridine	-0.94319	0.88218	-0.98690
Phenanthridine	-0.95754	0.90824	-0.98908
1-Naphthalenamine	-0.99933		
2-Naphthalenamine	-0.94741	0.88888	-0.98724
9-Methylcarbazole	-0.94968	0.89307	-0.98761

^aSee Sec. 1.6

TABLE 6. Densities of saturated liquid calculated from Eq. (6) at selected temperatures

$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$
1-Butanamine											
224.05	805.	298.15	739.3	370	670.0	450	575.4	521	416.	529	359.
230	800.	300	737.7	380	659.6	460	560.7	522	411.	530	346.
240	791.	310	728.4	390	648.8	470	544.9	523	405.	531	327.
250	782.	320	719.1	400	637.8	480	527.5	524	400.	531.9	264.
260	774.	330	709.6	410	626.3	490	508.	525	393.		
270	764.7	340	700.0	420	614.4	500	485.	526	386.		
280	755.8	350	690.2	430	602.1	510	458.	527	379.		
290	746.8	360	680.2	440	589.1	520	420.	528	370.		
2-Butanamine											
168.65	828.	240	771.	300	718.2	370	647.	440	555.	510	364.
180	819.	250	762.	310	708.8	380	635.	450	539.	511	355.
190	811.	260	754.	320	699.2	390	624.	460	521.	512	344.
200	803.	270	745.	330	689.	400	611.	470	502.	513	329.
210	795.	280	736.5	340	679.	410	598.	480	480.	514	302.
220	787.	290	727.5	350	668.	420	585.	490	453.	514.3	263.
230	779.	298.15	720.0		360	658.	430	571.	500	419.	
2-Methyl-1-propanamine											
186.45	827.	260	763.4	330	697.9	410	610.6	490	476.	516	359.
190	824.	270	754.4	340	688.0	420	597.8	500	446.	517	346.
200	816.	280	745.3	350	677.8	430	584.5	510	404.	518	328.
210	807.	290	736.3	360	667.4	440	570.3	511	398.	519	263.
220	798.	298.15	728.5	370	656.8	450	555.1	512	392.		
230	790.	300	726.8	380	645.8	460	538.6	513	385.		
240	781.	310	717.3	390	634.5	470	520.	514	377.		
250	772.	320	707.7	400	622.8	480	500.	515	369.		
2-Methyl-2-propanamine											
206.2	782.	280	709.5	350	629.	430	508.	474	385.	482	324.
210	778.	290	698.9	360	617.	440	488.	475	379.	483	306.
220	769.	298.15	690.1	370	603.	450	465.	476	374.	483.9	250.
230	759.	300	688.1	380	590.	460	438.	477	368.		
240	750.	310	677.0	390	575.	470	403.	478	361.		
250	740.	320	665.	400	560.	471	398.	479	354.		
260	730.	330	654.	410	544.	472	394.	480	346.		
270	719.	340	642.	420	527.	473	389.	481	336.		
Pyrrole											
249.75	1006.	320	946.1	400	870.	480	782.	560	670.	635	450.
260	998.0	330	937.0	410	860.	490	770.	570	652.	636	441.
270	989.6	340	927.9	420	849.	500	757.	580	633.	637	429.
280	981.1	350	918.7	430	839.	510	744.	590	612.	638	415.
290	972.5	360	909.3	440	828.	520	730.	600	589.	639	393.
298.15	965.4	370	899.	450	817.	530	716.	610	562.	639.7	335.
300	963.8	380	890.	460	806.	540	702.	620	530.		
310	955.0	390	880.	470	794.	550	686.	630	485.		
1-Methylpyrrole											
216.91	977.	298.15	904.5	370	832.	450	739.	530	616.	590	428.
230	966.	300	902.7	380	822.	460	726.	540	596.	592	410.
240	9570.	310	893.2	390	811.	470	713.	550	574.	594	386.
250	948.	320	883.5	400	799.	480	698.	560	549.	596	300.
260	939.	330	873.6	410	788.	490	684.	570	520.		
270	930.6	340	863.7	420	776.	500	668.	575	503.		
280	921.4	350	853.5	430	764.	510	652.	580	483.		
290	912.1	360	843.	440	752.	520	635.	585	460.		

TABLE 6. Densities of saturated liquid calculated from Eq. (6) at selected temperatures — Continued

$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$
Pyridine											
231.49	1045.	300	976.1	380	893.0	460	802.4	540	690.6	615	463.
240	1036.	310	966.0	390	882.2	470	790.1	550	673.2	616	454.
250	1026.	320	955.8	400	871.3	480	777.4	560	654.3	617	441.
260	1016.	330	945.5	410	860.3	490	764.4	570	633.6	618	426.
270	1006.	340	935.2	420	849.1	500	750.9	580	610.2	619	405.
280	996.3	350	924.8	430	837.8	510	736.9	590	582.9	620	326.
290	986.3	360	914.2	440	826.2	520	722.2	600	549.0		
298.15	978.0	370	903.7	450	814.4	530	706.9	610	501.3		
2-Methylpyridine											
206.47	1020.	290	947.1	360	880.3	440	794.2	520	688.5	600	517.
220	1009.	298.15	939.6	370	870.2	450	782.3	530	672.8	610	475.
230	1000.	300	937.9	380	859.9	460	770.2	540	656.2	615	443.
240	991.5	310	928.6	390	849.5	470	757.7	550	638.	620	384.
250	982.8	320	919.2	400	838.9	480	744.8	560	619.	621	318.
260	974.0	330	909.7	410	828.0	490	731.6	570	598.		
270	965.1	340	900.0	420	817.0	500	717.8	580	575.		
280	956.2	350	890.2	430	805.7	510	703.5	590	549.		
3-Methylpyridine											
255.01	989.	330	923.9	410	847.	490	759.	570	645.	641	430.
270	976.1	340	914.9	420	837.	500	747.	580	627.	642	419.
280	967.6	350	905.7	430	827.	510	734.	590	607.	643	406.
290	959.1	360	896.4	440	816.	520	721.	600	586.	644	388.
298.15	952.0	370	887.0	450	805.	530	707.	610	561.	645	323.
300	950.4	380	877.	460	794.	540	693.	620	533.		
310	941.7	390	867.	470	783.	550	678.	630	496.		
320	932.9	400	857.	480	771.	560	662.	640	439.		
4-Methylpyridine											
276.81	969.	350	902.9	430	823.	510	729.	590	603.	643	411.
290	957.2	360	893.5	440	812.	520	716.	600	581.	644	397.
298.15	950.1	370	883.9	450	801.	530	702.	610	557.	645	376.
300	948.5	380	874.2	460	790.	540	688.	620	529.	645.7	319.
310	939.6	390	864.3	470	778.	550	673.	630	493.		
320	930.6	400	854.3	480	767.	560	657.	640	439.		
330	921.5	410	844.1	490	754.	570	640.	641	431.		
340	912.3	420	833.8	500	742.	580	622.	642	422.		
Pyrrolidine											
215.31	929.	280	871.0	340	812.	410	734.	480	639.	550	482.
220	925.	290	861.6	350	802.	420	722.	490	622.	560	436.
230	916.	298.15	853.8	360	791.	430	710.	500	605.	565	396.
240	908.	300	852.0	370	780.	440	697.	510	586.	566	384.
250	899.	310	842.3	380	769.	450	683.	520	565.	567	367.
260	889.	320	832.4	390	758.	460	669.	530	542.	568.2	299.
270	880.	330	822.	400	746.	470	654.	540	515.		
Piperidine											
262.12	888.9	320	836.6	390	767.2	460	686.	530	582.	591	386.
270	882.0	330	827.2	400	756.	470	673.	540	563.	592	374.
280	873.2	340	817.6	410	745.	480	660.	550	542.	593	357.
290	864.2	350	807.9	420	734.	490	646.	560	518.	594	295.
298.15	856.8	360	798.0	430	723.	500	631.	570	490.		
300	855.1	370	787.9	440	711.	510	616.	580	455.		
310	846.0	380	777.6	450	699.	520	600.	590	396.		

TABLE 6. Densities of saturated liquid calculated from Eq. (6) at selected temperatures — Continued

$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$
Quinoline											
258.37	1124.	350	1048.	450	967.	550	885.	650	792.	750	634.
270	1114.	360	1040.	460	959.	560	876.	660	781.	760	602.
280	1106.	370	1032.	470	951.	570	868.	670	769.	770	557.
290	1098.	380	1024.	480	943.	580	859.	680	757.	775	522.
298.15	1091.	390	1016.	490	934.	590	850.	690	744.	780	462.
300	1089.	400	1008.	500	926.	600	841.	700	730.	781	438.
310	1081.	410	999.	510	918.	610	832.	710	715.	782	348.
320	1073.	420	991.	520	910.	620	822.	720	699.		
330	1064.	430	983.	530	902.	630	812.	730	680.		
340	1056.	440	975.	540	893.	640	802.	740	659.		
Isoquinoline											
299.62	1094.	400	1014.	500	930.	600	838.	700	724.	800	454.
310	1086.	410	1006.	510	921.	610	828.	710	710.	801	440.
320	1078.	420	997.	520	913.	620	818.	720	695.	802	420.
330	1070.	430	989.	530	904.	630	807.	730	679.	803	346.
340	1062.	440	981.	540	895.	640	796.	740	661.		
350	1054.	450	973.	550	886.	650	785.	750	642.		
360	1046.	460	964.	560	876.	660	774.	760	621.		
370	1038.	470	956.	570	867.	670	762.	770	596.		
380	1030.	480	947.	580	857.	680	750.	780	566.		
390	1022.	490	939.	590	848.	690	737.	790	526.		
Carbazole											
519.3	1007.	600	947.	680	879.	760	796.	840	680.	898	476.
530	999.	610	939.	690	870.	770	784.	850	660.	900	446.
540	992.	620	931.	700	860.	780	772.	860	637.	901.8	368.
550	985.	630	923.	710	850.	790	758.	870	611.		
560	978.	640	914.	720	840.	800	745.	880	580.		
570	970.	650	906.	730	830.	810	730.	890	536.		
580	962.	660	897.	740	819.	820	714.	895	504.		
590	955.	670	888.	750	808.	830	698.	896	496.		
Acridine											
383.24	1081.	470	1024.	560	955.	650	871.	740	767.	830	620.
390	1077.	480	1017.	570	946.	660	861.	750	753.	840	599.
400	1071.	490	1010.	580	937.	670	850.	760	739.	850	575.
410	1064.	500	1002.	590	928.	680	839.	770	725.	860	547.
420	1058.	510	995.	600	919.	690	828.	780	709.	870	515.
430	1051.	520	987.	610	910.	700	816.	790	694.	880	473.
440	1045.	530	979.	620	901.	710	804.	800	677.	885	443.
450	1038.	540	971.	630	891.	720	792.	810	659.	890	389.
460	1031.	550	963.	640	881.	730	780.	820	641.	891.1	327.
Phenanthridine											
379.94	1088.	480	1014.	580	934.	680	842.	780	727.	875	535.
390	1080.	490	1006.	590	925.	690	832.	790	713.	880	514.
400	1073.	500	998.	600	916.	700	822.	800	698.	885	490.
410	1066.	510	991.	610	908.	710	811.	810	683.	890	454.
420	1059.	520	983.	620	899.	720	800.	820	666.	892	433.
430	1051.	530	975.	630	890.	730	789.	830	648.	894	399.
440	1044.	540	967.	640	881.	740	778.	840	629.	895	327.
450	1036.	550	959.	650	871.	750	766.	850	607.		
460	1029.	560	950.	660	862.	760	753.	860	582.		
470	1022.	570	942.	670	852.	770	740.	870	553.		

TABLE 6. Densities of saturated liquid calculated from Eq. (6) at selected temperatures — Continued

$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{T}{K}$	$\frac{\rho_l}{\text{kg}\cdot\text{m}^{-3}}$
1-Naphthalenamine											
322.35	1096.	420	1003.	520	902.	620	794.	720	671.	820	501.
330	1089.	430	993.	530	892.	630	782.	730	657.	830	474.
340	1079.	440	983.	540	881.	640	771.	740	643.	835	458.
350	1070.	450	973.	550	871.	650	759.	750	629.	840	439.
360	1060.	460	963.	560	860.	660	747.	760	613.	845	412.
370	1051.	470	953.	570	849.	670	735.	770	598.	848	338.
380	1041.	480	943.	580	838.	680	723.	780	581.	850	327.
390	1032.	490	933.	590	827.	690	710.	790	564.		
400	1022.	500	923.	600	816.	700	697.	800	454.		
410	1012.	510	913.	610	805.	710	684.	810	524.		
2-Naphthalenamine											
386	1075.	480	1000.	570	921.	660	831.	750	717.	835	521.
400	1064.	490	992.	580	911.	670	820.	760	702.	840	495.
410	1056.	500	983.	590	902.	680	809.	770	685.	845	458.
420	1048.	510	974.	600	892.	690	797.	780	667.	848	422.
430	1041.	520	965.	610	883.	700	785.	790	648.	850	327.
440	1033.	530	957.	620	873.	710	773.	800	627.		
450	1025.	540	948.	630	862.	720	759.	810	603.		
460	1016.	550	939.	640	853.	730	746.	820	576.		
470	1008.	560	930.	650	842.	740	732.	830	542.		
9-Methylcarbazole											
362.49	1052.	460	984.	560	908.	660	823.	760	717.	860	547.
370	1047.	470	977.	570	900.	670	813.	770	705.	865	532.
380	1040.	480	970.	580	892.	680	804.	780	692.	870	516.
390	1033.	490	962.	590	883.	690	794.	790	678.	875	496.
400	1027.	500	955.	600	875.	700	784.	800	664.	880	472.
410	1020.	510	947.	610	867.	710	774.	810	648.	884	446.
420	1013.	520	939.	620	858.	720	763.	820	632.	888	404.
430	1006.	530	931.	630	850.	730	752.	830	614.	890	317.
440	999.	540	924.	640	841.	740	741.	840	595.		
450	992.	550	916.	650	832.	750	729.	850	573.		

TABLE 7. Coefficients and standard deviations^a of Eq. (7) for the rectilinear diameter line (from low reduced temperature density data)

Compound	$\frac{\rho_c}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{\sigma(\rho_c)}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{\alpha_m}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{\sigma(\alpha_m)}{\text{kg}\cdot\text{m}^{-3}}$	$C(\rho_c, \alpha_m)$	$\frac{\alpha_m}{\rho_c}$
1-Butanamine	264.	0.5	240.99	1.3	-0.962726	0.9137
2-Butanamine	263.	3.9	232.10	9.3	-0.999103	0.8832
2-Methyl-1-propanamine	263.	0.6	238.21	1.5	-0.962835	0.9063
2-Methyl-2-propanamine	250.	4.4	249.41	11.3	-0.999149	0.9974
Pyrrole	335.	2.4	275.76	4.4	-0.999587	0.8220
Pyridine	326.	0.3	313.78	0.5	-0.997543	0.9621
2-Methylpyridine	318.	0.3	291.20	0.6	-0.997799	0.9144
3-Methylpyridine	323.	1.9	284.56	3.5	-0.999722	0.8809
4-Methylpyridine	319.	1.1	289.53	2.1	-0.999507	0.9069
Pyrrolidine	299.	0.1	269.92	0.4	-0.999886	0.9039
Piperidine	295.	1.4	267.29	2.7	-0.999094	0.9050
Quinoline	348.	1.7	319.57	3.0	-0.994981	0.9192
Isoquinoline	346.	0.5	321.19	0.8	-0.996737	0.9292
Carbazole	368.	0.4	322.09	1.0	-0.997918	0.8761

^aSee Sec. 1.6.^bData not used for adopted ρ_c ; experimental data available.TABLE 8. Coefficients of Eq. (10) with their correlation coefficients^a for the second virial coefficients

Compound	$\frac{A_b}{\text{cm}^3\cdot\text{mol}^{-1}}$	$\frac{\sigma(A_b)}{\text{cm}^3\cdot\text{mol}^{-1}}$	$\frac{C_b}{\text{cm}^3\cdot\text{mol}^{-1}}$	$\frac{\sigma(C_b)}{\text{cm}^3\cdot\text{mol}^{-1}}$	$\frac{D_b}{\text{K}}$	$\frac{\sigma(D_b)}{\text{K}}$	rmswd ^b	(A_b, C_b)	(A_b, D_b)	(C_b, D_b)
1-Butanamine	542.07	16.31	-296.34	9.68	663.43	9.04	0.36	-0.996377	-0.984553	0.995863
2-Butanamine	395.00	15.91	-223.86	9.15	640.43	10.63	0.46	-0.995297	-0.982252	0.995780
2-Methyl-1-propanamine	431.44	22.76	-243.09	14.06	624.71	15.04	0.49	-0.997194	-0.986862	0.996039
2-Methyl-2-propanamine	396.29	14.61	-226.18	8.90	591.39	9.55	0.36	-0.996604	-0.983836	0.995062
Pyrrole	205.34	34.57	-121.71	15.15	996.49	39.72	1.48	-0.996700	-0.992453	0.998733
1-Methylpyrrole	377.66	13.91	-210.70	7.87	752.11	11.30	0.43	-0.995011	-0.981867	0.995864
Pyridine	307.58	19.37	-185.38	10.59	746.77	16.70	0.76	-0.995768	-0.984558	0.996462
2-Methylpyridine	329.82	24.95	-184.57	12.80	841.07	21.58	0.98	-0.998368	-0.993845	0.998536
3-Methylpyridine	493.57	28.54	-285.57	17.69	773.96	18.69	0.40	-0.997282	-0.989362	0.997172
4-Methylpyridine	356.72	17.79	-198.04	8.83	893.10	13.79	0.49	-0.996903	-0.991863	0.998388
Pyrrolidine	350.83	13.14	-200.26	7.84	693.91	10.82	0.49	-0.997586	-0.987483	0.995932
Piperidine	380.95	13.84	-220.94	8.32	714.13	10.93	0.33	-0.996943	-0.986388	0.996030
Quinoline	583.65	31.49	-318.13	17.95	981.68	21.92	0.29	-0.997144	-0.990168	0.997728
Isoquinoline ^c	496.85	12.79	-280.86	7.34	990.79	10.27	0.15	-0.997056	-0.989418	0.997440
Carbazole ^c	1088.23	10.69	-549.96	6.21	1151.2	5.28	0.28	-0.998459	-0.995024	0.998963
Acridine ^c	952.78	9.25	-450.73	5.18	1183.4	5.39	0.03	-0.998298	-0.994639	0.998917
Phenanthridine ^c	963.48	7.92	-466.21	4.57	1172.6	4.64	0.02	-0.998526	-0.995246	0.999015
1-Naphthalenamine ^c	592.11	9.25	-283.32	4.96	1166.2	7.73	0.08	-0.997207	-0.990907	0.998055
2-Naphthalenamine ^c	613.41	10.25	-284.59	5.27	1189.3	8.29	0.09	-0.997062	-0.990574	0.998016
9-Methylcarbazole ^c	1003.97	14.99	-494.46	8.08	1313.7	8.23	0.06	-0.997492	-0.992251	0.998439

^aSee Sec. 1.6.^brmswd = root-mean-squared-weighted deviation.^cValues used in fit calculated from Eq. (9).

TABLE 9. Second virial coefficients calculated from Eq. (10) at selected temperatures

T K	B_m $\text{cm}^3\text{mol}^{-1}$	T K	B_m $\text{cm}^3\text{mol}^{-1}$	T K	B_m $\text{cm}^3\text{mol}^{-1}$	T K	B_m $\text{cm}^3\text{mol}^{-1}$	T K	B_m $\text{cm}^3\text{mol}^{-1}$	T K	B_m $\text{cm}^3\text{mol}^{-1}$
1-Butanamine											
280	-3176.	340	-1585.	400	-964.	460	-636.	520	-434.	580	-299.
290	-2764.	350	-1446.	410	-896.	470	-596.	530	-408.	590	-280.
300	-2433.	360	-1325.	420	-835.	480	-559.	540	-383.	600	-263.
310	-2161.	370	-1218.	430	-778.	490	-524.	550	-360.	610	-247.
320	-1936.	380	-1124.	440	-727.	500	-492.	560	-338.	620	-231.
330	-1747.	390	-1040.	450	-680.	510	-462.	570	-318.	630	-216.
2-Butanamine											
260	-2564.	320	-1300.	380	-818.	440	-561.	500	-401.	560	-292.
270	-2230.	330	-1192.	390	-765.	450	-529.	510	-380.	570	-277.
280	-1965.	340	-1097.	400	-716.	460	-500.	520	-360.	580	-263.
290	-1751.	350	-1015.	410	-672.	470	-472.	530	-342.	590	-250.
300	-1574.	360	-942.	420	-632.	480	-447.	540	-324.	600	-237.
310	-1426.	370	-876.	430	-595.	490	-423.	550	-308.	610	-225.
2-Methyl-1-butanamine											
270	-2138.	330	-1176.	390	-770.	450	-543.	510	-398.	570	-297.
280	-1895.	340	-1087.	400	-724.	460	-515.	520	-378.	580	-283.
290	-1697.	350	-1009.	410	-682.	470	-488.	530	-360.	590	-270.
300	-1533.	360	-939.	420	-643.	480	-463.	540	-343.	600	-257.
310	-1395.	370	-877.	430	-607.	490	-440.	550	-327.	610	-245.
320	-1277.	380	-821.	440	-574.	500	-418.	560	-311.	620	-234.
2-Methyl-2-butanamine											
240	-2389.	300	-1206.	360	-764.	420	-529.	480	-381.	540	-281.
250	-2071.	310	-1107.	370	-716.	430	-500.	490	-362.	550	-267.
260	-1822.	320	-1021.	380	-672.	440	-473.	500	-344.	560	-254.
270	-1622.	330	-945.	390	-631.	450	-447.	510	-327.	570	-242.
280	-1458.	340	-878.	400	-594.	460	-424.	520	-311.	580	-230.
290	-1322.	350	-818.	410	-560.	470	-402.	530	-295.		
Pyrrole											
320	-2505.	390	-1247.	460	-775.	530	-527.	600	-375.	670	-272.
330	-2216.	400	-1155.	470	-730.	540	-501.	610	-358.	680	-260.
340	-1979.	410	-1073.	480	-690.	550	-477.	620	-341.	690	-248.
350	-1782.	420	-1000.	490	-652.	560	-454.	630	-326.	700	-237.
360	-1616.	430	-935.	500	-617.	570	-432.	640	-311.	710	-227.
370	-1475.	440	-876.	510	-585.	580	-412.	650	-298.	720	-217.
380	-1353.	450	-823.	520	-555.	590	-393.	660	-284.	730	-207.
1-Methylpyrrole											
300	-2378.	370	-1231.	440	-785.	510	-546.	580	-395.	650	-291.
310	-2116.	380	-1145.	450	-743.	520	-520.	590	-378.	660	-279.
320	-1900.	390	-1068.	460	-704.	530	-496.	600	-361.	670	-268.
330	-1721.	400	-1000.	470	-667.	540	-473.	610	-346.	680	-257.
340	-1569.	410	-938.	480	-634.	550	-452.	620	-331.	690	-246.
350	-1440.	420	-883.	490	-602.	560	-432.	630	-317.	700	-236.
360	-1328.	430	-832.	500	-573.	570	-413.	640	-304.		
Pyridine											
310	-1910.	380	-1043.	450	-687.	520	-490.	590	-363.	660	-276.
320	-1717.	390	-975.	460	-653.	530	-469.	600	-349.	670	-265.
330	-1556.	400	-914.	470	-620.	540	-449.	610	-335.	680	-255.
340	-1421.	410	-860.	480	-591.	550	-430.	620	-322.	690	-246.
350	-1305.	420	-811.	490	-563.	560	-412.	630	-310.	700	-237.
360	-1206.	430	-766.	500	-537.	570	-395.	640	-298.	710	-228.
370	-1119.	440	-725.	510	-513.	580	-379.	650	-286.	720	-219.

TABLE 9. Second virial coefficients calculated from Eq. (10) at selected temperatures — Continued

$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3 \cdot \text{mol}^{-1}}$	$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3 \cdot \text{mol}^{-1}}$	$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3 \cdot \text{mol}^{-1}}$	$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3 \cdot \text{mol}^{-1}}$	$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3 \cdot \text{mol}^{-1}}$	$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3 \cdot \text{mol}^{-1}}$
2-Methylpyridine											
320	-2311.	390	-1276.	460	-840.	530	-596.	600	-439.	670	-329.
330	-2084.	400	-1194.	470	-797.	540	-569.	610	-421.	680	-317.
340	-1894.	410	-1120.	480	-757.	550	-544.	620	-404.	690	-304.
350	-1732.	420	-1053.	490	-721.	560	-521.	630	-387.	700	-292.
360	-1594.	430	-992.	500	-686.	570	-498.	640	-372.	710	-281.
370	-1474.	440	-937.	510	-654.	580	-477.	650	-357.	720	-270.
380	-1369.	450	-887.	520	-624.	590	-458.	660	-343.		
3-Methylpyridine											
340	-2420.	410	-1373.	480	-912.	550	-650.	620	-479.	690	-360.
350	-2196.	420	-1286.	490	-866.	560	-621.	630	-460.	700	-346.
360	-2005.	430	-1209.	500	-824.	570	-594.	640	-441.	710	-333.
370	-1842.	440	-1138.	510	-784.	580	-568.	650	-423.	720	-320.
380	-1701.	450	-1074.	520	-747.	590	-544.	660	-407.	730	-307.
390	-1578.	460	-1016.	530	-713.	600	-522.	670	-390.	740	-295.
400	-1469.	470	-962.	540	-680.	610	-500.	680	-375.	750	-284.
4-Methylpyridine											
340	-2412.	410	-1351.	480	-891.	550	-630.	620	-462.	690	-345.
350	-2184.	420	-1265.	490	-845.	560	-602.	630	-443.	700	-332.
360	-1990.	430	-1187.	500	-803.	570	-575.	640	-425.	710	-318.
370	-1825.	440	-1116.	510	-764.	580	-550.	650	-407.	720	-306.
380	-1683.	450	-1052.	520	-727.	590	-527.	680	-391.	730	-294.
390	-1558.	460	-994.	530	-693.	600	-504.	660	-375.	740	-282.
400	-1449.	470	-940.	540	-661.	610	-483.	670	-360.	750	-271.
Pyrrolidine											
280	-2173.	350	-1088.	420	-688.	490	-475.	560	-343.	630	-253.
290	-1918.	360	-1010.	430	-650.	500	-453.	570	-328.	640	-242.
300	-1711.	370	-941.	440	-615.	510	-432.	580	-314.	650	-232.
310	-1542.	380	-880.	450	-583.	520	-412.	590	-300.	660	-222.
320	-1400.	390	-824.	460	-553.	530	-393.	600	-287.		
330	-1280.	400	-774.	470	-525.	540	-375.	610	-275.		
340	-1178.	410	-729.	480	-499.	550	-359.	620	-264.		
Piperidine											
300	-2107.	370	-1127.	440	-733.	510	-516.	580	-378.	650	-283.
310	-1886.	380	-1051.	450	-694.	520	-492.	590	-362.	660	-271.
320	-1703.	390	-984.	460	-659.	530	-471.	600	-347.	670	-261.
330	-1550.	400	-924.	470	-626.	540	-450.	610	-333.	680	-250.
340	-1420.	410	-869.	480	-596.	550	-430.	620	-319.	690	-240.
350	-1309.	420	-819.	490	-567.	560	-412.	630	-307.		
360	-1212.	430	-774.	500	-541.	570	-394.	640	-294.		
Quinoline											
440	-2579.	520	-1538.	600	-1035.	680	-737.	760	-540.	840	-401.
450	-2392.	530	-1457.	610	-990.	690	-708.	770	-520.	850	-386.
460	-2226.	540	-1382.	620	-947.	700	-681.	780	-501.	860	-372.
470	-2080.	550	-1313.	630	-907.	710	-655.	790	-483.	870	-359.
480	-1948.	560	-1250.	640	-869.	720	-630.	800	-465.	880	-346.
490	-1830.	570	-1190.	650	-834.	730	-606.	810	-448.		
500	-1723.	580	-1135.	660	-800.	740	-583.	820	-432.		
510	-1626.	590	-1084.	670	-768.	750	-561.	830	-416.		

TABLE 9. Second virial coefficients calculated from Eq. (10) at selected temperatures — Continued

$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3 \cdot \text{mol}^{-1}}$	$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3 \cdot \text{mol}^{-1}}$	$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3 \cdot \text{mol}^{-1}}$	$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3 \cdot \text{mol}^{-1}}$	$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3 \cdot \text{mol}^{-1}}$	$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3 \cdot \text{mol}^{-1}}$
Isoquinoline											
440	-2221.	520	-1381.	600	-963.	680	-710.	760	-540.	840	-417.
450	-2071.	530	-1314.	610	-925.	690	-685.	770	-522.	850	-404.
460	-1939.	540	-1252.	620	-889.	700	-662.	780	-505.	860	-392.
470	-1821.	550	-1195.	630	-855.	710	-639.	790	-489.	870	-380.
480	-1715.	560	-1142.	640	-823.	720	-617.	800	-474.	880	-368.
490	-1619.	570	-1093.	650	-793.	730	-597.	810	-459.	890	-357.
500	-1532.	580	-1047.	660	-764.	740	-577.	820	-445.	900	-346.
510	-1453.	590	-1004.	670	-736.	750	-558.	830	-431.		
Carbazole											
600	-2291.	670	-1672.	740	-1268.	810	-983.	880	-772.	950	-610.
610	-2183.	680	-1604.	750	-1221.	820	-949.	890	-747.	960	-590.
620	-2083.	690	-1540.	760	-1177.	830	-917.	900	-722.	970	-571.
630	-1989.	700	-1480.	770	-1134.	840	-885.	910	-698.	980	-552.
640	-1902.	710	-1422.	780	-1094.	850	-855.	920	-675.	990	-534.
650	-1820.	720	-1368.	790	-1055.	860	-827.	930	-653.	1000	-517.
660	-1744.	730	-1317.	800	-1018.	870	-799.	940	-631.		
Acridine											
590	-2384.	660	-1735.	730	-1313.	800	-1016.	870	-797.	940	-628.
600	-2271.	670	-1664.	740	-1264.	810	-981.	880	-770.	950	-607.
610	-2166.	680	-1598.	750	-1218.	820	-947.	890	-744.	960	-587.
620	-2068.	690	-1534.	760	-1174.	830	-914.	900	-719.	970	-568.
630	-1976.	700	-1475.	770	-1132.	840	-883.	910	-695.	980	-549.
640	-1891.	710	-1418.	780	-1092.	850	-853.	920	-672.		
650	-1811.	720	-1364.	790	-1053.	860	-824.	930	-650.		
Phenanthridine											
610	-2231.	680	-1649.	750	-1262.	820	-985.	890	-778.	960	-618.
620	-2131.	690	-1585.	760	-1217.	830	-952.	900	-753.	970	-598.
630	-2037.	700	-1524.	770	-1174.	840	-920.	910	-728.	980	-579.
640	-1950.	710	-1466.	780	-1133.	850	-889.	920	-705.	990	-560.
650	-1868.	720	-1411.	790	-1093.	860	-860.	930	-682.	1000	-542.
660	-1790.	730	-1359.	800	-1056.	870	-832.	940	-660.		
670	-1718.	740	-1309.	810	-1020.	880	-804.	950	-638.		
1-Naphthalenamine											
510	-2223.	590	-1447.	670	-1021.	750	-750.	830	-564.	910	-428.
520	-2092.	600	-1380.	680	-981.	760	-723.	840	-545.	920	-414.
530	-1974.	610	-1319.	690	-942.	770	-698.	850	-526.	930	-400.
540	-1867.	620	-1261.	700	-906.	780	-673.	860	-508.	940	-387.
550	-1768.	630	-1207.	710	-872.	790	-649.	870	-491.	950	-374.
560	-1678.	640	-1156.	720	-839.	800	-627.	880	-475.		
570	-1595.	650	-1108.	730	-808.	810	-605.	890	-459.		
580	-1518.	660	-1063.	740	-779.	820	-584.	900	-443.		
2-Naphthalenamine											
510	-2345.	590	-1515.	670	-1063.	750	-777.	830	-580.	910	-438.
520	-2205.	600	-1444.	680	-1020.	760	-748.	840	-560.	920	-423.
530	-2078.	610	-1379.	690	-980.	770	-721.	850	-541.	930	-408.
540	-1963.	620	-1317.	700	-942.	780	-695.	860	-522.	940	-394.
550	-1858.	630	-1260.	710	-905.	790	-670.	870	-504.	950	-381.
560	-1762.	640	-1206.	720	-871.	800	-646.	880	-486.		
570	-1673.	650	-1155.	730	-838.	810	-624.	890	-470.		
580	-1591.	660	-1108.	740	-807.	820	-602.	900	-454.		

TABLE 9. Second virial coefficients calculated from Eq. (10) at selected temperatures — Continued

$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3\cdot\text{mol}^{-1}}$	$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3\cdot\text{mol}^{-1}}$	$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3\cdot\text{mol}^{-1}}$	$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3\cdot\text{mol}^{-1}}$	$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3\cdot\text{mol}^{-1}}$	$\frac{T}{K}$	$\frac{B_m}{\text{cm}^3\cdot\text{mol}^{-1}}$
9-Methylcarbazole											
600	-2361.	670	-1746.	740	-1339.	810	-1049.	880	-832.	950	-664.
610	-2254.	680	-1678.	750	-1292.	820	-1014.	890	-805.	960	-643.
620	-2155.	690	-1614.	760	-1246.	830	-980.	900	-780.	970	-623.
630	-2063.	700	-1553.	770	-1203.	840	-948.	910	-755.	980	-604.
640	-1976.	710	-1496.	780	-1162.	850	-918.	920	-731.	990	-585.
650	-1895.	720	-1441.	790	-1123.	860	-888.	930	-708.		
660	-1818.	730	-1389.	800	-1085.	870	-859.	940	-686.		

TABLE 10. Enthalpy of vaporization or sublimation and conversion to the ideal gas at 298.15 K

Compound	Phase x	$\Delta_f^{\text{id}} H_m / \text{kJ}\cdot\text{mol}^{-1}, ^a$
1-Butanamine	l	35.70 ± 0.10
2-Butanamine	l	32.85 ± 0.10
2-Methyl-1-propanamine	l	33.81 ± 0.10
2-Methyl-2-propanamine	l	29.64 ± 0.10
Pyrrole	l	45.09 ± 0.2 ^a
1-Methylpyrrole	l	40.65 ± 0.20
2-Methylpyrrole	l	50.7 ± 0.5
3-Methylpyrrole	l	49.7 ± 0.5
Pyridine	l	40.21 ± 0.20
2-Methylpyridine	l	42.47 ± 0.20
3-Methylpyridine	l	44.44 ± 0.20
4-Methylpyridine	l	44.56 ± 0.20
Pyrrolidine	l	37.52 ± 0.20
Piperidine	l	39.29 ± 0.20
Indole	cr	69.9 ± 1.0
Quinoline	l	59.3 ± 1.0
Isoquinoline	l	60.3 ± 1.0
Acridine	cr	94.5 ± 4.0
Carbazole	cr	99.0 ± 4.0
Phenanthridine	cr	98.6 ± 4.0
1-Naphthalenamine	cr	65.0 ± 4.0
2-Naphthalenamine	cr	74.1 ± 4.0
9-Methylcarbazole	cr	95.5 ± 4.0

^aUncertainties are standard error estimates.

TABLE 11. Selected enthalpies of formation^{a,b} at 0 and 298.15 K for the ideal gas and condensed phases

Temperature Compound	Ideal gas		Liquid or crystal	
	0 K	298.15 K $\Delta_f H^\circ/\text{kJ}\cdot\text{mol}^{-1}$	298.15 K	Phase ^c
1-Butanamine	-60.59 ± 1.27	-91.90 ± 1.27	-127.60 ± 1.26	l
2-Butanamine	-71.11 ± 1.06	-104.65 ± 1.06	-137.50 ± 1.05	l
2-Methyl-1-propanamine	-65.64 ± 0.51	-98.74 ± 0.51	-132.55 ± 0.50	l
2-Methyl-2-propanamine	-87.11 ± 0.52	-120.98 ± 0.52	-150.62 ± 0.50	l
Pyrrole	124.85 ± 0.81	108.18 ± 0.81	63.09 ± 0.80	l
1-Methylpyrrole	125.88 ± 0.60	103.14 ± 0.54	62.38 ± 0.50	l
2-Methylpyrrole	96.5 ± 2.3	74.0 ± 2.2	23.3 ± 2.0	l
3-Methylpyrrole	92.7 ± 2.3	70.2 ± 2.2	20.5 ± 2.0	l
Pyridine	157.20 ± 0.54	140.37 ± 0.54	100.16 ± 0.50	l
2-Methylpyridine	121.66 ± 0.79	99.16 ± 0.78	56.69 ± 0.75	l
3-Methylpyridine	128.86 ± 0.61	106.36 ± 0.61	61.92 ± 0.58	l
4-Methylpyridine	126.29 ± 0.91	103.76 ± 0.90	59.20 ± 0.88	l
Pyrrolidine	26.89 ± 0.82	-3.59 ± 0.80	-41.11 ± 0.80	l
Piperidine	-9.04 ± 0.62	-47.15 ± 0.62	-86.44 ± 0.58	l
Indole	179.57 ± 1.30	156.50 ± 1.25	86.65 ± 0.75	cr
Quinoline	223.42 ± 1.40	200.52 ± 1.36	141.22 ± 0.92	l
Isoquinoline	227.49 ± 1.35	204.61 ± 1.33	144.35 ± 0.88	l
Carbazole	232.8 ± 5.2	200.7 ± 4.9	101.7 ± 2.8	cr
Acridine	302.4 ± 4.3	273.9 ± 4.1	179.41 ± 1.04	cr
Phenanthridine	268.8 ± 4.4	240.5 ± 4.2	141.93 ± 1.36	cr
1-Naphthalenamine	159.9 ± 7.0	132.8 ± 6.7 ^d	67.8 ± 5.4	cr
2-Naphthalenamine	161.1 ± 5.4	134.3 ± 5.2 ^d	60.2 ± 3.3	cr
9-Methylcarbazole	234.1 ± 4.3	201.0 ± 4.1	105.52 ± 1.05	cr

^aFor formation reactions $n\text{C}(\text{graphite}) + (m/2)\text{H}_2(\text{g}) + (1/2)\text{N}_2(\text{g}) \rightarrow \text{C}_n\text{H}_m\text{N}(\text{cr, l, or g})^\circ$ ^bUncertainties are two standard error estimates.^ccr for crystal, and l for liquid.^dEstimated.TABLE 12. Thermodynamic properties for the condensed phases at vapor saturation.^a

$\frac{T}{\text{K}}$	$\frac{C_{\text{sat}}}{R}$	$\frac{\Delta_f^\circ S}{R}$	$-\frac{\Delta_f^\circ G}{RT}$	$\frac{\Delta_f^\circ H}{RT}$
Pyrrole (crII,l)				
0	0.000	0.000	0.000	0.000
10	0.195	0.066	0.017	0.049
15	0.574	0.211	0.055	0.156
20	1.068	0.443	0.121	0.322
25	1.604	0.738	0.214	0.524
30	2.118	1.077	0.329	0.748
35	2.601	1.440	0.462	0.978
40	3.046	1.817	0.608	1.210
45	3.440	2.199	0.763	1.436
50	3.796	2.580	0.926	1.654
60	4.423	3.329	1.265	2.065
64	4.681	3.622	1.402	2.220
65.5	5.038	3.735	1.455	2.280
66	4.739	3.772	1.472	2.300
70	4.788	4.052	1.612	2.441
80	5.031	4.707	1.958	2.749
90	5.273	5.314	2.298	3.016
100	5.492	5.880	2.628	3.252
110	5.696	6.413	2.948	3.465
120	5.897	6.917	3.258	3.659
130	6.105	7.398	3.558	3.840
140	6.324	7.858	3.849	4.009
150	6.559	8.302	4.131	4.171
160	6.822	8.734	4.405	4.329
170	7.107	9.156	4.672	4.483

TABLE 12. Thermodynamic properties for the condensed phases at vapor saturation^a — Continued

$\frac{T}{\text{K}}$	$\frac{C_{\text{sat}}}{R}$	$\frac{\Delta_f^\circ S}{R}$	$-\frac{\Delta_f^\circ G}{RT}$	$\frac{\Delta_f^\circ H}{RT}$
Pyrrole (crII,l) — Continued				
180	7.416	9.571	4.934	4.638
190	7.755	9.981	5.188	4.793
200	8.121	10.388	5.438	4.950
210	8.506	10.793	5.683	5.110
220	8.932	11.199	5.925	5.274
230	9.391	11.606	6.163	5.443
240	9.850	12.015	6.398	5.617
249.74	10.297	12.416	6.625	5.791
Pyrrole (l)				
249.74	13.954	16.224	6.625	9.599
250	13.960	16.237	6.633	9.603
260	14.235	16.791	7.015	9.776
270	14.529	17.330	7.383	9.947
280	14.827	17.863	7.748	10.115
290	15.121	18.392	8.109	10.283
298.15	15.367	18.815	8.396	10.419
300	15.422	18.910	8.461	10.450
310	15.722	19.419	8.804	10.615
320	16.023	19.922	9.143	10.780
330	16.323	20.420	9.477	10.943
340	16.624	20.913	9.808	11.106
350	16.920	21.401	10.134	11.267
360	17.221	21.879	10.450	11.429

TABLE 12. Thermodynamic properties for the condensed phases at vapor saturation^a — Continued

$\frac{T}{K}$	$\frac{C_{sat}}{R}$	$\frac{\Delta_f S}{R}$	$-\frac{\Delta_f G}{RT}$	$\frac{\Delta_f H}{RT}$
Pyrrole (l) — Continued				
370	17.522	22.357	10.768	11.589
380	17.823	22.825	11.075	11.750
390	18.124	23.293	11.384	11.909
400	18.425	23.756	11.687	12.068
2-Methyl-2-propanamine (crIII)				
0	0.000	0.000	0.000	0.000
10	0.298	0.100	0.025	0.076
15	0.867	0.322	0.083	0.239
20	1.569	0.665	0.183	0.482
25	2.268	1.091	0.321	0.770
30	2.897	1.561	0.488	1.073
35	3.438	2.049	0.676	1.373
40	3.912	2.540	0.879	1.662
45	4.323	3.025	1.090	1.935
50	4.703	3.501	1.308	2.193
60	5.430	4.422	1.751	2.671
70	6.174	5.313	2.196	3.117
80	7.042	6.193	2.641	3.552
90	7.976	7.075	3.084	3.991
91.30	8.107	7.191	3.142	4.049
2-Methyl-2-propanamine (crII)				
91.30	7.217	7.340	3.142	4.198
100	7.643	8.016	3.537	4.479
110	8.217	8.771	3.978	4.792
120	8.808	9.511	4.409	5.103
130	9.403	10.239	4.829	5.411
140	10.009	10.959	5.241	5.717
150	10.621	11.670	5.646	6.024
160	11.259	12.375	6.044	6.331
170	11.932	13.078	6.438	6.640
180	12.686	13.781	6.826	6.955
190	13.579	14.490	7.211	7.279
200	14.625	15.212	7.593	7.620
202.27	14.884	15.379	7.679	7.700
2-Methyl-2-propanamine (crI)				
202.27	20.099	18.977	7.679	11.298
206.20	20.252	19.364	7.900	11.464
2-Methyl-2-propanamine (l)				
206.20	21.289	19.877	7.900	11.977
210	21.442	20.265	8.122	12.143
220	21.764	21.272	8.695	12.577
230	22.024	22.249	9.264	12.985
240	22.223	23.190	9.822	13.368
250	22.392	24.102	10.376	13.726
260	22.527	24.983	10.924	14.059
270	22.655	25.834	11.458	14.377
280	22.790	26.660	11.986	14.674
290	22.939	27.461	12.504	14.956
298.15	23.062	28.100	12.922	15.178
300	23.092	28.241	13.018	15.223
310	23.276	29.001	13.521	15.480
320	23.490	29.746	14.019	15.726
330	23.720	30.470	14.502	15.968
340	23.960	31.185	14.985	16.199

TABLE 12. Thermodynamic properties for the condensed phases at vapor saturation^a — Continued

$\frac{T}{K}$	$\frac{C_{sat}}{R}$	$\frac{\Delta_f S}{R}$	$-\frac{\Delta_f G}{RT}$	$\frac{\Delta_f H}{RT}$
1-Methylpyrrole (cr)				
0	0.000	0.000	0.000	0.000
10	0.204	0.068	0.017	0.051
15	0.621	0.224	0.058	0.166
20	1.186	0.476	0.128	0.348
25	1.830	0.809	0.229	0.579
30	2.482	1.200	0.357	0.842
35	3.109	1.630	0.508	1.122
40	3.693	2.084	0.677	1.408
45	4.225	2.550	0.860	1.691
50	4.703	3.020	1.052	1.969
60	5.527	3.953	1.458	2.496
70	6.177	4.856	1.880	2.976
80	6.683	5.715	2.306	3.409
90	7.098	6.527	2.730	3.796
100	7.473	7.295	3.148	4.146
110	7.797	8.023	3.559	4.463
120	8.086	8.713	3.960	4.753
130	8.370	9.371	4.350	5.021
140	8.669	10.002	4.732	5.270
150	8.971	10.611	5.104	5.507
160	9.307	11.200	5.466	5.734
170	9.646	11.775	5.821	5.954
180	10.017	12.336	6.167	6.169
190	10.430	12.889	6.507	6.382
200	10.855	13.435	6.840	6.595
210	11.318	13.975	7.166	6.809
216.912	11.652	14.347	7.389	6.958
1-Methylpyrrole (l)				
216.912	16.363	18.685	7.389	11.296
220	16.411	18.917	7.549	11.368
230	16.560	19.650	8.060	11.590
240	16.722	20.358	8.558	11.801
250	16.912	21.044	9.043	12.002
260	17.125	21.713	9.519	12.194
270	17.350	22.363	9.982	12.381
280	17.586	22.998	10.435	12.563
290	17.834	23.619	10.879	12.740
298.15	18.048	24.117	11.235	12.882
300	18.098	24.228	11.314	12.914
310	18.369	24.826	11.740	13.086
320	18.641	25.414	12.159	13.255
330	18.915	25.992	12.569	13.423
340	19.200	26.560	12.972	13.588
350	19.498	27.121	13.368	13.753
360	19.787	27.675	13.758	13.917
370	20.092	28.221	14.142	14.079
Pyridine (cr)				
0	0.000	0.000	0.000	0.000
10	0.249	0.084	0.021	0.063
15	0.721	0.267	0.069	0.198
20	1.302	0.554	0.153	0.402
25	1.905	0.909	0.267	0.642
30	2.485	1.309	0.407	0.902
35	3.003	1.731	0.566	1.165
40	3.457	2.127	0.704	1.424
45	3.846	2.593	0.921	1.672
50	4.174	3.016	1.110	1.906
60	4.720	3.827	1.495	2.332

TABLE 12. Thermodynamic properties for the condensed phases at vapor saturation^a - Continued

$\frac{T}{K}$	$\frac{C_{sat}}{R}$	$\frac{\Delta G^0}{R}$	$-\frac{\Delta G^0}{RT}$	$\frac{\Delta H^0}{RT}$
Pyridine (cr)				
70	5.136	4.587	1.883	2.703
80	5.482	5.296	2.266	3.029
90	5.796	5.959	2.640	3.319
100	6.084	6.585	3.004	3.581
110	6.367	7.178	3.356	3.822
120	6.652	7.744	3.698	4.046
130	6.944	8.288	4.031	4.257
140	7.251	8.814	4.460	4.354
150	7.570	9.325	4.657	4.668
160	7.906	9.824	4.975	4.849
170	8.265	10.314	5.275	5.040
180	8.646	10.797	5.568	5.229
190	9.065	11.276	5.856	5.420
200	9.497	11.752	6.139	5.613
210	9.951	12.226	6.417	5.809
220	10.447	12.700	6.692	6.008
230	10.974	13.176	6.964	6.212
231.49	11.055	13.246	7.002	6.244
Pyridine (l)				
231.49	14.577	17.545	7.002	10.543
240	14.719	18.073	7.383	10.689
250	14.901	18.677	7.823	10.854
260	15.106	19.266	8.253	11.013
270	15.313	19.840	8.672	11.169
280	15.531	20.404	9.083	11.321
290	15.771	20.953	9.483	11.470
298.15	15.965	21.396	9.805	11.591
300	16.010	21.492	9.874	11.618
310	16.256	22.020	10.257	11.763
320	16.511	22.538	10.631	11.908
330	16.776	23.052	11.000	12.052
340	17.047	23.555	11.360	12.195
350	17.322	24.053	11.716	12.337
Pyrrolidine (crII)				
0	0.000	0.000	0.000	0.000
10	0.194	0.065	0.016	0.049
15	0.598	0.213	0.055	0.158
20	1.153	0.459	0.123	0.336
25	1.792	0.794	0.231	0.562
30	2.437	1.167	0.346	0.821
35	3.032	1.589	0.493	1.096
40	3.571	2.030	0.658	1.372
45	4.038	2.477	0.835	1.642
50	4.446	2.923	1.021	1.902
60	5.134	3.797	1.412	2.386
70	5.668	4.631	1.813	2.818
80	6.106	5.416	2.214	3.202
90	6.488	6.158	2.612	3.546
100	6.825	6.859	3.002	3.857
110	7.140	7.524	3.383	4.141
120	7.451	8.160	3.755	4.404
130	7.756	8.767	4.117	4.650
140	8.065	9.353	4.470	4.883
150	8.392	9.921	4.815	5.106
160	8.729	10.474	5.152	5.322
170	9.087	11.013	5.480	5.533
180	9.488	11.543	5.802	5.741
190	9.939	12.068	6.119	5.950
200	10.445	12.591	6.429	6.162
207.14	10.849	12.964	6.648	6.316

TABLE 12. Thermodynamic properties for the condensed phases at vapor saturation^a - Continued

$\frac{T}{K}$	$\frac{C_{sat}}{R}$	$\frac{\Delta G^0}{R}$	$-\frac{\Delta G^0}{RT}$	$\frac{\Delta H^0}{RT}$
Pyrrolidine (crI)				
207.14	10.710	13.278	6.648	6.630
210	11.089	13.427	6.739	6.688
215.31	11.785	13.714	6.909	6.805
Pyrrolidine (l)				
215.31	17.986	18.503	6.909	11.595
220	18.104	18.892	7.160	11.732
230	18.338	19.698	7.683	12.015
240	18.497	20.483	8.201	12.282
250	18.594	21.244	8.711	12.533
260	18.654	21.974	9.207	12.767
270	18.692	22.679	9.693	12.986
280	18.733	23.359	10.168	13.191
290	18.781	24.013	10.631	13.383
298.15	18.834	24.537	11.006	13.531
300	18.844	24.652	11.089	13.563
310	18.923	25.271	11.536	13.735
320	19.012	25.875	11.977	13.899
330	19.121	26.459	12.404	14.055
340	19.260	27.033	12.827	14.206
350	19.425	27.596	13.243	14.353
2-Methylpyridine (cr)				
0	0.000	0.000	0.000	0.000
10	0.220	0.074	0.018	0.056
15	0.655	0.242	0.062	0.180
20	1.206	0.504	0.138	0.366
25	1.807	0.837	0.244	0.594
30	2.406	1.220	0.374	0.846
35	2.975	1.635	0.525	1.110
40	3.509	2.067	0.690	1.378
45	3.993	2.509	0.868	1.642
50	4.441	2.953	1.054	1.900
60	5.255	3.836	1.444	2.392
70	5.942	4.699	1.848	2.852
80	6.547	5.533	2.257	3.276
90	7.097	6.337	2.666	3.671
100	7.589	7.110	3.071	4.038
110	8.037	7.855	3.473	4.382
120	8.456	8.572	3.868	4.704
130	8.854	9.265	4.257	5.008
140	9.232	9.935	4.639	5.296
150	9.612	10.585	5.013	5.571
160	9.994	11.217	5.381	5.836
170	10.380	11.834	5.743	6.092
180	10.768	12.439	6.098	6.341
190	11.166	13.032	6.448	6.584
200	11.573	13.615	6.792	6.823
206.45	11.837	13.987	7.011	6.976
2-Methylpyridine (l)				
206.45	17.017	19.650	7.011	12.640
210	17.054	19.938	7.224	12.714
220	17.178	20.733	7.820	12.914
230	17.346	21.504	8.401	13.103
240	17.545	22.244	8.960	13.284
250	17.763	22.964	9.506	13.458
260	17.999	23.664	10.035	13.629
270	18.259	24.349	10.554	13.795
280	18.531	25.019	11.059	13.960

TABLE 12. Thermodynamic properties for the condensed phases at vapor saturation^a — Continued

$\frac{T}{K}$	$\frac{C_{sat}}{R}$	$\frac{\Delta_f S}{R}$	$-\frac{\Delta_f G}{RT}$	$\frac{\Delta_f H}{RT}$
2-Methylpyridine (l) — Continued				
290	18.816	25.673	11.551	14.122
298.15	19.056	26.201	11.948	14.254
300	19.111	26.317	12.034	14.284
310	19.421	26.946	12.502	14.445
320	19.737	27.570	12.965	14.605
330	20.057	28.184	13.419	14.765
340	20.388	28.788	13.862	14.926
350	20.723	29.382	14.295	15.087
360	21.064	29.970	14.723	15.248
370	21.390	30.554	15.144	15.410
3-Methylpyridine (cr)				
0	0.000	0.000	0.000	0.000
10	0.178	0.059	0.015	0.045
15	0.567	0.197	0.050	0.147
20	1.166	0.436	0.114	0.323
25	1.837	0.767	0.211	0.557
30	2.528	1.164	0.335	0.829
35	3.178	1.603	0.485	1.118
40	3.774	2.067	0.653	1.414
45	4.296	2.542	0.837	1.706
50	4.755	3.019	1.031	1.988
60	5.532	3.958	1.441	2.517
70	6.127	4.857	1.865	2.992
80	6.607	5.707	2.293	3.414
90	7.026	6.510	2.718	3.792
100	7.403	7.270	3.135	4.135
110	7.757	7.992	3.544	4.448
120	8.102	8.682	3.944	4.738
130	8.442	9.344	4.334	5.010
140	8.784	9.981	4.714	5.267
150	9.131	10.599	5.086	5.513
160	9.495	11.200	5.450	5.751
170	9.870	11.787	5.805	5.982
180	10.253	12.362	6.153	6.209
190	10.646	12.927	6.495	6.432
200	11.037	13.483	6.830	6.652
210	11.446	14.031	7.160	6.871
220	11.856	14.573	7.484	7.089
230	12.281	15.108	7.805	7.304
240	12.713	15.642	8.122	7.520
250	13.174	16.171	8.434	7.737
255.01	13.427	16.433	8.586	7.847
3-Methylpyridine (l)				
255.01	18.020	23.120	8.586	14.535
260	18.130	23.473	8.871	14.602
270	18.355	24.158	9.421	14.737
280	18.602	24.832	9.962	14.870
290	18.866	25.487	10.483	15.004
298.15	19.091	26.015	10.903	15.112
300	19.146	26.131	10.994	15.138
310	19.431	26.765	11.492	15.273
320	19.731	27.389	11.985	15.404
330	20.042	27.998	12.458	15.540
340	20.352	28.602	12.921	15.681
350	20.663	29.196	13.379	15.817
360	20.984	29.784	13.827	15.957
370	21.315	30.363	14.265	16.098
380	21.636	30.936	14.697	16.239
390	21.952	31.500	15.120	16.380

TABLE 12. Thermodynamic properties for the condensed phases at vapor saturation^a — Continued

$\frac{T}{K}$	$\frac{C_{sat}}{R}$	$\frac{\Delta_f S}{R}$	$-\frac{\Delta_f G}{RT}$	$\frac{\Delta_f H}{RT}$
4-Methylpyridine (crII)				
0	0.000	0.000	0.000	0.000
10	0.541	0.201	0.052	0.148
15	1.160	0.542	0.155	0.386
20	1.731	0.954	0.302	0.652
25	2.317	1.404	0.478	0.926
30	2.874	1.876	0.671	1.206
35	3.385	2.358	0.877	1.482
40	3.849	2.841	1.093	1.749
45	4.264	3.319	1.313	2.006
50	4.631	3.788	1.538	2.250
60	5.251	4.689	1.988	2.701
70	5.773	5.537	2.435	3.102
80	6.225	6.339	2.874	3.465
90	6.641	7.096	3.301	3.795
100	7.057	7.817	3.717	4.100
110	7.450	8.509	4.122	4.387
120	7.838	9.174	4.516	4.658
130	8.207	9.816	4.899	4.917
140	8.597	10.438	5.271	5.166
150	8.992	11.045	5.636	5.408
160	9.407	11.638	5.992	5.645
170	9.835	12.221	6.342	5.878
180	10.288	12.796	6.684	6.111
190	10.760	13.365	7.021	6.343
200	11.271	13.930	7.353	6.576
210	11.818	14.493	7.680	6.812
220	12.430	15.056	8.001	7.054
230	13.136	15.624	8.321	7.303
240	13.987	16.200	8.637	7.563
250	15.329	16.795	8.952	7.843
255.000	17.452	17.115	9.108	8.007
4-Methylpyridine (crI)				
255.000	13.886	17.115	9.108	8.007
260	14.042	17.386	9.264	8.122
270	14.378	17.922	9.575	8.347
276.818	14.629	18.285	9.786	8.499
4-Methylpyridine (l)				
276.818	18.540	23.751	9.786	13.965
280	18.623	23.963	9.945	14.018
290	18.897	24.622	10.441	14.181
298.15	19.122	25.148	10.835	14.313
300	19.173	25.267	10.924	14.343
310	19.461	25.900	11.396	14.504
320	19.763	26.523	11.860	14.663
330	20.077	27.136	12.314	14.822
340	20.394	27.740	12.758	14.982
350	20.719	28.336	13.195	15.141
360	21.047	28.924	13.624	15.300
370	21.380	29.505	14.045	15.460
380	21.717	30.080	14.460	15.620
390	22.074	30.648	14.867	15.781
400	22.428	31.212	15.269	15.943
Piperidine (cr)				
0	0.000	0.000	0.000	0.000
10	0.188	0.063	0.016	0.047
15	0.591	0.208	0.053	0.155

TABLE 12. Thermodynamic properties for the condensed phases at vapor saturation* — Continued

T K	C_{sat} R	$\frac{\Delta_f S}{R}$	$-\frac{\Delta_f G}{RT}$	$\frac{\Delta_f H}{RT}$
Piperidine (cr) — Continued				
20	1.162	0.453	0.120	0.333
25	1.788	0.779	0.217	0.561
30	2.383	1.158	0.342	0.815
35	2.918	1.567	0.487	1.080
40	3.384	1.988	0.650	1.339
45	3.787	2.410	0.822	1.589
50	4.147	2.828	1.002	1.826
60	4.760	3.640	1.374	2.267
70	5.276	4.413	1.753	2.660
80	5.734	5.148	2.132	3.016
90	6.157	5.848	2.506	3.341
100	6.594	6.519	2.874	3.644
110	7.014	7.168	3.235	3.932
120	7.411	7.794	3.588	4.206
130	7.808	8.403	3.936	4.467
140	8.202	8.997	4.277	4.720
150	8.602	9.576	4.611	4.965
160	9.015	10.144	4.938	5.206
170	9.439	10.704	5.262	5.442
180	9.875	11.255	5.579	5.676
190	10.329	11.801	5.892	5.909
200	10.789	12.343	6.202	6.141
210	11.269	12.881	6.507	6.374
220	11.778	13.417	6.809	6.609
230	12.291	13.951	7.107	6.845
240	12.832	14.486	7.404	7.083
250	13.383	15.022	7.698	7.324
260	13.953	15.557	7.990	7.567
262.124	14.076	15.672	8.052	7.620
Piperidine (l)				
262.124	21.409	22.487	8.052	14.435
270	21.430	23.121	8.482	14.639
280	21.472	23.901	9.019	14.882
290	21.549	24.656	9.546	15.110
298.15	21.632	25.254	9.967	15.287
300	21.653	25.388	10.061	15.327
310	21.789	26.100	10.567	15.533
320	21.956	26.794	11.063	15.731
330	22.149	27.473	11.551	15.922
340	22.387	28.137	12.028	16.109
350	22.671	28.790	12.498	16.292
360	22.970	29.433	12.959	16.474
370	23.281	30.067	13.414	16.653
Quinoline (crII)				
0	0.000	0.000	0.000	0.000
10	0.380	0.136	0.035	0.101
15	0.971	0.399	0.108	0.291
20	1.621	0.766	0.224	0.542
25	2.210	1.192	0.375	0.816
30	2.827	2.826	1.177	1.650
35	3.342	2.125	0.740	1.386
40	3.807	2.603	0.944	1.660
45	4.226	3.075	1.154	1.922
50	4.602	3.540	1.369	2.172
60	5.282	4.442	1.807	2.635
70	5.858	5.299	2.245	3.054
80	6.389	6.117	2.679	3.438
90	6.886	6.898	3.105	3.793
100	7.365	7.648	3.521	4.127
110	7.857	8.373	3.930	4.443

TABLE 12. Thermodynamic properties for the condensed phases at vapor saturation* — Continued

T K	C_{sat} R	$\frac{\Delta_f S}{R}$	$-\frac{\Delta_f G}{RT}$	$\frac{\Delta_f H}{RT}$
Quinoline (crII) — Continued				
120	8.356	9.079	4.329	4.749
130	8.865	9.767	4.721	5.046
140	9.382	10.443	5.106	5.337
150	9.916	11.108	5.484	5.624
160	10.475	11.766	5.856	5.910
170	11.026	12.417	6.222	6.195
180	11.592	13.064	6.585	6.479
190	12.161	13.706	6.943	6.763
200	12.740	14.344	7.297	7.047
210	13.363	14.980	7.647	7.333
220.000	14.004	15.617	7.996	7.621
Quinoline (crI)				
220.000	14.566	15.654	7.996	7.658
230	15.343	16.318	8.343	7.975
240	16.118	16.988	8.690	8.299
250	16.892	17.662	9.035	8.627
258.369	17.625	18.239	9.323	8.906
Quinoline (l)				
258.369	21.776	23.193	9.323	13.870
260	21.842	23.331	9.411	13.920
270	22.252	24.163	9.942	14.221
280	22.674	24.979	10.464	14.515
290	23.095	25.782	10.978	14.804
298.15	23.440	26.427	11.392	15.035
300	23.521	26.572	11.485	15.087
310	23.965	27.351	11.985	15.366
320	24.398	28.119	12.477	15.642
330	24.858	28.876	12.962	15.914
340	25.312	29.625	13.441	16.184
350	25.775	30.336	13.885	16.451
360	26.216	31.098	14.382	16.716
370	26.669	31.822	14.843	16.979
380	27.127	32.540	15.300	17.240
390	27.576	33.250	15.751	17.499
400	28.025	33.954	16.197	17.757
410	28.458	34.651	16.638	18.013
420	28.891	35.342	17.075	18.267
430	29.327	36.027	17.508	18.519
440	29.757	36.706	17.937	18.769
450	30.192	37.380	18.362	19.018
460	30.635	38.048	18.782	19.266
470	31.073	38.712	19.200	19.512
480	31.507	39.371	19.613	19.758
490	31.940	40.025	20.023	20.002
500	32.374	40.674	20.429	20.245
Isoquinoline (crIII)				
0	0.000	0.000	0.000	0.000
10	0.235	0.079	0.020	0.059
15	0.720	0.259	0.067	0.192
20	1.365	0.550	0.147	0.403
25	2.026	0.927	0.265	0.661
30	2.634	1.351	0.410	0.941
35	3.172	1.798	0.576	1.223
40	3.639	2.253	0.758	1.496
45	4.078	2.707	0.949	1.759
50	4.459	3.157	1.148	2.010
60	5.113	4.030	1.555	2.475
70	5.735	4.866	1.970	2.896
80	6.256	5.666	2.382	3.284

TABLE 12. Thermodynamic properties for the condensed phases at vapor saturation^a — Continued

T K	$\frac{C_{sat}}{R}$	$\frac{\Delta_f^0 S}{R}$	$-\frac{\Delta_f^0 G}{RT}$	$\frac{\Delta_f^0 H}{RT}$
Isoquinoline (crIII) — Continued				
90	6.755	6.432	2.790	3.642
100	7.223	7.168	3.190	3.977
110	7.709	7.879	3.584	4.294
120	8.229	8.572	3.972	4.600
130	8.737	9.250	4.351	4.899
140	9.247	9.917	4.726	5.191
150	9.768	10.572	5.093	5.479
160	10.320	11.220	5.456	5.764
170	10.879	11.862	5.814	6.048
180	11.453	12.500	6.168	6.332
190	12.198	13.138	6.518	6.620
200	13.417	13.792	6.865	6.927
210	15.115	14.487	7.211	7.276
220	18.036	15.240	7.559	7.681
221.00	18.733	15.323	7.594	7.729
Isoquinoline (crII)				
221.00	14.811	15.323	7.594	7.729
230	15.211	15.921	7.909	8.012
240	15.809	16.581	8.256	8.326
250	16.484	17.239	8.602	8.638
260	17.184	17.900	8.947	8.953
270	18.405	18.568	9.291	9.277
275.00	19.416	18.915	9.463	9.452
Isoquinoline (crI)				
275.00	19.415	18.915	9.463	9.452
280	19.691	19.267	9.635	9.632
290	20.486	19.971	9.979	9.992
298.15	21.371	20.550	10.260	10.290
299.620	21.563	20.656	10.311	10.345
Isoquinoline (l)				
299.620	23.653	26.093	10.311	15.782
300	23.668	26.123	10.331	15.792
310	24.048	26.905	10.853	16.052
320	24.479	27.675	11.366	16.309
330	24.905	28.435	11.872	16.563
340	25.343	29.185	12.370	16.815
350	25.781	29.926	12.861	17.065
360	26.226	30.659	13.346	17.313
370	26.668	31.383	13.823	17.560
380	27.106	32.100	14.295	17.805
390	27.565	32.810	14.760	18.050
400	27.993	33.514	15.221	18.293
410	28.427	34.210	15.675	18.535
420	28.864	34.900	16.125	18.775
430	29.299	35.585	16.570	19.015
440	29.741	36.263	17.009	19.254
450	30.180	36.937	17.445	19.492
Acridine (cr)				
0	0.000	0.000	0.000	0.000
10	0.421	0.151	0.039	0.112
15	1.049	0.436	0.120	0.316
20	1.754	0.833	0.246	0.587
25	2.447	1.300	0.410	0.890
30	3.095	1.804	0.600	1.205
35	3.689	2.326	0.809	1.518

TABLE 12. Thermodynamic properties for the condensed phases at vapor saturation^a — Continued

T K	$\frac{C_{sat}}{R}$	$\frac{\Delta_f^0 S}{R}$	$-\frac{\Delta_f^0 G}{RT}$	$\frac{\Delta_f^0 H}{RT}$
40	4.239	2.855	1.032	1.824
45	4.744	3.385	1.264	2.121
50	5.198	3.908	1.502	2.406
60	6.041	4.932	1.989	2.943
70	6.785	5.918	2.480	3.438
80	7.483	6.870	2.970	3.900
90	8.162	7.791	3.455	4.336
100	8.823	8.685	3.933	4.752
110	9.495	9.558	4.406	5.152
120	10.177	10.412	4.869	5.543
130	10.877	11.254	5.328	5.926
140	11.591	12.087	5.782	6.305
150	12.308	12.911	6.229	6.682
160	13.072	13.729	6.672	7.057
170	13.843	14.545	7.112	7.433
180	14.629	15.358	7.547	7.811
190	15.428	16.171	7.980	8.191
200	16.240	16.983	8.410	8.573
210	17.071	17.795	8.837	8.958
220	17.906	18.608	9.263	9.345
230	18.751	19.423	9.687	9.736
240	19.602	20.239	10.110	10.129
250	20.474	21.056	10.531	10.526
260	21.341	21.877	10.952	10.925
270	22.207	22.699	11.372	11.327
280	23.086	23.522	11.791	11.731
290	23.959	24.348	12.210	12.138
298.15	24.664	25.021	12.551	12.470
300	24.824	25.174	12.628	12.546
310	25.690	26.002	13.046	12.956
320	26.580	26.832	13.464	13.368
330	27.483	27.664	13.882	13.782
340	28.363	28.497	14.299	14.198
350	29.256	29.332	14.717	14.615
360	30.160	30.169	15.134	15.035
370	31.101	31.008	15.552	15.456
380	32.047	31.850	15.970	15.880
383.242	32.347	32.123	16.105	16.018
Acridine (l)				
383.242	36.966	38.614	16.105	22.509
390	37.403	39.265	16.502	22.763
400	37.992	40.219	17.082	23.137
410	38.578	41.164	17.658	23.506
420	39.157	42.101	18.229	23.872
430	39.714	43.029	18.795	24.234
440	40.274	43.948	19.356	24.592
450	40.847	44.860	19.913	24.947
460	41.422	45.764	20.465	25.299
470	41.995	46.661	21.013	25.648
480	42.568	47.551	21.556	25.995
490	43.142	48.434	22.095	26.339
500	43.715	49.312	22.632	26.680
Phenanthridine (crII)				
0	0.000	0.000	0.000	0.000
10	0.358	0.124	0.031	0.093
15	0.947	0.376	0.101	0.275
20	1.650	0.742	0.212	0.530
25	2.363	1.187	0.361	0.825
30	3.042	1.679	0.541	1.139
35	3.667	2.195	0.740	1.456

TABLE 12. Thermodynamic properties for the condensed phases at vapor saturation^a — Continued

$\frac{T}{K}$	$\frac{C_{sat}}{R}$	$\frac{\Delta_f^0 S}{R}$	$-\frac{\Delta_f^0 G}{RT}$	$\frac{\Delta_f^0 H}{RT}$
Phenanthridine (crII) — Continued				
40	4.237	2.722	0.954	1.769
45	4.760	3.253	1.180	2.073
50	5.230	3.779	1.414	2.365
60	6.090	4.809	1.894	2.915
70	6.835	5.804	2.382	3.422
80	7.541	6.764	2.871	3.893
90	8.193	7.690	3.355	4.335
100	8.841	8.587	3.834	4.753
110	9.506	9.461	4.306	5.155
120	10.167	10.316	4.771	5.545
130	10.846	11.156	5.229	5.927
140	11.532	11.985	5.682	6.303
150	12.240	12.805	6.130	6.675
160	12.976	13.618	6.572	7.046
170	13.721	14.427	7.011	7.416
180	14.483	15.233	7.446	7.787
190	15.261	16.037	7.877	8.160
200	16.048	16.839	8.304	8.535
210	16.858	17.642	8.730	8.912
220	17.682	18.445	9.153	9.292
230	18.501	19.249	9.575	9.674
240	19.332	20.054	9.995	10.059
250	20.188	20.860	10.413	10.448
260	21.027	21.668	10.831	10.838
270	21.876	22.479	11.248	11.231
280	22.724	23.289	11.662	11.627
290	23.586	24.102	12.078	12.024
298.15	24.280	24.765	12.415	12.350
300	24.434	24.916	12.492	12.424
310	25.272	25.731	12.906	12.825
320	26.134	26.547	13.320	13.227
330	26.983	27.364	13.733	13.631
340	27.827	28.182	14.146	14.036
350	28.669	29.001	14.559	14.442
354.00	29.007	29.328	14.723	14.605
Phenanthridine (crI)				
354.00	29.330	29.335	14.723	14.612
360	30.004	29.554	14.971	14.863
370	31.109	30.671	15.384	15.287
379.740	32.185	31.493	15.786	15.707
Phenanthridine (l)				
379.740	36.656	38.724	15.786	22.938
380	36.670	38.750	15.803	22.947
390	37.247	39.710	16.404	23.306
400	37.816	40.660	16.998	23.662
410	38.362	41.600	17.586	24.014
420	38.936	42.532	18.170	24.362
430	39.496	43.454	18.746	24.708
440	40.052	44.369	19.319	25.050
450	40.609	45.275	19.885	25.390
460	41.167	46.174	20.447	25.727
470	41.724	47.065	21.004	26.061
480	42.281	47.949	21.556	26.393
490	42.839	48.827	22.104	26.723
500	43.396	49.698	22.647	27.051

TABLE 12. Thermodynamic properties for the condensed phases at vapor saturation^a — Continued

$\frac{T}{K}$	$\frac{C_{sat}}{R}$	$\frac{\Delta_f^0 S}{R}$	$-\frac{\Delta_f^0 G}{RT}$	$\frac{\Delta_f^0 H}{RT}$
9-Methylcarbazole (cr)				
0	0.000	0.000	0.000	0.000
10	0.526	0.183	0.046	0.136
15	1.353	0.552	0.148	0.403
20	2.205	1.056	0.309	0.747
25	3.017	1.636	0.516	1.121
30	3.756	2.254	0.754	1.500
35	4.413	2.883	1.013	1.870
40	5.021	3.512	1.285	2.227
45	5.579	4.136	1.568	2.568
50	6.105	4.751	1.855	2.896
60	7.065	5.951	2.438	3.513
70	7.923	7.105	3.024	4.081
80	8.703	8.215	3.604	4.611
90	9.440	9.282	4.175	5.107
100	10.182	10.315	4.738	5.577
110	10.900	11.320	5.291	6.029
120	11.599	12.298	5.835	6.464
130	12.298	13.254	6.369	6.886
140	13.008	14.191	6.893	7.298
150	13.727	15.113	7.411	7.702
160	14.463	16.022	7.920	8.102
170	15.220	16.922	8.424	8.498
180	16.002	17.814	8.921	8.893
190	16.798	18.700	9.412	9.288
200	17.608	19.582	9.898	9.684
210	18.432	20.461	10.381	10.080
220	19.268	21.338	10.859	10.479
230	20.116	22.213	11.334	10.879
240	20.980	23.087	11.805	11.282
250	21.859	23.961	12.274	11.688
260	22.746	24.837	12.741	12.096
270	23.639	25.712	13.205	12.507
280	24.536	26.588	13.667	12.921
290	25.453	27.464	14.127	13.337
298.15	26.200	28.180	14.502	13.678
300	26.369	28.343	14.587	13.756
310	27.280	29.922	15.744	14.178
320	28.213	30.103	15.501	14.602
330	29.167	30.986	15.958	15.028
340	30.120	31.871	16.413	15.458
350	31.083	32.758	16.867	15.891
360	32.005	33.646	17.320	16.326
362.490	32.252	33.868	17.434	16.434
9-Methylcarbazole (l)				
362.490	37.197	39.560	17.434	22.126
370	37.583	40.326	17.890	22.436
380	38.123	41.335	18.494	22.841
390	38.670	42.332	19.092	23.240
400	39.039	43.317	19.686	23.631

^aThe percentage imprecision in the listed properties is 2 for 10 to 50 K and 0.2 above 50 K.

TABLE 13. Thermodynamic properties for the ideal gas at 0.1 MPa

$\frac{T}{K}$	$-\frac{\Delta_f G^\circ}{RT}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f S^\circ}{R}$	$\frac{C_p^\circ}{R}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f G^\circ}{RT}$
1-Butanamine						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	22.54	4.41	26.95	5.51	-161.212	-128.287
100	26.01	5.80	31.81	8.63	-88.943	-44.053
150	28.61	7.04	35.65	10.26	-63.031	-13.573
200	30.77	8.00	38.77	11.48	-49.942	2.587
273.15	33.44	9.20	42.64	13.56	-39.487	16.447
298.15	34.27	9.60	43.87	14.37	-37.072	19.787
300	34.32	9.63	43.95	14.43	-36.908	20.026
400	37.32	11.25	48.57	17.82	-30.128	29.624
500	40.00	12.89	52.89	20.97	-25.709	35.850
600	42.49	14.47	56.96	23.70	-22.490	40.240
700	44.84	15.96	60.80	26.05	-19.976	43.504
800	47.06	17.35	64.41	28.08	-17.924	46.086
900	49.18	18.64	67.82	29.85	-16.201	48.044
1000	51.21	19.84	71.05	31.39	-14.720	49.670
1100	53.16	20.95	74.11	32.74	-13.435	51.005
1200	55.01	21.99	77.00	33.91	-12.298	52.142
1300	56.82	22.94	79.76	34.94	-11.304	53.076
1400	58.55	23.83	82.38	35.84	-10.416	53.879
1500	60.22	24.66	84.88	36.62	-9.619	54.572
2-Butanamine						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	23.72	4.21	27.93	4.69	-186.715	-154.770
100	26.84	4.92	31.76	6.69	-102.474	-57.532
150	29.01	5.86	34.87	8.76	-72.645	-22.408
200	30.83	6.82	37.65	10.64	-57.447	-3.799
273.15	33.16	8.22	41.38	13.49	-45.098	12.096
298.15	33.90	8.70	42.60	14.49	-42.216	15.914
300	33.95	8.74	42.69	14.57	-42.015	16.178
400	36.73	10.69	47.42	18.44	-33.851	27.051
500	39.33	12.58	51.91	21.77	-28.549	33.989
600	41.78	14.35	56.13	24.52	-24.718	38.841
700	44.12	15.97	60.09	26.80	-21.773	42.417
800	46.34	17.45	63.79	28.75	-19.406	45.225
900	48.48	18.80	67.28	30.43	-17.447	47.339
1000	50.53	20.04	70.57	31.90	-15.785	49.085
1100	52.49	21.18	73.67	33.18	-14.356	50.525
1200	54.37	22.23	76.60	34.30	-13.112	51.728
1300	56.20	23.19	79.39	35.28	-12.027	52.723
1400	57.94	24.09	82.03	36.13	-11.060	53.586
1500	59.63	24.92	84.55	36.88	-10.203	54.318
2-Methyl-1-propanamine						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	23.19	4.26	27.45	4.83	-173.522	-141.097
100	26.36	5.05	31.41	6.93	-95.773	-50.483
150	28.60	6.03	34.63	9.01	-68.094	-17.617
200	30.47	7.01	37.48	10.87	-53.972	-0.153
273.15	32.86	8.41	41.27	13.58	-42.503	14.801
298.15	33.61	8.88	42.49	14.52	-39.832	18.408
300	33.67	8.91	42.58	14.59	-39.655	18.649
400	36.49	10.80	47.29	18.23	-32.098	28.934
500	39.10	12.61	51.71	21.42	-27.205	35.534
600	41.55	14.31	55.86	24.11	-23.663	40.166
700	43.87	15.88	59.75	26.40	-20.925	43.605
800	46.09	17.32	63.41	28.37	-18.714	46.296
900	48.21	18.64	66.85	30.09	-16.877	48.339
1000	50.24	19.86	70.10	31.59	-15.308	50.032
1100	52.19	20.99	73.18	32.90	-13.948	51.423

TABLE 13. Thermodynamic properties for the ideal gas at 0.1 MPa — Continued

T K	$-\frac{\Delta_f G^\circ}{RT}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f S^\circ}{R}$	$\frac{C_p^\circ}{R}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f G^\circ}{RT}$
2-Methyl-1-propanamine — Continued						
1200	54.06	22.03	76.09	34.05	-12.764	52.586
1300	55.86	23.00	78.86	35.06	-11.712	53.568
1400	57.60	23.89	81.49	35.93	-10.791	54.395
1500	59.27	24.72	83.99	36.70	-9.965	55.116
2-Methyl-2-propanamine						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	21.08	4.07	25.15	4.29	-225.361	-190.636
100	24.04	4.62	28.66	6.28	-122.027	-73.987
150	26.08	5.57	31.65	8.61	-85.770	-32.313
200	27.83	6.59	34.42	10.69	-67.304	-10.426
273.15	30.10	8.07	38.17	13.53	-52.297	8.107
298.15	30.83	8.57	39.40	14.49	-48.803	12.526
300	30.88	8.61	39.49	14.56	-48.563	12.831
400	33.63	10.56	44.19	18.25	-38.794	25.337
500	36.18	12.44	48.62	21.52	-32.540	33.289
600	38.61	14.19	52.80	24.29	-28.087	38.802
700	40.92	15.80	56.72	26.62	-24.694	42.866
800	43.13	17.28	60.41	28.62	-21.982	46.028
900	45.24	18.64	63.88	30.34	-19.746	48.439
1000	47.27	19.89	67.16	31.84	-17.860	50.419
1100	49.23	21.03	70.26	33.14	-16.256	52.035
1200	51.10	22.09	73.19	34.28	-14.856	53.394
1300	52.91	23.07	75.97	35.26	-13.628	54.542
1400	54.65	23.97	78.62	36.13	-12.555	55.501
1500	56.33	24.81	81.14	36.88	-11.596	56.335
Pyrrole						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	19.78	4.00	23.78	4.00	294.288	302.371
100	22.56	4.01	26.57	4.09	143.119	156.905
150	24.19	4.11	28.30	4.61	93.179	109.695
200	25.40	4.36	29.76	5.68	68.204	86.656
273.15	26.85	4.99	31.84	7.82	48.147	68.676
298.15	27.30	5.26	32.56	8.61	43.640	64.657
300	27.33	5.28	32.61	8.67	43.333	64.390
400	29.02	6.51	35.53	11.67	31.197	53.757
500	30.61	7.80	38.41	14.16	24.162	47.616
600	32.14	9.03	41.17	16.13	19.632	43.640
700	33.62	10.16	43.78	17.70	16.506	40.860
800	35.04	11.19	46.23	18.98	14.244	38.839
900	36.42	12.11	48.53	20.05	12.531	37.234
1000	37.74	12.95	50.69	20.95	11.210	35.986
1100	39.01	13.72	52.73	21.72	10.168	34.969
1200	40.24	14.41	54.65	22.39	9.312	34.116
1300	41.41	15.05	56.46	22.96	8.616	33.410
1400	42.55	15.63	58.18	23.46	8.023	32.787
1500	43.64	16.17	59.81	23.90	7.526	32.256
1-Methylpyrrole						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	21.45	4.34	25.79	4.59	293.809	309.250
100	24.54	4.63	29.17	5.26	141.302	164.717
150	26.48	4.98	31.46	6.15	91.248	118.264
200	27.97	5.43	33.40	7.48	66.239	95.784
273.15	29.79	6.30	36.09	10.00	46.166	78.425
298.15	30.36	6.65	37.01	10.93	41.606	74.582
300	30.40	6.68	37.08	11.00	41.304	74.327
400	32.53	8.22	40.75	14.65	29.153	64.285
500	34.54	9.83	44.37	17.80	22.167	58.592
600	36.47	11.38	47.85	20.38	17.725	54.971
700	38.33	12.82	51.15	22.50	14.707	52.483

TABLE 13. Thermodynamic properties for the ideal gas at 0.1 MPa — Continued

$\frac{T}{K}$	$-\frac{\Delta_f G^\circ}{RT}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f S^\circ}{R}$	$\frac{C_p^\circ}{R}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f G^\circ}{RT}$
1-Methylpyrrole — Continued						
800	40.13	14.15	54.28	24.25	12.570	50.698
900	41.87	15.35	57.22	25.74	10.982	49.279
1000	43.54	16.46	60.00	27.00	9.793	48.192
1100	45.16	17.46	62.62	28.07	8.857	47.301
1200	46.72	18.39	65.11	28.99	8.128	46.563
1300	48.23	19.23	67.46	29.79	7.528	45.934
1400	49.68	20.01	69.69	30.47	7.038	45.394
1500	51.09	20.73	71.82	31.07	6.631	44.916
2-Methylpyrrole						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	21.95	4.51	26.46	4.54	223.287	238.058
100	25.14	4.64	29.75	5.13	105.967	128.802
150	27.05	4.97	32.02	6.21	67.674	94.131
200	28.54	5.46	34.00	7.66	48.597	77.541
273.15	30.38	6.38	36.76	10.23	33.307	64.896
298.15	30.94	6.75	37.69	11.16	29.851	62.147
300	30.99	6.77	37.76	11.23	29.612	61.955
400	33.15	8.34	41.49	14.83	20.437	54.829
500	35.19	9.96	45.15	17.93	15.228	50.872
600	37.14	11.51	48.65	20.47	11.964	48.410
700	39.03	12.94	51.97	22.55	9.778	46.734
800	40.84	14.25	55.09	24.27	8.252	45.570
900	42.59	15.45	58.04	25.73	7.155	44.632
1000	44.27	16.54	60.81	26.96	6.339	43.928
1100	45.89	17.54	63.43	28.02	5.724	43.358
1200	47.46	18.45	65.91	28.93	5.242	42.877
1300	48.97	19.29	68.26	29.72	4.869	42.475
1400	50.43	20.06	70.49	30.41	4.563	42.119
1500	51.84	20.77	72.61	31.00	4.314	41.810
3-Methylpyrrole						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	21.97	4.50	26.47	4.53	214.196	228.957
100	25.12	4.64	29.76	5.13	101.426	124.251
150	27.06	4.97	32.03	6.21	64.647	91.094
200	28.56	5.45	34.01	7.66	46.316	75.251
273.15	30.38	6.38	36.76	10.22	31.644	63.233
298.15	30.96	6.74	37.70	11.14	28.319	60.604
300	30.99	6.77	37.76	11.21	28.098	60.441
400	33.15	8.34	41.49	14.81	19.302	53.694
500	35.19	9.95	45.14	17.91	14.310	49.964
600	37.14	11.49	48.64	20.45	11.187	47.643
700	39.02	12.93	51.95	22.53	9.119	46.095
800	40.84	14.24	55.08	24.26	7.674	45.002
900	42.58	15.44	58.02	25.72	6.641	44.137
1000	44.27	16.53	60.80	26.96	5.875	43.474
1100	45.89	17.53	63.42	28.02	5.301	42.945
1200	47.45	18.44	65.89	28.93	4.854	42.509
1300	48.96	19.28	68.24	29.72	4.510	42.136
1400	50.42	20.05	70.47	30.41	4.229	41.805
1500	51.83	20.76	72.59	31.00	4.002	41.517
Pyridine						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	20.67	4.00	24.67	4.00	372.081	379.305
100	23.44	4.05	27.49	4.27	181.994	194.974
150	25.11	4.24	29.35	5.04	119.102	134.798
200	26.38	4.58	30.96	6.24	87.645	105.268
273.15	27.91	5.32	33.23	8.51	62.387	82.091
298.15	28.39	5.62	34.01	9.35	56.625	76.883
300	28.43	5.64	34.07	9.41	56.235	76.529

TABLE 13. Thermodynamic properties for the ideal gas at 0.1 MPa — Continued

$\frac{T}{K}$	$-\frac{\Delta_f G^\circ}{RT}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f S^\circ}{R}$	$\frac{C_p^\circ}{R}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f G^\circ}{RT}$
Pyridine — Continued						
400	30.23	7.00	37.23	12.71	40.785	62.693
500	31.94	8.44	40.38	15.53	31.761	54.648
600	33.60	9.82	43.42	17.82	25.906	49.412
700	35.21	11.10	46.31	19.65	21.841	45.742
800	36.78	12.26	49.04	21.15	18.871	43.041
900	38.28	13.32	51.60	22.39	16.631	40.937
1000	39.74	14.28	54.02	23.43	14.885	39.273
1100	41.14	15.15	56.29	24.31	13.910	37.925
1200	42.49	15.95	58.44	25.05	12.361	36.804
1300	43.80	16.67	60.47	25.69	11.417	35.851
1400	45.06	17.34	62.40	26.25	10.628	35.030
1500	46.27	17.95	64.22	26.72	9.950	34.326
2-Methylpyridine						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	22.69	4.33	27.02	4.81	283.632	297.874
100	25.81	4.73	30.54	5.52	135.858	158.018
150	27.81	5.17	32.98	6.69	87.911	113.638
200	29.37	5.74	35.11	8.24	63.781	91.986
273.15	31.31	6.77	38.08	11.00	44.405	75.280
298.15	31.91	7.17	39.08	12.01	40.001	71.597
300	31.96	7.20	39.16	12.08	39.705	71.345
400	34.27	8.92	43.19	16.05	27.957	61.697
500	36.45	10.70	47.15	19.50	21.200	56.248
600	38.55	12.41	50.96	22.33	16.908	52.792
700	40.58	14.00	54.58	24.65	14.000	50.422
800	42.56	15.45	58.01	26.57	11.930	48.712
900	44.45	16.78	61.23	28.17	10.416	47.375
1000	46.28	17.99	64.27	29.52	9.271	46.342
1100	48.05	19.09	67.14	30.68	8.381	45.499
1200	49.75	20.10	69.85	31.66	7.682	44.806
1300	51.40	21.02	72.42	32.50	7.116	44.212
1400	52.99	21.87	74.86	33.23	6.652	43.696
1500	54.52	22.65	77.17	33.85	6.263	43.254
3-Methylpyridine						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	22.69	4.52	27.21	4.60	301.141	315.193
100	25.88	4.73	30.61	5.40	144.917	167.007
150	27.87	5.16	33.03	6.67	93.674	119.351
200	29.43	5.73	35.16	8.26	68.101	96.256
273.15	31.36	6.77	38.13	11.02	47.575	78.400
298.15	31.97	7.17	39.14	12.03	42.905	74.441
300	32.01	7.20	39.21	12.10	42.592	74.181
400	34.32	8.92	43.24	16.05	30.122	63.811
500	36.51	10.70	47.21	19.49	22.932	57.920
600	38.61	12.41	51.02	22.32	18.351	54.176
700	40.64	14.00	54.64	24.64	15.237	51.599
800	42.61	15.45	58.06	26.56	13.012	49.745
900	44.50	16.78	61.28	28.16	11.378	48.287
1000	46.33	17.99	64.32	29.52	10.137	47.158
1100	48.10	19.09	67.19	30.67	9.169	46.236
1200	49.81	20.09	69.90	31.65	8.394	45.467
1300	51.45	21.02	72.47	32.50	7.782	44.828
1400	53.05	21.86	74.91	33.22	7.260	44.254
1500	54.58	22.64	77.22	33.85	6.831	43.772
4-Methylpyridine						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	21.99	4.52	26.51	4.61	294.947	309.698
100	25.18	4.74	29.92	5.41	141.830	164.609
150	27.17	5.16	32.33	6.66	91.609	117.986

TABLE 13. Thermodynamic properties for the ideal gas at 0.1 MPa — Continued

$\frac{T}{K}$	$\frac{-\Delta_f G^\circ}{RT}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f S^\circ}{R}$	$\frac{C_p^\circ}{R}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f G^\circ}{RT}$
4-Methylpyridine — Continued						
200	28.74	5.72	34.46	8.24	66.542	95.397
273.15	30.67	6.76	37.43	11.01	46.431	77.956
298.15	31.27	7.16	38.43	12.02	41.857	74.102
300	31.32	7.19	38.51	12.09	41.549	73.839
400	33.62	8.92	42.54	16.05	29.347	63.737
500	35.80	10.70	46.50	19.49	22.313	58.010
600	37.90	12.41	50.31	22.32	17.835	54.370
700	39.94	13.99	53.93	24.64	14.784	51.856
800	41.90	15.45	57.35	26.56	12.625	50.068
900	43.80	16.77	60.57	28.16	11.024	48.643
1000	45.63	17.98	63.61	29.52	9.817	47.548
1100	47.40	19.08	66.48	30.67	8.877	46.654
1200	49.10	20.09	69.19	31.66	8.136	45.919
1300	50.74	21.02	71.76	32.50	7.544	45.300
1400	52.34	21.86	74.20	33.23	7.039	44.743
1500	53.87	22.64	76.51	33.85	6.624	44.275
Pyrrolidine						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	21.23	4.54	25.77	5.22	52.626	77.393
100	24.56	5.07	29.63	5.85	19.147	54.102
150	26.67	5.38	32.05	6.18	8.935	48.562
200	28.26	5.66	33.92	6.94	3.748	46.764
273.15	30.10	6.26	36.36	9.00	-0.498	46.301
298.15	30.67	6.52	37.19	9.88	-1.448	46.374
300	30.70	6.55	37.25	9.94	-1.501	46.394
400	32.76	7.86	40.63	13.71	-3.779	47.168
500	34.68	9.39	44.07	17.21	-4.714	48.135
600	36.53	10.95	47.48	20.18	-5.011	49.028
700	38.33	12.45	50.78	22.67	-4.982	49.803
800	40.09	13.86	53.95	24.76	-4.779	50.493
900	41.79	15.18	56.97	26.54	-4.477	51.008
1000	43.46	16.39	59.85	28.05	-4.143	51.455
1100	45.07	17.51	62.58	29.35	-3.792	51.839
1200	46.65	18.54	65.19	30.46	-3.445	52.143
1300	48.16	19.50	67.66	31.42	-3.099	52.418
1400	49.64	20.38	70.02	32.25	-2.782	52.630
1500	51.07	21.20	72.27	32.97	-2.476	52.814
Piperidine						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	21.82	4.02	25.84	4.11	-37.615	-3.550
100	24.68	4.34	29.02	5.36	-28.471	19.323
150	26.55	4.94	31.49	6.92	-23.940	29.907
200	28.07	5.64	33.71	8.60	-21.532	36.427
273.15	29.99	6.83	36.82	11.67	-19.532	42.827
298.15	30.61	7.28	37.89	12.85	-19.020	44.510
300	30.65	7.32	37.97	12.94	-18.978	44.632
400	33.03	9.34	42.37	17.83	-17.166	49.834
500	35.34	11.49	46.83	22.25	-15.530	53.491
600	37.63	13.60	51.23	25.94	-14.027	56.180
700	39.87	15.59	55.46	28.98	-12.651	58.245
800	42.08	17.42	59.50	31.51	-11.410	59.895
900	44.23	19.11	63.34	33.65	-10.275	61.123
1000	46.32	20.66	66.98	35.46	-9.245	62.157
1100	48.37	22.07	70.44	37.00	-8.323	62.981
1200	50.34	23.37	73.71	38.32	-7.484	63.675
1300	52.26	24.57	76.83	39.46	-6.716	64.243
1400	54.12	25.67	79.79	40.45	-6.032	64.712
1500	55.93	26.68	82.61	41.30	-5.415	65.101

TABLE 13. Thermodynamic properties for the ideal gas at 0.1 MPa — Continued

T K	$-\frac{\Delta_f G^\circ}{RT}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f S^\circ}{R}$	$\frac{C_p^\circ}{R}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f G^\circ}{RT}$
Indole						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	23.28	4.02	27.30	4.14	422.570	436.593
100	26.14	4.33	30.47	5.27	205.359	227.817
150	28.00	4.93	32.93	7.07	133.811	160.048
200	29.53	5.74	35.27	9.38	98.139	126.925
273.15	31.53	7.23	38.76	13.24	69.613	101.018
298.15	32.18	7.79	39.97	14.58	63.132	95.218
300	32.24	7.83	40.07	14.68	62.694	94.818
400	34.80	10.19	44.99	19.71	45.381	79.417
500	37.34	12.52	49.86	23.86	35.308	70.448
600	39.81	14.70	54.51	27.16	28.803	64.633
700	42.23	16.67	58.90	29.79	24.293	60.548
800	44.57	18.45	63.02	31.92	21.023	57.564
900	46.84	20.05	66.89	33.68	18.558	55.202
1000	49.02	21.49	70.51	35.15	16.645	53.359
1100	51.13	22.79	73.92	36.39	15.124	51.847
1200	53.17	23.97	77.14	37.45	13.890	50.580
1300	55.13	25.04	80.17	38.36	12.869	49.515
1400	57.02	26.02	83.04	39.15	12.008	48.588
1500	58.85	26.92	85.77	39.82	11.278	47.779
Quinoline						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	23.77	4.07	27.84	4.34	528.094	541.608
100	26.71	4.52	31.23	5.67	258.225	280.038
150	28.67	5.20	33.87	7.57	169.101	194.628
200	30.28	6.09	36.37	10.01	124.630	152.687
273.15	32.41	7.68	40.09	14.10	88.999	119.680
298.15	33.10	8.28	41.38	15.53	80.889	112.256
300	33.16	8.32	41.48	15.64	80.339	111.749
400	35.89	10.84	46.73	21.03	58.590	91.934
500	38.58	13.35	51.93	25.53	45.863	80.338
600	41.22	15.69	56.91	29.11	37.583	72.761
700	43.80	17.82	61.62	31.98	31.816	67.426
800	46.31	19.74	66.05	34.30	27.600	63.496
900	48.74	21.46	70.20	36.21	24.396	60.403
1000	51.08	23.02	74.10	37.79	21.905	57.971
1100	53.34	24.42	77.77	39.12	19.905	55.971
1200	55.52	25.70	81.22	40.25	18.282	54.322
1300	57.62	26.86	84.48	41.21	16.935	52.921
1400	59.66	27.91	87.57	42.04	15.782	51.690
1500	61.61	28.88	90.49	42.74	14.806	50.642
Isoquinoline						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	23.78	4.07	27.85	4.35	537.873	551.377
100	26.72	4.53	31.25	5.71	263.124	284.917
150	28.68	5.23	33.91	7.63	172.391	197.877
200	30.30	6.12	36.42	10.03	127.105	155.112
273.15	32.44	7.70	40.14	14.07	90.809	121.440
298.15	33.14	8.29	41.43	15.49	82.539	113.856
300	33.19	8.34	41.53	15.59	81.989	113.349
400	35.93	10.84	46.77	20.96	59.812	93.116
500	38.62	13.33	51.95	25.46	46.821	81.276
600	41.26	15.66	56.92	29.06	38.368	73.536
700	43.83	17.79	61.62	31.93	32.484	68.095
800	46.33	19.71	66.04	34.25	28.181	64.087
900	48.76	21.43	70.19	36.16	24.909	60.926
1000	51.09	22.99	74.08	37.75	22.364	58.450
1100	53.36	24.39	77.75	39.09	20.319	56.405
1200	55.54	25.66	81.20	40.22	18.650	54.709

TABLE 13. Thermodynamic properties for the ideal gas at 0.1 MPa — Continued

$\frac{T}{K}$	$-\frac{\Delta_f G^\circ}{RT}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f S^\circ}{R}$	$\frac{C_p^\circ}{R}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f G^\circ}{RT}$
Isoquinoline — Continued						
1300	57.64	26.82	84.46	41.18	17.271	53.277
1400	59.66	27.88	87.54	42.01	16.101	52.039
1500	61.62	28.84	90.46	42.72	15.092	50.958
Carbazole						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	24.41	4.26	28.67	4.97	537.046	559.160
100	27.63	5.19	32.83	7.39	261.126	293.797
150	29.96	6.40	36.36	10.35	170.418	207.575
200	31.99	7.81	39.80	13.81	125.257	165.358
273.15	34.77	10.16	44.92	19.37	89.162	132.244
298.15	35.69	11.01	46.70	21.27	80.962	124.797
300	35.76	11.07	46.83	21.41	80.407	124.297
400	39.42	14.56	53.99	28.48	58.502	104.474
500	43.04	17.95	60.99	34.26	45.757	92.908
600	46.59	21.06	67.66	38.83	37.495	85.338
700	50.05	23.87	73.92	42.44	31.769	80.023
800	53.41	26.38	79.79	45.35	27.595	76.103
900	56.65	28.62	85.27	47.75	24.436	73.001
1000	59.77	30.64	90.41	49.74	21.990	70.561
1100	62.78	32.45	95.23	51.41	20.033	68.558
1200	65.67	34.09	99.77	52.83	18.874	67.311
1300	68.46	35.58	104.04	54.04	17.133	65.471
1400	71.15	36.94	108.09	55.08	16.023	64.229
1500	73.74	38.18	111.92	55.98	15.074	63.155
Acridine						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	24.75	4.29	29.04	5.16	714.829	736.603
100	28.04	5.39	33.43	7.79	350.141	382.327
150	30.46	6.64	37.10	10.56	229.771	266.418
200	32.55	8.02	40.57	13.85	169.678	209.380
273.15	35.38	10.31	45.69	19.35	121.478	164.395
298.15	36.32	11.15	47.47	21.29	110.491	154.246
300	36.39	11.21	47.60	21.43	109.749	153.565
400	40.09	14.70	54.79	28.79	80.236	126.456
500	43.75	18.16	61.91	34.98	62.923	110.556
600	47.35	21.39	68.74	39.92	51.638	100.149
700	50.87	24.33	75.20	43.87	43.764	92.815
800	54.29	26.98	81.27	47.06	38.000	87.412
900	57.61	29.36	86.97	49.67	33.619	83.157
1000	60.82	31.50	92.32	51.83	30.194	79.797
1100	63.91	33.44	97.35	53.65	27.459	77.057
1200	66.89	35.19	102.08	55.18	25.218	74.773
1300	69.78	36.77	106.55	56.48	23.349	72.827
1400	72.56	38.22	110.78	57.60	21.768	71.142
1500	75.24	39.55	114.79	58.55	20.421	69.686
Phenanthridine						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	25.47	4.20	29.67	4.78	633.979	655.123
100	28.61	5.05	33.66	7.18	309.421	341.377
150	30.89	6.28	37.17	10.44	202.491	239.068
200	32.89	7.79	40.68	14.25	149.258	188.850
273.15	35.68	10.31	45.99	20.16	106.695	149.313
298.15	36.63	11.22	47.85	22.15	97.017	140.393
300	36.69	11.29	47.98	22.30	96.369	139.805
400	40.45	14.98	55.43	29.66	70.421	116.001
500	44.18	18.55	62.73	35.72	55.237	102.050
600	47.85	21.83	69.68	40.54	45.348	92.919
700	51.45	24.78	76.23	44.38	38.445	86.466
800	54.94	27.43	82.37	47.48	33.402	81.715

TABLE 13. Thermodynamic properties for the ideal gas at 0.1 MPa — Continued

T K	$\frac{-\Delta G^\circ}{RT}$	$\frac{\Delta H^\circ}{RT}$	$\frac{\Delta S^\circ}{R}$	$\frac{C_p^\circ}{R}$	$\frac{\Delta H^\circ}{RT}$	$\frac{\Delta G^\circ}{RT}$
Phenanthridine — Continued						
900	58.30	29.81	88.11	50.02	29.582	77.980
1000	61.55	31.94	93.49	52.14	26.596	75.029
1100	64.69	33.86	98.55	53.91	24.208	72.606
1200	67.71	35.59	103.30	55.41	22.253	70.588
1300	70.62	37.17	107.79	56.69	20.642	68.880
1400	73.43	38.60	112.03	57.78	19.264	67.387
1500	76.14	39.91	116.05	58.71	18.089	66.094
1-Naphthalenamine						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	22.80	4.35	27.15	4.66	372.248	395.820
100	25.96	4.99	30.95	6.85	178.605	212.927
150	28.19	6.11	34.30	9.93	115.441	154.198
200	30.13	7.47	37.60	13.21	84.149	125.709
273.15	32.78	9.66	42.44	18.06	59.220	103.571
298.15	33.66	10.43	44.09	19.68	53.571	98.636
300	33.72	10.49	44.21	19.80	53.195	98.311
400	37.17	13.58	50.75	25.79	38.163	85.279
500	40.52	16.54	57.06	30.75	29.498	77.774
600	43.78	19.25	63.03	34.72	23.943	72.920
700	46.94	21.69	68.63	37.88	20.134	69.526
800	49.98	23.88	73.86	40.44	17.399	67.068
900	52.91	25.84	78.75	42.55	15.359	65.099
1000	55.72	27.60	83.32	44.30	13.794	63.572
1100	58.43	29.19	87.62	45.78	12.565	62.314
1200	61.02	30.63	91.65	47.03	11.577	61.277
1300	63.53	31.93	95.46	48.10	10.764	60.382
1400	65.94	33.12	99.06	49.02	10.080	59.600
1500	68.26	34.21	102.47	49.81	9.504	58.925
2-Naphthalenamine						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	22.80	4.36	27.16	4.67	375.151	398.713
100	25.99	5.01	31.00	6.93	180.071	214.343
150	28.23	6.16	34.39	10.05	116.456	155.123
200	30.19	7.54	37.73	13.37	84.942	126.372
273.15	32.86	9.76	42.62	18.28	59.850	104.021
298.15	33.75	10.55	44.30	19.92	54.176	99.031
300	33.81	10.61	44.42	20.04	53.797	98.703
400	37.30	13.74	51.04	26.08	38.685	85.510
500	40.69	16.72	57.41	31.04	29.967	77.893
600	43.98	19.45	63.43	34.98	24.384	72.961
700	47.17	21.90	69.07	38.11	20.550	69.502
800	50.24	24.09	74.33	40.65	17.790	66.989
900	53.19	26.05	79.24	42.73	15.730	64.980
1000	56.02	27.81	83.83	44.47	14.148	63.416
1100	58.75	29.39	88.14	45.93	12.896	62.125
1200	61.38	30.82	92.20	47.17	11.888	61.038
1300	63.89	32.12	96.01	48.23	11.065	60.133
1400	66.31	33.31	99.62	49.13	10.374	59.334
1500	68.65	34.39	103.04	49.91	9.781	58.631
9-Methylcarbazole						
0	0.00	0.00	0.00	0.00	infinite	infinite
50	25.46	4.34	29.86	5.36	547.423	577.714
100	28.86	5.71	34.58	8.84	264.767	307.918
150	31.49	7.34	38.83	12.40	172.262	220.610
200	33.83	9.07	42.90	16.15	126.261	177.995
273.15	37.05	11.74	48.79	21.97	89.445	144.678
298.15	38.12	12.69	50.80	23.98	81.083	137.226
300	38.20	12.75	50.95	24.13	80.511	136.716
400	42.39	16.56	58.95	31.68	58.338	117.142

TABLE 13. Thermodynamic properties for the ideal gas at 0.1 MPa — Continued

$\frac{T}{K}$	$-\frac{\Delta_f G^\circ}{RT}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f S^\circ}{R}$	$\frac{C_p^\circ}{R}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f G^\circ}{RT}$
9-Methylcarbazole — Continued						
500	46.49	20.24	66.73	38.03	45.134	105.476
600	50.48	23.65	74.13	43.16	36.754	98.045
700	54.36	26.74	81.11	47.29	30.974	92.830
800	58.12	29.53	87.65	50.67	26.806	89.036
900	61.74	32.04	93.78	53.46	23.685	86.023
1000	65.24	34.30	99.54	55.80	21.279	83.654
1100	68.61	36.35	104.95	57.78	19.387	81.725
1200	71.85	38.20	110.05	59.45	17.853	80.100
1300	74.98	39.90	114.87	60.88	16.613	78.733
1400	77.99	41.44	119.43	62.10	15.555	77.523
1500	80.90	42.85	123.75	63.15	14.659	76.475

3. Data Sources

3.1. Freezing, Normal Boiling and Critical Temperatures with Critical Pressure and Volume

3.1.1. Freezing and Normal Boiling Temperatures

The selected values of the normal boiling temperatures ($p_{\text{sat}} = 101.325$ kPa) were determined from the least squares fits to the Cox equation. If a reliable value for the triple point temperature was available, this was selected rather than the freezing point, because unspecified impurities usually alter freezing points much more than the change that one atmosphere of non-reacting air over the sample would produce in establishing the difference between the freezing point and the triple point. In addition, prolonged exposure of an amine to air produces a significant amount of impurities which cannot be easily characterized. Measured values of the freezing and normal boiling temperature, along with estimated uncertainties are listed in Table 14.

1-Butanamine

Our selected value for the normal boiling temperature agrees with the results of Werner (1919–57), Timmermans and Mattaar (1921–17), Erickson (1926–46), Lycan *et al.* (1931–249), Butler and Ramchandani (1935–366), Brown and Jones (1946–175), Schuerch and Huntress (1949–167), Few and Smith (1949–482), Arnett *et al.* (1950–248), Dilke *et al.* (1950–591), Ross and Finkelstein (1957–212), Holmberg (1962–353), Sudaricov *et al.* (1963–316), Humphrey and van Winkle (1967–204), Christie and Crisp (1967–324), Union Carbide Corp. (1968–195), and Letcher and Bayles (1971–42) within our estimated uncertainties of those measurements. Other measurements of the normal boiling temperature, generally of lower accuracy, are listed in (1870–6), (1871–9), (1872–18), (1874–11), (1919–57), (1926–46), (1947–146), (1951–569), (1952–42), (1957–76), (1959–313), (1962–356), (1967–218), and (1969–2).

The selected value of the freezing temperature was based on the careful measurement carried out at Union

Carbide laboratories (1968–195) on a sample with 100 percent purity. The freezing temperature listed by Timmermans and Mattaar (1921–17), is low due to impurities.

2-Butanamine

Our selected value for the normal boiling temperature agrees with the results of Evans *et al.* (1959–313) within the estimated uncertainties. The other published results of Sabatier and Mailhe (1909–1), Schuerch and Huntress (1949–167) and Holmberg (1962–353) are higher, which is consistent with the presence of involatile impurities in their samples. The selected freezing temperature was based on the results of Timmermans and Mattaar (1921–17).

2-Methyl-1-propanamine

Our selected value for the normal boiling temperature was based on the ebulliometric measurements of Osborn and Scott (1980–1). It also agrees with that of Timmermans and Mattaar (1921–17), Barcelo *et al.* (1951–569) and Costello and Bowden (1959–218) within the limits of their uncertainty. The other published results of Perkin (1889–26), Schuerch and Huntress (1949–167) and Holmberg (1962–353) are higher, which is consistent with the presence of involatile impurities in the samples. The selected value of the freezing temperature was based on the value of Timmermans and Mattaar (1921–17).

2-Methyl-2-propanamine

Our selected value for the normal boiling temperature agrees with the results of Timmermans and Mattaar (1921–17) and Osborn and Douslin (1968–206) within the estimated uncertainties. The presence of impurities probably account for the high values of Timmermans (1921–19), Costello and Bowden (1959–218) and Holmberg (1962–353). The selected value of the freezing temperature comes from the triple point temperature value published by Finke *et al.* (1972–140).

Pyrrole

The selected value of the normal boiling temperature agrees with Scott *et al.* (1967–166), API (1942–300 and 1957–605) and Robles (1939–3) within the estimated uncertainties. Other measurements of the normal boiling temperature, generally of lower accuracy, are listed in (1941–378), (1946–260), (1947–346), (1955–485), (1957–76), (1959–335), (1962–406), and (1969–163). The selected value of the freezing temperature was based upon the triple point temperature measured by Scott *et al.* (1967–116), McCullough and Waddington (1957–539), and by Helm *et al.* (1958–216). The agreement with the freezing temperature listed are commensurate with the purities and accuracies of the measurements.

1-Methylpyrrole

Our selected value for the normal boiling temperature agrees with the results of Osborn and Douslin (1968–206), API (1958–417) and Lecat (1947–346) within the estimated uncertainties. The selected value of the freezing temperature was based upon the triple point temperature measured by Messerly *et al.* (1988–93) which agrees very well with the freezing temperature measured by Guanquan *et al.* (1986–69). The value listed by Milazzo (1941–378), which is 141K higher, is obviously in error. Other measurements of the normal boiling temperature, generally of lower accuracy, are listed in (1941–378), (1962–392), and (1969–163).

2-Methylpyrrole

Our selected value for the normal boiling temperature is based on the normal boiling temperature measured by Lecat (1947–346). Other measurements which agree within their accuracy include (1971–379), (1912–167), (1928–70), and (1952–71). There is a low pressure measurement by (1952–705). The selected freezing point was that given by API (1957–605) and by Lanum and Morris (1969–51). They were identical.

3-Methylpyrrole

The normal boiling point measured by (1958–446), (1971–380), (1963–480), and (1990–502) are in agreement with the recommended value within the estimated uncertainty. The value also agrees with the normal boiling point estimated from the temperature equivalent to a vapor pressure of 98.66 kPa measured by Lancaster and Van der Werf (1958–415) and the low pressure measurements of (1913–194). The freezing point value measured by Lanum and Morris (1969–51) was selected.

Pyridine

Our selected value for the normal boiling temperature agrees with the published results within the estimated uncertainties. Measurements which agree with our value are listed in (1906–115), (1931–349), (1943–220), (1950–591), (1950–599), (1958–216), (1958–388), (1959–360), (1959–361), (1962–411), (1965–341), (1967–319), and (1971–214). Other measurements of the normal boiling temperature with lower accuracy, are listed in (1884–15),

(1889–26), (1899–11), (1908–126), (1908–127), (1909–134), (1910–58), (1911–54), (1912–127), (1913–179), (1917–65), (1921–19), (1921–129), (1923–3), (1923–73), (1926–71), (1927–12), (1929–341), (1931–278), (1934–392), (1935–417), (1937–146), (1941–100), (1946–100), (1947–346), (1948–464), (1950–591), (1952–363), (1954–670), (1955–11), (1956–607), (1957–176), (1958–385), (1958–391), (1959–358), (1960–333), (1961–303), (1961–305), (1961–307), (1961–308), (1962–97), (1962–406), (1963–379), (1963–381), (1964–434), (1965–583), (1966–485), (1967–320), (1967–325), (1968–48), (1968–281), (1970–233), (1970–239), (1971–220), (1972–234), (1972–235), (1973–222), (1974–227), (1974–255), (1975–127), (1976–183), (1986–2), and (1989–79).

The selected value of the freezing temperature was based upon the triple point temperature measured by McCullough *et al.* (1957–176) and by Helm *et al.* (1958–216). This value agrees with most of published results within their estimated uncertainties. Timmermans (1921–19) listed a higher normal boiling point temperature and a lower freezing point which is consistent with the presence of involatile impurities in the sample. Other published values for the freezing point are listed in (1906–115), (1909–134), (1910–58), (1911–54), (1912–127), (1916–38), (1917–65), (1926–210), (1936–163), (1937–146), (1946–296), (1948–464), (1954–24), (1954–31), (1958–391), (1966–222), (1966–485), (1973–225), and (1986–96).

2-Methylpyridine

Our selected value for the normal boiling temperature agrees with Scott *et al.* (1963–156) within the estimated uncertainties. Other measurements which agree with our value within their estimated uncertainties are given in (1942–300), (1948–442), (1951–314), (1955–635), (1958–387), (1959–337), and (1959–358). Measurements of the normal boiling temperature with lower accuracy are listed in (1895–49), (1921–19), (1921–129), (1927–12), (1929–178), (1934–392), (1943–29), (1943–255), (1945–205), (1947–346), (1951–86), (1955–485), (1957–217), (1958–389), (1958–391), (1959–358), (1960–333), (1961–303), (1961–305), (1961–307), (1959–336), (1960–9), (1961–304), (1962–406), (1964–434), (1964–523), (1966–485), (1967–325), (1968–195), and (1968–285).

The selected value of the freezing temperature was based upon the triple point temperature measured by Scott *et al.* (1963–156) and by Helm *et al.* (1958–216). This value agrees with that published by API (1942–300), Freiser and Glowacki (1948–442), Biddiscombe *et al.* (1954–31) and Ait-Kaci and Merlin (1979–131, 1979–132, 1979–133, and 1979–134), within the estimated uncertainties. Other published values for the freezing point with lower accuracy are listed in (1921–19), (1946–296), (1955–485), (1966–485), (1968–195), and (1981–138).

3-Methylpyridine

Our selected value for the normal boiling temperature agrees with Scott *et al.* (1963–156) within the estimated uncertainties. Other measurements which agree with our

value within their estimated uncertainties are listed in (1895–49), (1909–47), (1921–129), (1946–308), (1947–346), (1958–390), (1959–359), (1961–306), (1964–250), (1964–434), (1966–485), and (1968–285). Measurements of the normal boiling temperature with lower accuracy are listed in (1934–392), (1943–255), (1948–465), (1948–467), (1951–184), (1951–314), (1966–257), and (1967–325).

The selected value of the freezing temperature was based upon the triple point temperature measured by Scott *et al.* (1963–156). This value agrees with that published by Hoffman and Vander Werf (1946–296), Coulson and Jones (1946–308), Witschonke (1954–24), Biddiscombe *et al.* (1954–31), Assal (1966–485), and Den Adel *et al.* (1981–138), within the estimated uncertainties. Liplavk and Boliter (1951–184) measured a lower freezing point which is consistent with the presence of involatile impurities in the sample.

4-Methylpyridine

Our selected value for the normal boiling temperature was based on the ebulliometric measurements of Osborn and Douslin (1968–206). It also agrees with that of Flaschner (1909–47), Coulson and Jones (1946–308), Lecat (1947–346), Liplavk and Boliter (1951–184), Kyte *et al.* (1960–119), Bylicki and Jankun-Pinska (1964–250), Assal (1966–485), API (1968–195), and Wilson and Worrall (1968–285) and Cabezos *et al.* (1990–77) within the limits of their uncertainties. Other measurements of the normal boiling temperature with lower accuracy are listed in (1943–256), (1948–465), (1948–467), (1951–86), (1951–314), (1958–390), and (1967–325).

The selected value of the freezing temperature was based upon the triple point temperature measured by Soulard *et al.* (1986–227) and Messerly *et al.* (1988–93). This value agrees with that published in (1946–296), (1951–184), (1954–24), (1954–31), (1966–485), (1966–485), (1968–195), and (1981–138), within the estimated uncertainties. Other published values for the freezing point with lower accuracy are listed in (1946–308), (1948–465), and (1960–119).

Pyrrolidine

Our selected value for the normal boiling temperature agrees with Boord *et al.* (1950–546), API (1956–676), Helm *et al.* (1958–216), McCullough *et al.* (1959–355), Hildenbrand *et al.* (1959–374), and Anderson and Shimanskaya (1969–163). Other measurements of the normal boiling temperature of lower accuracy are those of Yur'ev *et al.* (1946–260) and Lecat (1947–346). The selected value of the freezing temperature was based upon the triple point published by Helm *et al.* (1958–216), by McCullough *et al.* (1959–355) and by Hildenbrand *et al.* (1959–374). The freezing point published by Boord *et al.* (1950–546) was too low.

Piperidine

Our selected value for the normal boiling temperature agrees with those of Osborn and Douslin (1968–206),

Kahlbaum (1884–15), Perkin (1988–26), Louguinine (1899–11), Kurnakow and Zemczun (1913–179), Riley and Bailey (1929–178), Semb and McElvain (1931–371), Rau and Narayanaswamy (1934–392), Timmermans and Hennaut-Roland (1937–146), Magnusson and Schierz (1940–364), Lecat (1947–346), Dilke *et al.* (1950–591), Kalman and Smyth (1960–369), and Vedal *et al.* (1976–211) within their limits of accuracy. Other measurements of the normal boiling temperature of lower accuracy are given by Bedford *et al.* (1963–357), Moelwyn-Hughes and Thorpe (1964–572), and Nakanishi *et al.* (1975–283).

The selected value of the freezing point was based upon the triple point published by Kalman and Smyth (1960–369) and by Messerly *et al.* (1988–93). The freezing point published by Altschul and Von Schneider (1895–61) is very low, while that published by Vedal *et al.* (1976–211) is higher than the selected value. The freezing point listed by Pushin and Sladovic (1928–220) and by Timmermans and Hennaut-Roland (1937–146) agree with our selected value within their limits of accuracy.

Indole

The selected value of the normal boiling temperature at atmospheric pressure was that given by Lecat (1947–346). The selected value of the freezing point was based on those reported by Cowley and Partington (1936–459), and Aihara (1955–710). Other freezing point values with less accuracy were reported by Weerman (1910–141), and by Serpinski *et al.* (1958–398).

Quinoline

Our selected value for the normal boiling temperature agrees with Steele *et al.* (1988–551). Also it agrees with that by Timmermans and Hennaut-Roland (1937–146), Lecat (1943–221 and 1947–346), Malanowski (1961–368), Mavzynski and Maczynska (1965–688), Cooper *et al.* (1967–293), and Sundaram (1969–243) within the limits of accuracy. Other measurements of the normal boiling temperature with lower accuracy are listed in (1884–15), (1911–54), (1922–55), (1923–73), (1935–428), (1943–255), (1951–444), and (1957–76).

The selected value of the freezing point was based upon the triple point published by Steele *et al.* (1988–551). This value agrees with those published by Pushin and Sladovic (1928–20), Park *et al.* (1936–163), Witschonke (1954–24), Mallikarjun and Hill (1965–231), and Lanum and Morris (1969–51) within the limits of their estimated accuracies. Other freezing point values with less accuracy were listed in (1895–61), (1911–54), (1916–38), (1926–28), (1937–146), (1951–444), (1952–50), (1954–674), (1955–11), and (1957–551).

Isoquinoline

Our selected value for the normal boiling temperature agrees with that published by Steele *et al.* (1988–551). Also it agrees with that listed by Malanowski (1961–368). Other normal boiling temperatures were listed in (1922–155), (1934–392), (1943–255), (1947–346), and (1967–293). The selected value of the freezing point was based

upon the triple point published by Steele *et al.* (1988–551). This value agrees with that published by Freiser and Glowacki (1949–545), and by Mallikarjun and Hill (1965–231). Other freezing point values with lower accuracy are listed in (1922–155), (1953–712), (1953–715), and (1957–567).

Carbazole

Our selected value for the normal boiling temperature agrees with that published by Graeber and Glaser (1872–31). Other normal boiling temperatures with low accuracy are listed in (1872–30) and (1891–58). The selected value of the freezing point was based upon the freezing point published by Robinson and Scott (1969–244). This value agrees with that published by Marsh (1987–598) and that by NIST (1988–9). Other freezing point values with less accuracy were listed in (1872–30), (1872–31), (1891–58), (1908–128), (1919–40), (1921–90), (1923–166), (1923–167), (1931–8), (1936–459), (1954–24), and (1955–710).

Acridine

Our selected value for the normal boiling temperature agrees with that published by Steele *et al.* (1988–76). The selected value of the freezing point was based upon the triple point published by Steele *et al.* (1989–76). This value agrees with the freezing point published by Kalman and Smyth (1960–391). Other freezing point values with less accuracy are listed in (1953–698), (1962–472), (1975–228), and (1986–32).

Phenanthridine

In the case of phenanthridine we found no reported normal boiling temperature at atmospheric pressure. Our value was obtained by extrapolating the values published by Steel *et al.* (1989–76) using the Cox equation.

Our selected value of the freezing point was based on the triple point published by Steele *et al.* (1989–76). This value agrees with the freezing point published by Taylor and Kalenda (1954–764) and by Cumper *et al.* (1962–472). A value considerably below the selected value is given in (1952–665).

1-Naphthalenamine

Our selected value for the normal boiling temperature agrees with that published by Stillmann and Swain (1899–63) and by Stull (1947–83). The selected value for the freezing point was based on that listed by Witschonke (1954–24). This value agrees with values listed by Stillmann and Swain (1899–63), Beck and Smith (1906–123), Beck (1907–112), Cowley and Partington (1938–372), and Assal (1966–514). Other freezing point values with less accuracy were listed in (1899–68), (1905–101), (1906–78), (1914–155), (1926–228), (1947–83), (1947–406), (1953–700), and (1979–205).

2-Naphthalenamine

Our selected value for the normal boiling temperature agrees with that published by Stull (1947–83). The

selected value for the freezing point was based on that given by Karyakin *et al.* (1968–3). Other freezing point values are reported in (1938–372), (1940–231), (1947–83), (1947–406), (1953–700), and (1979–205).

9-Methylcarbazole

Our selected value for the normal boiling temperature is based on the vapor pressures published by Steele *et al.* (1992–3). The selected value of the freezing point was based upon the triple point published by Messerly *et al.* (1988–93). The freezing point published by Burton and Gibson (1924–187) agrees within the estimated uncertainty.

3.1.2. Critical Temperature, Pressure and Volume

Both measured and estimated values of the critical temperature, pressure and volume are listed in Table 15.

1-Butanamine

The critical temperature and the critical pressure were determined by Glasser and Rüland (1957–76) and by Toczylkin and Young (1980–25). The critical temperature determined by Glasser and Rüland is much lower than that determined by Toczylkin and Young. The critical molar volume was estimated by Toczylkin and Young (1980–25). The critical temperature and the critical pressure determined by Toczylkin and Young was selected while the critical molar volume calculated from the rectilinear diameter agrees with that estimated by Toczylkin and Young within the combined uncertainties.

2-Butanamine

The critical temperature measured by Toczylkin and Young (1980–25) was selected. These authors believe that their critical pressure was too high so the selected critical pressure was that obtained by extrapolation of the Cox equation to the selected critical temperature. The selected critical molar volume was calculated from the rectilinear diameter. This value agrees within the estimated uncertainty with the value estimated by Toczylkin and Young.

2-Methyl-1-propanamine

The critical constants of 2-methyl-1-propanamine have not been measured. They were estimated by ESDU (1976–328) using Ambrose's method, and by Somayajulu (1989–1). We adopted the critical temperature and the critical pressure estimated using Ambrose's method. The critical molar volume was calculated from the rectilinear diameter.

2-Methyl-2-propanamine

The selected values of the critical temperature and pressure were those measured by Kobe and Mathews (1970–5). The critical molar volume was calculated from the rectilinear diameter.

Pyrrole

Glaser and Rüland (1957-76) measured the critical temperature and pressure of pyrrole. Their critical temperature is very low compared with the value of Cheng *et al.* (1962-239) which was adopted. The critical pressure obtained by extrapolation of the Cox equation to the selected critical temperature has a considerably higher value than that reported in (1957-76). The critical molar volume was calculated from the rectilinear diameter.

1-Methylpyrrole

The critical constants of this compound have not been measured. They were all estimated using Ambrose's method.

2-Methylpyrrole

The critical constants of this compound have not been measured. They were all estimated using Ambrose's method.

3-Methylpyrrole

The critical constants of this compound have not been measured. They were all estimated using Ambrose's method.

Pyridine

The critical temperature was measured by Radice (1899-59), Livingston *et al.* (1908-112), Herz and Neukirch (1923-3), Swietoslawski and Kreglewski (1954-37), Kobe *et al.* (1956-9), Ambrose and Grant (1957-423), and by Brunner (1987-588). Swietoslawski and Kreglewski purified their sample by fractional distillation. Ambrose and Grant used a sample of 99.91 mol per cent purity and their value was selected. Herz and Neukirch (1923-3), Kobe *et al.* (1956-7) and Brunner (1987-588) measured the critical pressure. The only determination of the critical volume was by Kobe *et al.* (1956-9). The selected critical pressure obtained by extrapolation of the Cox equation to the selected critical temperature agrees with (1956-7) and (1987-588) within the estimated uncertainties. The selected critical molar volume calculated from the rectilinear diameter is higher than that reported in (1956-9) but just outside the combined estimated uncertainties.

2-Methylpyridine

Ambrose and Grant (1957-423) measured the critical temperature on a 99.85 mol per cent pure sample and their value was adopted. Kobe and Mathews (1970-5) measured both the critical temperature and pressure. The selected critical pressure obtained by extrapolation of the Cox equation to the selected critical temperature and the selected critical molar volume calculated from the rectilinear diameter agrees with (1970-5) within the combined uncertainties.

3-Methylpyridine

Ambrose and Grant (1957-423) measured the critical

temperature on a 99.71 mol percent pure sample and their value was adopted. The selected critical pressure was obtained by extrapolation of the Cox equation to the selected critical temperature and the selected critical molar volume was calculated from the rectilinear diameter.

4-Methylpyridine

Ambrose and Grant (1957-423) measured the critical temperature of this compound and their value was adopted. They used a sample of 99.97 mol per cent purity. Kobe and Mathews (1970-5) measured both the critical temperature and pressure. The selected critical pressure obtained by extrapolation of the Cox equation to the selected critical temperature and the selected critical molar volume calculated from the rectilinear diameter agree with (1970-5) within the combined uncertainties.

Pyrrolidine

Kobe *et al.* (1956-9) determined all the critical properties of pyrrolidine but they reported that the sample decomposed near the critical temperature. Cheng *et al.* (1962-239) also determined the critical temperature using a 99.85 mol per cent purity sample further purified by distillation *in vacuo*. The precision of their measurement is ± 0.1 K. We selected their critical temperature. The selected critical pressure obtained by extrapolation of the Cox equation to the selected critical temperature and the selected critical molar volume calculated from the rectilinear diameter agrees with (1956-9) within the combined estimated uncertainties.

Piperidine

Cheng *et al.* (1962-239) measured the critical temperature using a commercial sample. Ambrose (1963-213) used a National Chemical Laboratory sample of 99.90 mol per cent purity to determine the critical temperature. On the basis of purity, we selected the value of Ambrose. The critical pressure determined by Guye and Mallet (1902-64) is considerably lower than, but within the combined estimated uncertainties, of the selected critical pressure obtained by extrapolation of the Cox equation to the selected critical temperature. The selected critical molar volume was calculated from the rectilinear diameter.

Indole

The critical constants of indole have not been measured. They were estimated using the Joback group contribution method (1984-560).

Quinoline

The selected critical temperature was measured by Ambrose (1963-213) using a sample of 99.69 mol per cent purity. The selected critical pressure was obtained by extrapolation of the Cox equation to the selected critical temperature and the selected critical molar volume was calculated from the rectilinear diameter. The values of Glasser and Rüland (1957-75) and Livingston *et al.* (1980-112) are considerably higher.

Isoquinoline

The selected critical temperature was measured by Ambrose (1963–213) using a sample of 99.95 mol percent purity. The selected critical pressure was that obtained by extrapolation of the Cox equation to the selected critical temperature and the selected critical molar volume was calculated from the rectilinear diameter.

Carbazole

The critical constants of carbazole have not been measured. The critical temperature and the critical pressure estimated by Sivaraman *et al.* (1983–189) were selected. The selected critical molar volume was estimated using the Joback group contribution method (1984–560).

Acridine

The critical constants of acridine have not been measured. The critical temperature and the critical pressure estimated by Sivaraman *et al.* (1983–189) were selected. The selected critical molar volume was estimated using the Joback group contribution method (1984–560).

Phenanthridine

The critical constants of phenanthridine were not measured. They were estimated using the Joback group contribution method (1984–560).

1-Naphthalenamine

The critical constants of 1-naphthalenamine have not been measured. The critical temperature and critical pressure were estimated using Ambrose's method and the critical molar volume was estimated using the Joback group contribution method (1984–560).

2-Naphthalenamine

The critical constants of 2-naphthalenamine have not been measured. The critical temperature and critical pressure were estimated using Ambrose's method and the critical molar volume was estimated using the Joback group contribution method (1984–560).

9-Methylcarbazole

The critical constants of 9-methylcarbazole estimated by Steele *et al.* (1992–3) were selected.

3.2. Vapor Pressure

The temperature and pressure ranges over which measurements of vapor pressure have been reported are listed in Table 16. Also included are the method of measurement as well as the estimated accuracy in both the temperature and pressure. If the results were determined by an ebulliometric (dynamic) method, these were given greater weight among measurements made on samples with equal purity and with equal accuracies. This preference arises because the ebulliometric methods

expel light gases that may remain in the samples when they are subjected to static measurements. The smoothed vapor pressure values listed in Table 3 were calculated using the Cox equation [Eq. (3a and 3b)]. The coefficients of the equation are listed in Table 2, and the coefficients of the Antoine and the extended Antoine equations [Eq. (4 and 5)] respectively are listed in Table 4 for nine of the compounds involved in this study for which measurements are available.

1-Butanamine

Lieben and Rossi (1871–9), Coply *et al.* (1941–101), and Rogers (1947–146) did not mention the method of measurements or the purity of their samples so these results were excluded from the fit. Krichevskii *et al.* (1962–356), Siedler and Bittrich (1969–2), and Pradhan (1979–77) all used a static method but owing to questions of the degree of outgassing, these results were also excluded. The results of Majer *et al.* (1979–78) obtained using a dynamic method, were given the highest weight. To cover temperatures up to the critical temperature, the results of Glaser and Rüland (1957–76) were used but were given less weight. The critical temperature and pressure selected in this work was also used in the fitting. The isolated points reported in Refs. (1872–20, 1919–64, 1944–125, 1948–262, 1952–385, 1957–13, 1959–218, 1959–313, 1967–324, 1973–229, 1974–134, and 1979–76) were also excluded. Percent deviations of the experimental values from the vapor pressures calculated from the Cox equation are shown in Fig. 1.

2-Butanamine

The measurements of Majer *et al.* (1979–78), Copley *et al.* (1941–101), the boiling temperature at one atmosphere measured by Evans *et al.* (1959–313) and the selected critical temperature and pressure were used in the fitting. The results of Majer *et al.* obtained using a dynamic method were given the highest weight. The isolated points reported in Refs. (1895–49, 1948–262, and 1959–313) were excluded. Percent deviations of the experimental values from the vapor pressures calculated from the Cox equation are plotted in Fig. 2.

2-Methyl-1-propanamine

For 2-methyl-1-propanamine the results of Copley *et al.* (1941–101) were excluded. All other values were used but the values of Osborn and Douslin (1968–206) were given the highest weight while those of Simon and Huter (1935–278) were given the lowest. The selected critical temperature and pressure were also used in the fitting. The isolated points reported in Refs. (1895–49 and 1948–262) were also excluded. Fig. 3 shows the percent deviations from the vapor pressures calculated from the Cox equation.

2-Methyl-2-propanamine

The values of Osborn and Douslin (1968–206) obtained by an ebulliometric method and the selected critical temperature and pressure were used in the fitting.

Valero *et al.*'s (1979–80) results were excluded. Fig. 4 shows the percent deviations from the vapor pressures calculated from the Cox equation.

Pyrrole

The low temperature results of Milazzo (1941–378), the medium temperature results of Scott *et al.* (1967–116) and the results of Glaser and Rüland (1957–76) at the higher temperatures up to the critical temperature were used in the analysis. Measurements by Kobe *et al.* (1956–9) and by Eon *et al.* (1971–47) were excluded. The isolated points reported in Refs. (1927–165, 1952–5, and 1956–9) were also excluded. The results of Scott *et al.* were given the highest weight while Glaser and Rüland's were given the lowest. Fig. 5 shows the percent deviations from the vapor pressures calculated from the Cox equation.

1-Methylpyrrole

The results of Milazzo (1941–378) and Osborn and Douslin (1968–206) together with the critical temperature and pressure selected in this work were used in the analysis. The measurements of Osborn and Douslin were given higher weight than those of Milazzo. Valero *et al.*'s (1979–80) results were excluded. The results of Eon *et al.* (1971–47) and the isolated values reported in Refs. (1952–5 and 1954–771) were excluded. Fig. 6 shows the percent deviations from the vapor pressures calculated from the Cox equation.

2- and 3-Methylpyrrole

No extensive set of vapor pressure measurements appear to have been made on these compounds. No evaluation was made.

Pyridine

Many vapor pressure measurements have been reported for pyridine in the last hundred years. The measurements used in the fitting were those by McCullough *et al.* (1957–176), Chan and Van Hook (1976–182), Herington and Martin (1953–518), and Kanakbaeva *et al.* (1974–227). For the high pressure region up to the critical point, the measurements by Kobe *et al.* (1956–9) using a static method were used. Values which were not used are those by Bruhl (1895–49), Kahlenberg (1901–63), Arndt and Nachtway (1926–210), van der Meulen and Mann (1931–349), Hieber and Woerner (1934–26), Bratton *et al.* (1935–418), Ibl *et al.* (1954–757, 1956–615 and 1978–131), Andon *et al.* (1957–537), Maczynska (1963–382), Findlay and Kenyon (1969–224), Findlay and Copp (1969–226), Nakanishi *et al.* (1976–132), Weclawski and Bylicki (1983–11), and Gardner and Day (1984–49). The isolated results reported in Refs. (1900–81, 1908–125, 1914–136, 1915–45, 1917–66, 1929–205, 1929–341, 1943–29, 1945–205, 1946–296, 1950–594, 1954–736, 1961–292, 1962–408, 1962–409, 1963–381, 1971–183, 1973–226, 1975–129, 1977–46, 1977–161, 1977–162, 1980–142, 1985–72, and 1986–21) were also excluded. Percent deviations of the

experimental values from those calculated from the Cox equation are shown in Fig. 7.

2-Methylpyridine

The vapor pressures of Riley and Bailey (1929–178), Herington and Martin (1953–518) and Scott *et al.* (1963–156) were used in the analysis along with the selected critical temperature and pressures. The measurements of Nakanishi *et al.* (1976–132), Abe *et al.* (1978–131) and the single result of Refs. (1880–2, 1895–49, 1901–64, 1935–418, 1938–82, 1943–29, 1946–296, 1953–690, 1966–482, 1970–5, 1975–129, 1977–46, 1977–162, and 1985–300) were not used in the evaluation. The deviations of the experimental values from those calculated from the Cox equation are shown in Fig. 8.

3-Methylpyridine

The final evaluation was made using the measurements of Herington and Jones (1953–518) at low temperatures and those of Scott *et al.* (1963–157) at intermediate temperatures. The results of Coulson and Jones (1946–308), Othmer and Savitt (1948–467), Lipilvak and Boliter (1951–184), Andon *et al.* (1957–537), Abe *et al.* (1978–131), Semeniuk *et al.* (1988–1133) and the isolated results of Refs. (1946–296, 1955–11, 1960–119, 1966–257, 1975–129, 1977–46, 1977–161, and 1977–162) were excluded. Percent deviations of the experimental vapor pressures from values calculated with the Cox equation are shown in Fig. 9.

4-Methylpyridine

The final evaluation was made using the measurements of Herington and Jones (1953–518) at low temperatures and those of Osborn and Douslin (1968–206) at intermediate temperatures. The results of Coulson and Jones (1946–308), Othmer and Savitt (1948–467), Lipilvak and Boliter (1951–184), Andon *et al.* (1957–537), Abe *et al.* (1978–131), Semeniuk *et al.* (1988–1133) and the isolated results of Refs. (1938–82, 1946–296, 1968–195, 1970–5, 1975–129, and 1977–46) were excluded. Percent deviations of experimental values from those calculated with the Cox equation are shown in Fig. 10.

Pyrrolidine

The final evaluation was made using the measurements of McCullough *et al.* (1959–355) at intermediate temperatures and those of Kobe *et al.* (1956–9) at high temperatures up to the critical temperature. The measurements of McCullough *et al.*, who used an ebulliometric method, were given higher weight. The results of Hildenbrand *et al.* (1959–374) and Wu *et al.* (1990–32) show good agreement with our smoothed results. Percent deviations of the experimental values from those calculated with the Cox equation are shown in Fig. 11.

Piperidine

The measurements of Osborn and Douslin (1968–206) were used in the final evaluation. The measurements of Riley and Bailey (1929–178) and Nakanishi *et al.* (1975–

283) were excluded. Fig. 12 shows the percent deviations from the vapor pressures calculated from the Cox equation.

Indole

There appear to be no vapor pressure measurements on liquid indole. For the crystalline phase the experimental values reported by Aihara (1955–710) together with the high temperature values of Serpinskii *et al.* (1958–398) were used in the fitting. The low temperature values reported by Serpinskii *et al.* was excluded. Fig. 13 shows the percent deviations from the vapor pressures calculated from the Antoine equation.

Quinoline

The measurements of Steele *et al.* (1988–551) were used for the final evaluation. The results of Young (1889–25), Glaser and Rüländ (1957–76), Malanowski (1961–32), Van De Rostyne and Prausnitz (1980–6), Krevor *et al.* (1986–24), Klara *et al.* (1987–21), Neisen and Yesavage (1988–70), and Flanigan *et al.* (1988–555) were excluded. Fig. 14 shows the percent deviations from the vapor pressures calculated from the Cox equation.

Isoquinoline

The measurements of Steele *et al.* (1988–551) were used for the final evaluation. The results of Malanowski (1961–32) were excluded. Fig. 15 shows the percent deviations from the vapor pressures calculated from the Cox equation.

Carbazole

For carbazole, there are vapor pressure measurements on both the crystalline and the liquid phase.

For the crystalline phase the results of Aihara (1955–710) was used while those by Jimenez *et al.* (1990–65) was excluded. Fig. 16 shows the percent deviations from the vapor pressures calculated from the Antoine equation.

For the liquid phase the results reported by Sivaraman *et al.* (1983–185) together with the selected critical temperature and pressure were used. The measurements by Senseman and Nelson (1923–166) and Moritimer and Murphy (1923–167) were not used. Fig. 17 shows the percent deviations from the vapor pressures calculated from the Cox equation.

Acridine

For acridine, there are vapor pressure measurements on both the crystalline and the liquid phase. For the crystalline phase, the single set of measurements by McEachern *et al.* (1975–229) were used in the evaluation. Fig. 18 shows the percent deviations from the vapor pressures calculated from the Antoine equation. For the liquid phase, the results reported by Steele *et al.* (1989–76) together with the critical temperature and pressure selected in this work were used. The values of Sivaraman *et al.* (1983–185) was excluded. Fig. 19 shows the percent deviations from the vapor pressures calculated from the Cox equation.

Phenanthridine

For phenanthridine, the only measurements on the crystalline phase are those by McEachern *et al.* (1975–229) and on the liquid phase by Steele *et al.* (1989–76). These two sets of results were used in this evaluation. The critical temperature and pressure selected in this work were used in the fitting of the liquid results. Figure 20 shows the percent deviations from the vapor pressures calculated from the Antoine equation for the crystalline phase and from the Cox equation Fig. 21 for the liquid phase.

1-Naphthalenamine

The vapor pressures selected for the liquid are the smoothed values reported by Stull (1947–83). The critical temperature and pressure selected in this work were also used. Fig. 22 shows the percent deviations from the vapor pressures calculated using the Cox equation.

2-Naphthalenamine

The vapor pressures selected are the smoothed values published by Karyakin *et al.* (1968–3) for the crystalline phase and the smoothed values reported by Stull (1947–83) for the liquid phase. The critical temperature and pressure selected in this work were also used. Fig. 23 shows the percent deviations from the vapor pressures calculated using the Antoine equation for the crystalline phase and Fig. 24 for the percent deviations from the vapor pressures calculated using the Cox equation for the liquid phase.

9-Methylcarbazole

For the crystalline phase, the selected measurements are those reported by Jimenez *et al.* (1990–65) which was used in this fitting. Fig. 25 shows the percent deviations from the vapor pressures calculated using the Antoine equation. For the liquid phase, the only measurements are those of Steele *et al.* (1992–3). These results together with the critical temperature and pressure reported by the same authors were used in this evaluation. Fig. 26 shows the percent deviations from the vapor pressures calculated using the Cox equation for the liquid phase.

3.3. Saturated Liquid Density

The temperature and density ranges over which measurements of density have been reported are listed in Table 17. Also included are the estimated accuracies for both temperature and density along with the number of experimental determinations. For some compounds, either vapor densities or rectilinear diameter lines were reported and are noted in this section. Details of measurements at isolated temperatures are not given in the table, but are discussed in the text.

1-Butanamine

The values of Costello and Bowden (1959–218) and of Sreenivasulu and Naidu (1978–77) were used to fit Eq. (6). The deviations of the results of Friend and

Hargeaves (1944–125) are much higher than expected. The values of Vogel (1948–262) and of Zhigunov and Ampelogyva (1972–237) were about 0.5 percent lower and the values of Lieben and Rossi (1871–21) were about 1.0 percent lower than the selected values. The remaining values at isolated temperatures (1872–20, 1919–64, 1947–146, 1952–385, 1967–218, 1968–195, 1971–42, 1972–151, 1974–134, 1977–84, 1978–78, 1979–97, and 1970–164) were represented to within ± 1.0 percent. The deviations are shown in Fig. 27.

2-Butanamine

The temperature range of the available measurements was so limited that only two constants in the fitting equation could be obtained reliably. As indicated in Table 17, values from only two sources were used for the fit together with some isolated results in (1903–28, 1930–63, and 1978–78) not listed in Table 17. Two isolated results from (1919–64, and 1954–310) were not used in the fitting. Deviations from the fitting equation of the experimental results are shown in Fig. 28.

2-Methyl-1-propanamine

The values reported by Vogel (1948–262) and Costello and Bowden (1959–218) were selected, and were represented to within their experimental accuracies by Eq. (6) with three adjustable parameters. The deviations are shown in Fig. 29. The remaining values at isolated temperatures (1919–64, 1970–167, and 1978–78) were represented to within ± 0.06 percent, while those measurements made prior to 1900 (1889–26 and 1895–49) were represented to within ± 0.1 percent.

2-Methyl-2-propanamine

The temperature range of the available results was so limited that only two constants in the fitting equation could be obtained reliably. As indicated in Table 17, all available results were used except two isolated point (1946–175 and 1978–78). The analysis was based on the values of Bruhl (1897–43), Krishnaji and Mansingh (1965–387), Otin *et al.* (1973–148), and Whitmer and Cyvin (1978–36). Deviations from the fitting equation of the experimental results are shown in Fig. 30.

Pyrrole

The temperature range of the available results was so limited that only two constants in the fitting equation could be obtained reliably. As indicated in Table 17, values from Timmermans *et al.* (1955–485) and Helm *et al.* (1958–216) were used in the fitting. The results of Dezelic (1937–487) and the isolated results (1895–49, 1934–404, 1942–300, 1949–223, 1955–696, and 1978–78) were excluded. Deviations from the fitting equation for some of the experimental results are shown in Fig. 31.

1-Methylpyrrole

There are high quality measurements from API Project 52 (1958–417) in the temperature range 293 to 303 K which are in reasonable agreement with those from

Auwers and Kohlhas (1924–198). The isolated results (1877–24, and 1904–106) were excluded from the fit. The density calculated with Eq. (6a) using the predicted critical density only gave values differing by 10 percent from the API 41 values. The values given in Table 6 were calculated by adjusting the critical density so that the predicted and experimental value from (1958–417) agreed. It is not unusual for predicted critical densities to be in error by 10 percent.

2-Methylpyrrole

A density of $942.6 \text{ kg}\cdot\text{m}^{-3}$ is reported by Mikhaleva *et al.* (1979–333) at 293.15 K and a value of $944.6 \text{ kg}\cdot\text{m}^{-3}$ at 288.15 K is reported by Pictet (1904–106). Both these values are unreliable so no recommended values are given.

3-Methylpyrrole

Our literature search indicated that there was no density data for this compound.

Pyridine

The values of Muller and Brenneis (1932–322), Lagemann *et al.* (1949–264), Toropov (1956–639), Helm *et al.* (1958–216), Mato and Sanchez (1967–321), Deshpande *et al.* (1971–130), Meyer *et al.* (1971–213), Rao and Naidu (1973–222), and Pikkarainen (1980–121) were used to fit Eq. (6). The values of Timmermans (1910–58, and 1937–146), Leis and Curran (1945–205), Hatem (1949–43), Biddiscombe *et al.* (1954–31), and Malanowski *et al.* (1979–207) agree within ± 0.05 percent while the values of Bruhl (1895–49), Livingston *et al.* (1908–112), Bramley (1916–37), and Naumova (1953–615) agreed to about ± 0.4 percent. The deviations of Gokavi *et al.* (1986–2) are much higher than expected. The values at isolated temperatures (1884–28, 1898–2, 1906–115, 1907–62, 1908–125, 1908–126, 1908–127, 1909–134, 1912–127, 1913–179, 1921–129, 1926–71, 1927–12, 1929–341, 1931–278, 1934–392, 1934–404, 1935–417, 1949–223, 1950–594, 1952–363, 1953–406, 1955–378, 1955–695, 1955–696, 1956–563, 1958–391, 1960–119, 1961–292, 1961–303, 1961–305, 1963–379, 1965–341, 1967–319, 1967–320, 1968–48, 1969–223, 1969–224, 1969–226, 1969–230, 1970–164, 1970–233, 1970–239, 1971–183, 1971–214, 1972–234, 1972–235, 1974–255, 1976–183, 1978–130, 1978–131, 1980–142, 1982–34, 1983–11, 1983–150, 1984–196, 1984–241, 1985–68, 1986–334, and 1989–79) were represented to within ± 1.0 percent. The deviations of some of the experimental results are shown in Fig. 32.

2-Methylpyridine

The temperature range of the available results was so limited that only two constants in the fitting equation could be obtained reliably. As indicated in Table 17, values from Freiser and Glowacki (1948–442), Meyer *et al.* (1971–213), and Minana Aznar *et al.* (1984–95) were used for the fit; they were represented to within better than ± 0.1 percent. Results of Bruhl (1895–49),

Biddiscombe *et al.* (1954–31), Timmermans *et al.* (1955–485), Toropov (1956–639), Helm *et al.* (1958–216), and Kyte *et al.* (1960–119) and the isolated results which were not indicated in Table 17, (1880–2, 1884–28, 1895–49, 1907–62, 1921–129, 1927–12, 1934–392, 1935–418, 1942–300, 1953–690, 1960–9, 1961–304, 1966–482, 1968–195, 1976–132, 1976–178, 1978–131, 1982–34, and 1984–241) were not used in the fitting. Deviations from the fitting equation for some of the experimental results are shown in Fig. 33.

3-Methylpyridine

Values were available over a limited range of temperatures, and only two constants could be determined for the fitting equation. The values included in the fit, indicated in Table 17, with some isolated results (1921–129, 1957–537, 1976–178, 1978–131, 1982–34, 1984–196, and 1985–68) were represented with the fitting equation to better than ± 0.1 percent. Some other isolated results (1895–49, 1907–62, 1936–285, 1946–308, 1951–184, and 1966–257), not indicated in Table 17, were excluded from the fit. Deviations from the fitting equation for some of the experimental results are shown in Fig. 34.

4-Methylpyridine

Two constants were determined for the fitting equation with the values available over the limited temperature range indicated in Table 17. The selected values were fitted to better than ± 0.1 percent. Isolated results (1946–308, 1951–184, 1957–537, 1968–195, 1972–41, 1967–178, 1978–131, 1982–34, and 1984–241) were not indicated in Table 17. The recommended values are in good agreement with the excellent results of (1972–41). Deviations from the fitting equation for some of the experimental results are shown in Fig. 35.

Pyrrolidine

The most reliable results reported were that by Helm *et al.* (1958–216), but the temperature range was 10 K. Values reported by Holland and Smyth (1955–11) are higher by about $9.5 \text{ kg}\cdot\text{m}^{-3}$. Therefore the values reported by Helm *et al.* and those of Holland and Smyth (after subtracting $9.5 \text{ kg}\cdot\text{m}^{-3}$ from each value) were used in the fit. Isolated results (1949–223, 1950–546, and 1978–78), were not indicated in Table 17, were represented to within ± 1.0 percent. Deviations from the fitting equation for some of the experimental results are shown in Fig. 36.

Piperidine

The temperature range of the available results was so limited that only two constants in the fitting equation could be obtained reliably. As indicated in Table 17, values reported by Perkin (1889–26), Timmermans and Hennaut-Roland (1937–146), Teitelbaum *et al.* (1947–404) and those published by API (1960–369) were used to fit Eq. (6). The deviations of the Friend and Hargreaves (1944–126) values are much higher than expected. The values of Kurnakow and Zemczny (1913–179) and the

isolated point (1889–41, 1892–46, 1895–49, 1895–58, 1898–2, 1902–64, 1930–307, 1934–392, 1937–487, 1937–506, 1940–364, 1949–223, 1951–656, 1964–572, 1968–370, 1972–41, 1975–283, and 1978–78) were not used in the fitting. Deviations from the fitting equation for some of the experimental results are shown in Fig. 37.

Quinoline

Results reported by Mallikarjun and Hill (1965–231) and by Steele *et al.* (1988–511) were used in the fit. The results of Steele *et al.* were given higher weight. The values of Lumsden (1907–64), Livingston *et al.* (1908–112), Schwes (1911–44), Bramley (1916–37), Timmermans and Hennaut-Roland (1937–146), Hatem (1949–43), Tschamler and Krischai (1951–444), Kovalenko and Trifonov (1954–674), Holland and Smyth (1955–11), Irwin *et al.* (1984–246), and Oshmyansky *et al.* (1986–551) were represented to within ± 0.5 percent. The values at isolated temperatures (1884–28, 1895–58, 1898–2, 1935–428, 1949–223, 1961–292, 1969–51, 1969–243, 1971–244, 1978–209, and 1982–321) were represented to within ± 1.0 percent. The deviations are shown in Fig. 38.

Isoquinoline

The temperature range of the available results was so limited that only two constants in the fitting equation could be obtained reliably. As indicated in Table 17, results reported by Freiser and Glowacki (1949–545) and by Steele *et al.* (1988–511) were used in the fit. The results of Steele *et al.* were given higher weight. Values reported by Holland and Smyth (1955–11) and Mallikarjun and Hill (1965–231) together with the isolated results reported in (1895–58 and 1972–41) were represented to within ± 0.1 percent. The deviations are shown in Fig. 39.

Carbazole

The measurements of Gurevich and Bednov (1972–326) were used in the analysis. The two values reported by Burriel (1931–8) appear to be too low. The deviations are shown in Fig. 40.

Acridine

The liquid densities were estimated using Eq. (6a) with the critical temperature and density reported in Table 1 and an acentric factor ω of 0.546.

1-Naphthalenamine

The only values used in the fit were those reported by Beck (1907–112). Isolated values given in (1892–22, 1913–194, and 1923–177) were not used in the fit. Deviations are shown in Fig. 41.

2-Naphthalenamine

Measurements of low quality have been reported by Bhatnagar and Singh (1929–353), and Perkin (1892–22). The temperature of measurement of the later work was considerable below the accepted melting point. The

densities were estimated using Eq. (6a) with the critical temperature and density reported in Table 1 and an acentric factor ω of 0.544.

9-Methylcarbazole

Our literature search indicated that there were no measurements on the liquid phase. The liquid densities were estimated using Eq. (6a) with the critical temperature and density reported in Table 1 and an acentric factor ω of 0.475.

3.4. Second Virial Coefficients

The temperature ranges over which second virial coefficients have been either measured or calculated by the authors from enthalpies of vaporization, along with the estimated uncertainties, are listed in Table 18.

1-Butanamine

Second virial coefficients were derived from the Claperyon equation with the enthalpy of vaporization results of Majer *et al.* (1979–78), the liquid density Eq. (6) constants from Table 5], and the Cox equation constants from Table 2. The derived values at 313.15, 328.15, 343.15 and 358.15 K were (-1793 ± 175), (-1795 ± 100), (-1554 ± 5) and (-1335 ± 20) $\text{cm}^3\text{mol}^{-1}$ respectively.

2-Butanamine

Second virial coefficients were derived from the Claperyon equation with the enthalpy of vaporization results of Majer *et al.* (1979–78), the liquid density Eq. (6) constants from Table 5], and the Cox equation constants from Table 2. The derived values at 298.15, 313.15, 328.15 and 343.15 K were (-1553 ± 90), (-1354 ± 50), (-1264 ± 140), and (-1080 ± 70) $\text{cm}^3\text{mol}^{-1}$ respectively.

2-Methyl-1-propanamine

Second virial coefficients were derived from the Claperyon equation with the enthalpy of vaporization results of Majer *et al.* (1979–78), the liquid density Eq. (6) constants from Table 5], and the Cox equation constants from Table 2. The derived values at 313.15 and 328.15 K were (-1212 ± 190) and (-1195 ± 40) $\text{cm}^3\text{mol}^{-1}$ respectively.

2-Methyl-2-propanamine

The second virial coefficient derived from the enthalpy of vaporization determined by Wadsö (1969–169) was (-1254 ± 100) $\text{cm}^3\text{mol}^{-1}$ at 298.15 K.

Pyrrole

The second virial coefficient results of Eon *et al.* (1971–47) were not used because of their high uncertainty. Only the values of Scott *et al.* (1967–116) were used.

1-Methylpyrrole

The values of Eon *et al.* (1971–47) were the only results available. The estimated uncertainty in the virial coefficient is $\pm 50 \text{ cm}^3\text{mol}^{-1}$.

Pyridine

The values of McCullough *et al.* (1957–176), Andon *et al.* (1957–420), and Cox and Andon (1958–272) were used in the analysis.

2-Methylpyridine

The values of Andon *et al.* (1957–420), Cox and Andon (1958–272), and Scott *et al.* (1963–157) were used in the analysis.

3-Methylpyridine

The values of Andon *et al.* (1957–420), Cox and Andon (1958–272), and Scott *et al.* (1963–157) were used in the analysis.

4-Methylpyridine

The values of Andon *et al.* (1957–420), Cox and Andon (1958–272), and Hossenlopp and Scott (1981–44) were used in the analysis.

Pyrrolidine

The values of McCullough *et al.* (1959–355) were the only results available. The estimated uncertainty in the virial coefficient is $\pm 20 \text{ cm}^3\text{mol}^{-1}$.

Piperidine

The selected values were those derived from enthalpies of vaporization determined by Hossenlopp and Archer (1988–556) were (-1385 ± 60), (-1261 ± 25), and (-1077 ± 30) $\text{cm}^3\text{mol}^{-1}$ at 338.34, 357.42 and 379.36 K respectively.

Quinoline

Values of the second virial coefficient derived from enthalpies of vaporization determined by Flanigan *et al.* (1988–555) were (-1322 ± 45), (-1154 ± 20), (-1012 ± 15), and (-850 ± 10) $\text{cm}^3\text{mol}^{-1}$ at 544.00, 595.80, 617.80 and 644.20 K respectively.

No second virial coefficients or direct enthalpy of vaporization measurements were available for the remaining compounds. Therefore the second virial coefficients were estimated from Eq. (9) at various temperatures. The constants of Eq. (10) were determined from a fit to these estimated values.

3.5 Enthalpies of Vaporization or Sublimation

Calorimetrically determined enthalpies of vaporization together with values calculated from vapor pressure measurements, along with estimated uncertainties are listed in Table 19. Values at 298.15 K calculated from Eq. (3) or (5) are also listed. The selected enthalpies of

vaporization at 298.15 K were corrected to the ideal gas state. Table 10 gives the enthalpy of vaporization and sublimation converted to the ideal gas at 298.15 K.

1-Butanamine

Wadsö (1969–169) and Kusano *et al.* (1982–127) measured calorimetrically the enthalpy of vaporization at 298.15 K. Majer *et al.* (1979–78) made similar measurements in the temperature range 298.15 to 358.15 K. An average weighted value at 298.15 K was selected.

2-Butanamine

Wadsö (1969–169) measured calorimetrically the enthalpy of vaporization at 298.15 K. Majer *et al.* (1979–78) made similar measurements between 298.15 and 358.15 K. An average weighted value at 298.15 K was selected, based on results of these two investigations and vapor pressure data evaluated in this work.

2-Methyl-1-propanamine

Wadsö (1969–169) measured calorimetrically the enthalpy of vaporization at 298.15 K. Majer *et al.* (1979–78) made similar measurements between 298.15 and 343.15 K. Good and Moore (1970–167) calculated the enthalpy of vaporization at 298.15 K from the vapor pressure measurements of Douslin and Osborn (1965–67). The selected value was an average of the values of Majer *et al.* (1979–78) and Wadsö (1969–169) at 298.15 K.

2-Methyl-2-propanamine

The enthalpy of vaporization determined calorimetrically by Wadsö (1969–169) at 298.15 K was selected. Smith and Good (1967–60) calculated the enthalpy of vaporization at 298.15 K from unpublished ebulliometric vapor pressure measurements.

Pyrrole

The enthalpy of vaporization of pyrrole was determined calorimetrically by Scott *et al.* (1967–116) at 362.11, 381.21 and 402.91 K. The standard enthalpy of vaporization at 298.15 K calculated using the second virial coefficients and other measurements reported in their paper was selected.

1-Methylpyrrole

No calorimetric value was available. The enthalpy of vaporization at 298.15 K calculated by Good (1972–41) from the vapor pressure measurements of Osborn and Doulsin (1968–206) was selected.

2-Methylpyrrole

No calorimetric or vapor pressure results were available. The enthalpy of vaporization at 298.15 K was estimated based on the additive procedure described in Ref. (1986–408).

3-Methylpyrrole

No calorimetric or vapor pressure results were available. The enthalpy of vaporization at 298.15 K was esti-

mated using an additive method described in Ref. (1986–408).

Pyridine

The enthalpy of vaporization of pyridine was determined calorimetrically by McCullough *et al.* (1957–176) at 346.65, 366.11 and 388.40 K and by Majer *et al.* (1984–94) between 298.15 and 368.15 K. Measurements were also reported by Louguinine (1899–11), Kahlenberg (1901–63), Constam and White (1903–66), Mathews (1926–71), Kolosovskii and Mezhenin (1931–49), Buck and Stewart (1961–293), and by Yarym-Agaev *et al.* (1963–2). The value determined by Majer *et al.* at 298.15 K was selected.

2-Methylpyridine

The enthalpy of vaporization of 2-methylpyridine was determined calorimetrically by Scott *et al.* (1963–157) at 359.35, 379.48 and 401.54 K and by Majer *et al.* (1984–94) between 298.15 and 368.15 K. It was also determined by Kahlenberg (1901–64) at 402.15 K and by Constam and White (1903–66) at 400.88 K. The value determined by Majer *et al.* at 298.15 K was selected.

3-Methylpyridine

The enthalpy of vaporization of 3-methylpyridine was determined calorimetrically by Scott *et al.* (1963–156) at 372.45, 393.36 and 417.29 K and by Majer *et al.* (1984–94) between 298.15 and 368.15 K. Measurements were also reported by Constam and White (1903–66) and by Kusano and Saito (1976–127). The average weighted value was selected on the basis of results obtained by Majer *et al.*, Kusano and Saito as well as vapor pressure data evaluated in this work.

4-Methylpyridine

The enthalpy of vaporization of 4-methylpyridine was determined calorimetrically by Hossenlopp and Scott (1981–44) at 355.04, 365.58, 373.53, 385.47, 394.51, 418.52, and 434.26 K and by Majer *et al.* (1984–94) at a range between 298.15 and 368.15 K. Measurements were also reported by Kustano and Saito (1976–127). Good (1972–41) calculated the enthalpy of vaporization at 298.15 K from the vapor pressure measurements of Osborn and Doulsin (1968–206). The value determined by Majer *et al.* was selected.

Pyrrolidine

McCullough *et al.* (1959–355) determined calorimetrically the enthalpy of vaporization of pyrrolidine at 321.90, 339.50, and 359.72 K. Hildenbrand *et al.* (1959–374) measured the enthalpy of vaporization at 298.15 K. The selected enthalpy of vaporization is taken from Majer and Svoboda (1985–23).

Piperidine

Hossenlopp and Archer (1988–556) determined calorimetrically the enthalpy of vaporization of piperidine at 338.34, 357.42 and 379.36 K. Both Good (1972–41) and

Bedford *et al.* (1963–357) calculated the enthalpy of vaporization for this compound at 298.15 K from vapor pressure measurements. The value calculated by Good was selected.

Indole

Aihara (1955–710) determined the enthalpy of sublimation of this compound at 298.15 K. This value was selected.

Quinoline

Flanigan *et al.* (1988–555) determined calorimetrically the enthalpy of vaporization of quinoline at 544.0, 595.8, 617.8, and 644.2 K. Steele *et al.* (1988–551) calculated the enthalpy of vaporization from vapor pressure measurements in the range between 260 and 600 K. The value calculated by Steele *et al.* was selected.

Isoquinoline

Steele *et al.* (1988–551) calculated the enthalpy of vaporization from the vapor pressure measurements in the range between 298.15 and 600 K. Their value was selected.

Carbazole

Aihara (1955–710) determined the enthalpy of sublimation of this compound at 298.15 K and Jimenez *et al.* (1990–65) at 355.27 K. The enthalpy of sublimation reported by Aihara was selected.

Acridine

Steele *et al.* (1989–76) calculated the enthalpy of vaporization from vapor pressure measurements in the range between 380 and 640 K. McEachern *et al.* (1975–228) calculated the enthalpy of sublimation of acridine at 300.0 K. The value of the enthalpy of sublimation extrapolated by Steele *et al.* to 298.15 K was accepted.

Phenanthridine

Steele *et al.* (1988–551) calculated the enthalpy of vaporization from vapor pressure measurements in the range between 380.0 and 520 K. The enthalpy of sublimation extrapolated in this study to 298.15 K was selected.

1-Naphthalenamine

No enthalpy of sublimation studies have been reported for 1-naphthalenamine. We assumed that the difference between the enthalpies of sublimation of 1- and 2-naphthalenamine were equal to the difference between their enthalpies of fusion, $9.1 \text{ kJ}\cdot\text{mol}^{-1}$ (1979–205). The enthalpy of sublimation of 1-naphthalenamine was calculated from the selected value for 2-naphthalenamine.

2-Naphthalenamine

The average enthalpy of sublimation of 2-naphthalenamine in the range of 283.15 and 313.15 K was calculated by Karyakin *et al.* (1968–3) from vapor pressure measurements. This value was adopted.

9-Methylcarbazole

The enthalpy of sublimation for this compound was calculated from the vapor pressure measurements at 322.69 K by Jimenez *et al.* (1990–65). Steele *et al.* (1992–3) calculated the enthalpy of vaporization from vapor pressure measurements in the range between 298.15 and 600 K. Their value at 298.15 K was selected.

3.6 Enthalpies of Combustion and Formation

Several determinations of enthalpies of combustion were made near the turn of the century. In general, these old values were found to deviate appreciably from recent determinations. The older measurements are included primarily for completeness, and we do not give them significant weight in our evaluation. The available enthalpy of combustion measurements along with estimated uncertainties are listed in Table 20. Enthalpies of formation were calculated using the enthalpies of formation of auxiliary substances listed in Table 21.

1-Butanamine

Lemoult (1907–116), Swietoslawski and Popov (1925–26), and Evans *et al.* (1959–313) determined the enthalpy of combustion of 1-butanamine in the liquid state at 298.15 K. The sample used by Evans *et al.* was obtained commercially and purified by fractional distillation. The purified sample was dried over solid KOH, and further fractionated. Gas-phase chromatography revealed no significant amounts of impurity. The value of Evans *et al.* was selected.

2-Butanamine

Lemoult (1907–116) determined the enthalpy of combustion of 2-butanamine in the liquid state at room temperature. Evans *et al.* (1959–313) made measurements on the liquid phase at 298.15 K. Their sample was obtained commercially, purified by fractional distillation, and dried over solid KOH. No significant impurities were found by gas-phase chromatography. The value of Evans *et al.* was selected.

2-Methyl-1-propanamine

Lemoult (1907–116) determined the enthalpy of combustion of 2-methyl-1-propanamine in the liquid state at room temperature while Good and Moore (1970–167) made measurements on the liquid state at 298.15 K. Their sample, obtained commercially, contained traces of 1-butanamine and 2-butanamine that would have little effect on the final value. The value determined by Good and Moore was selected.

2-Methyl-2-propanamine

Lemoult (1907–116), Swietoslawski and Popov (1925–236), Evans *et al.* (1959–313), and Smith and Good (1967–60) determined the enthalpy of combustion of 2-methyl-2-propanamine in the liquid state at 298.15 K. The sample used by Smith and Good was of the highest purity (99.90 ± 0.03) mol percent and was obtained from

API-USBM. The sample was dried by passing the vapors through activated molecular sieves. The values determined by Evans *et al.* and Smith and Good are in excellent agreement. The value determined by Smith and Good was selected.

Pyrrole

Berthelot and Andre (1899–60) determined the enthalpy of combustion of pyrrole in the liquid state at room temperature while Scott *et al.* (1967–116) made measurements on the liquid state at 298.15 K. The sample used by Scott *et al.* is stated to be 99.998 mol percent pure. The value determined by Scott *et al.* was selected.

1-Methylpyrrole

Good (1972–41) determined the enthalpy of combustion of 1-methylpyrrole in the liquid state at 298.15 K. The purity of the sample was stated to be 99.998 mol percent.

2-Methylpyrrole

Experimental measurements of the enthalpy of combustion have not been reported. The enthalpy of combustion of 2-methylpyrrole was estimated in the liquid state at 298.15 K based on an enthalpy of formation calculated using the additive method described in Ref. (1986–408).

3-Methylpyrrole

No experimental measurements on the enthalpy of combustion are available. This value was estimated in the liquid state at 298.15 K based on an enthalpy of formation calculated using the additive method described in Ref. (1986–408).

Pyridine

The enthalpy of combustion of pyridine in the liquid state at 298.15 K was determined by Delepine (1898–41), Constam and White (1903–66), Swietoslawski (1909–138), Cox *et al.* (1954–514), and Hubbard *et al.* (1961–295). Except for the determinations of Constam and White and Swietoslawski, the other three determinations are in good agreement. The purity of the sample used by Cox *et al.* was (99.85 ± 0.07) mol percent. The value determined by Hubbard *et al.* was selected.

2-Methylpyridine

Constam and White (1903–66), Cox *et al.* (1954–514), and Scott *et al.* (1963–156) determined the enthalpy of combustion of 2-methylpyridine in the liquid state at 298.15 K. The purity of the sample used by Cox *et al.* was (99.93 ± 0.04) mol percent. The sample used by Scott *et al.* was from the Standard Sample of Organic Nitrogen Compound API-USBM 52–4 Project. The sample was dried in the liquid state with calcium hydride and was always transferred and handled without exposure to air. The purity, determined by calorimetric studies of the melting point as a function of fraction melted, was 99.90

mol percent. The value determined by Scott *et al.* was selected.

3-Methylpyridine

Constam and White (1903–66), Cox *et al.* (1954–514), and Scott *et al.* (1963–157) determined the enthalpy of combustion of 3-methylpyridine in the liquid state at 298.15 K. The purity of the sample used by Cox *et al.* was (99.97 ± 0.02) mol percent. The sample of 3-methylpyridine used by Scott *et al.* was from the Standard Samples of Organic Nitrogen Compounds API-USBM 52–7 Project and the purity was 99.88 mol percent. The value determined by Scott *et al.* was selected.

4-Methylpyridine

Constam and White (1903–66), Cox *et al.* (1954–514), and Good (1972–41) determined the enthalpy of combustion of 4-methylpyridine in the liquid state at 298.15 K. The purity of the sample used by Cox *et al.* was (99.91 ± 0.05) mol percent. The sample used by Good was from the Samples of Standard Organic Nitrogen Compounds API-USBM 52–7 Project prepared by the Bureau of Mines, Laramie Energy Center. The purity of the sample used by Good is stated to be 99.97 mol percent. The value determined by Good was selected.

Pyrrolidine

McCullough *et al.* (1959–353) and Hildenbrand *et al.* (1959–131) determined the enthalpy of combustion of pyrrolidine in the liquid state at 298.15 K. The purity of the sample used by both groups was stated to be 99.85 mol percent. There is excellent agreement between these two determinations and an average value was selected.

Piperidine

Delepine (1898–42 and 1899–62) was the first to determine the enthalpy of combustion of this compound. Bedford *et al.* (1963–357) and Good (1972–41) determined the enthalpy of combustion of piperidine in the liquid state at 298.15 K. The purity of the sample used by Good was estimated to be 99.94 mol percent. The value determined by Good was selected.

Indole

Berthelot and Andre (1899–60 and 1899–61) were the first to determine the enthalpy of combustion of indole. Stern and Klebs (1932–334) and Good (1972–41) determined the enthalpy of combustion of indole in the crystalline state at 298.15 K. Good used a sample of purity 99.90 mol percent. The value determined by Good differed by $30 \text{ kJ}\cdot\text{mol}^{-1}$ from the value determined by Stern and Klebs. The value determined by Good was selected.

Quinoline

Delepine (1898–42 and 1899–62) and recently Steele *et al.* (1988–531) determined the enthalpy of combustion of quinoline in the liquid state at 298.15 K. For the later

measurements the sample purity was 99.991 mol percent. The value obtained by Steele *et al.* was selected.

Isoquinoline

Delepine (1898–42 and 1899–62) determined the enthalpy of combustion of isoquinoline in the crystalline state at 298.15 K. The enthalpy of combustion of the liquid at 304.15 K was determined by Good (1972–41). The purity of the sample used by Good was stated to be (99.9 ± 0.1) mol percent. His value was selected.

Carbazole

Berthelot and Andre (1899–60 and 1899–61), Tavernier and Lamoroux (1957–593), and Jimenez *et al.* (1990–65) determined the enthalpy of combustion of this compound. The value obtained by Jimenez *et al.* for a sample of purity 99.9 mol percent was selected.

Acridine

Albert and Willis (1946–316), Willis (1947–404) and Steele *et al.* (1984–76) have determined the enthalpy of combustion of acridine. Recently Steele *et al.* (1989–76) measured the enthalpy of combustion of acridine in a crystal state at 298.15 K using a highly purified sample (purity 99.988 mol percent). Their value was adopted.

Phenanthridine

The enthalpy of combustion reported by Steele *et al.* (1989–76) made on a sample of purity 99.975 mol percent was selected.

1-Naphthalenamine

The measurements of Lemoult (1907–116) and Swietoslawski and Popov (1925–236) at room temperature were of low accuracy. The more accurate measurement of Milone and Rosignoli (1932–52) at 298.15 K was selected.

2-Naphthalenamine

The measurements of Lemoult (1907–116) and Swietoslawski and Popov (1925–236) at room temperature were of low accuracy. Milone and Rosignoli (1932–52) and Willis (1947–404) determined the enthalpy of combustion of 2-naphthalenamine in the solid state at 298.15 K. These two determinations differed by $0.03 \text{ kJ} \cdot \text{mol}^{-1}$. The selected value is an average of these 2 determinations.

9-Methylcarbazole

The enthalpy of combustion of 9-methylcarbazole was determined calorimetrically in the crystalline state at 298.15 K by Good (1972–41) and recently by Jimenez *et al.* (1990–65). Both determinations were made on a highly purified samples and are in a good agreement. The value obtained by Good was selected.

3.7. Condensed Phase Calorimetric Properties.

Literature heat capacity and phase transition measurements for the condensed phases, along with estimated

uncertainties, are given in Table 22. Evaluation of the thermodynamic properties in the condensed phases (crystals and liquid) has been made only for compounds where heat capacities have been measured at least in the temperature range 10 to 300 K. These compounds are: 2-methyl-2-propanamine, pyrrole, 1-methylpyrrole, pyridine, 2-methylpyridine, 3-methylpyridine, 4-methylpyridine, pyrrolidine, piperidine, quinoline, isoquinoline, acridine, phenanthridine, and 9-methylcarbazole. For these compounds the values of the heat capacities of the condensed phases in equilibria with the saturated vapours ($C_{\text{sat},m}$), calculated from values of heat capacities at constant pressure ($C_{p,m}$), and the integrations of $C_{\text{sat},m}$ values were done satisfactorily in the original publications (including premelting effects, smoothing data procedures and extrapolation to 0 K). The results were not reanalysed except that the thermodynamic functions calculated originally on the basis of either IPTS–48 (1949–335) or IPTS–68 (1969–216) were corrected to ITS–90 (1990–427) using a procedure described in (1969–94). The following relationships were used to calculate the temperature scale corrections for heat capacity ($\Delta C_{\text{sat},m}$), absolute entropy (ΔS_m), enthalpy (as $\Delta\{H_m/T\}$) and Gibbs energy (as $\Delta\{G_m/T\}$):

$$\Delta C_{\text{sat},m} = -C_{\text{sat},m}(T) \frac{d\mu(T)}{dT} - \mu(T) \frac{dC_{\text{sat},m}(T)}{dT} \quad (11)$$

$$\Delta S_m = -\int_0^T \mu(T) C_{\text{sat},m}(T) \frac{dT}{T} - \frac{\mu(T) C_{\text{sat},m}(T)}{T} \quad (12)$$

$$\Delta\{H_m/T\} = -\frac{\mu(T) C_{\text{sat},m}(T)}{T} \quad (13)$$

$$\Delta\{G_m/T\} = \Delta\{H_m/T\} - \Delta S_m \quad (14)$$

where $\mu(T)$ is a difference between temperatures on the old and new temperature scale.

Differentiations in Eq. (11) and integration in Eq. (12) were done numerically. Equally spaced base points (1969–335) were used for the integral in Eq. (12). These base points were obtained by numerical non-linear extrapolation and interpolation of experimental results with quotients of polynomials (rational functions) (1986–789). Extrapolations below 10 K were done using the Debye heat capacity function (1912–160). Where the heat capacity and related enthalpy of transition results did not extend to temperatures low enough to apply the third law, the limited results were evaluated without attempts to derive related thermodynamic properties (entropy, Gibbs energy and enthalpy). The calculated results are presented as $C_{\text{sat},m}/R$, $\Delta_0^T S_m^\circ/R$, $\Delta_0^T H_m^\circ/RT$, and $\Delta_0^T G_m^\circ/RT$. For most cases the temperature scale corrections are significant for heat capacity, but they are negligible for the integrated thermodynamic functions. The thermodynamic quantities referenced to IPTS–68 were not corrected at temperatures higher than 270 K because of the absence of $\mu(T)$ results. The selections are discussed below.

1-Butanamine

No low-temperature heat capacity measurements have been reported. Timmermans and Mataar (1921–17) reported a melting point of $T_m = 222.65$ K and reference (1968–195) reported 224.05 K. Konicek and Wadsö measured $C_{p,m}(1, 298.15 \text{ K}) = 188.0 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ by drop calorimetry (1971–11).

2-Butanamine

No low-temperature heat capacities measurements have been reported. The only property value reported was $T_m = 168.65$ K (1921–17).

2-Methyl-1-propanamine

No low-temperature thermal measurements have been reported. The melting point has been measured by Timmermans and Mataar (1921–17) and twice by Simon and Huter (1935–278, 1935–280).

2-Methyl-2-propanamine

The heat capacity at 298.15 K for the liquid was reported by Smith and Good (1967–60) and by Konicek and Wadsö (1971–11). Finke *et al.* (1972–140) made low-temperature thermal measurements from 12 to 330 K, using adiabatic calorimetry. From these values, they evaluated the thermodynamic functions in the crystal (cIII, cII, cI) and liquid states. Their values were adopted after making corrections from IPTS–48 to ITS–90. The results are given in Table 12. A comparison $C_{sat,m}$ and $\Delta_f S_m^\circ$ at 298.15 K between the literature values and those adopted in this work follow (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 192.1, – (1967–60); 190.0, – (1971–11); 191.71, 233.63 (1972–140); 191.75, 233.63 (this work).

Pyrrole

The enthalpy of fusion has been reported as $7908 \text{ J}\cdot\text{mol}^{-1}$ (1956–676). Scott *et al.* (1967–116), using an adiabatic calorimeter, measured the heat capacity in the condensed phase from 11 to 359 K, the enthalpy of fusion and the triple point. A lambda-type transition between two crystal forms (cII and cI) was found near 65.5 K. The authors were not able to “separate” the thermodynamic results for crystal II and crystal I due to the very small value of the enthalpy of this transition (less than $15 \text{ J}\cdot\text{mol}^{-1}$). Therefore Scott *et al.* evaluated the thermodynamic functions for a mixture of crystals (cII, I) only and for the liquid state. These values were adopted after correcting from IPTS–48 to ITS–90. Table 12 lists the results. A comparison of the ITS–90 and initial values of heat capacity and entropy at 298.15 K are as follows (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 127.74, 156.44 (1967–116); 127.76, 156.43 (this work).

1-Methylpyrrole

The enthalpy of fusion has been reported in Ref. (1960–369). Messerly *et al.* (1988–93) measured the low-temperature heat capacity from 11 to 364 K, using adiabatic calorimetry. They calculated the thermody-

amic quantities in the crystal and liquid states on the basis of the original experimental results. We have corrected their values from IPTS–68 to ITS–90 and the results are listed in the Table 12. Literature and ITS–90 values of the heat capacity and entropy at 298.15 K have the same values of 150.06 and $200.52 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$, respectively.

2-Methylpyrrole

The low-temperature heat capacity has not been measured. The two measurements of the melting point (1957–605; 1969–51) agree within the assigned uncertainty.

3-Methylpyrrole

No low-temperature heat capacity values have been reported. The melting point was measured by Lanum and Morris (1969–51).

Pyridine

Several measurements of the heat capacity of pyridine in the liquid state over narrow temperature intervals or at a single temperature have been reported. Values of heat capacities from these studies are given below (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 142.8 at 337.6 K (1899–11); 133.9 at 293.2 K (1905–94); 129.1 at 294.2 K (1917–66); 135.4 at 290.2 K (1931–362); 129.3 at 289.2 K (1934–351); 146.9 at 332.2 K (1958–58). Bramley (1916–244) measured the specific heat of pyridine but it is not clear to which temperatures his results correspond. Rastorguev and Ganiev (1967–37) measured the heat capacity of pyridine under constant pressure in the adiabatic calorimeter from 293.15 K to 353.15 K. They reported the following results (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 132.09 at 293.15 K; 137.15 at 313.15 K; 142.21 at 333.15 K; 147.12 at 353.15 K. Pearce and Bakke (1936–442) and Parks *et al.* (1936–163) used adiabatic calorimetry to measure the heat capacity from 90 K. In both cases they extrapolated their results to 0 K and integrated to calculate the thermodynamic functions. Results of these two studies do not agree. For example, there are significant discrepancies between the enthalpies of fusion (3100 and $8270 \text{ J}\cdot\text{mol}^{-1}$) and the entropies in the liquid state at 298.15 K (210.41 and $179.08 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$). McCullough *et al.* (1957–176) measured the heat capacity from 13 to 347 K using adiabatic calorimetry. They also determined the enthalpy of fusion ($8278 \text{ J}\cdot\text{mol}^{-1}$) and the triple point temperature (231.489 K) and calculated the thermodynamic functions in the crystal and liquid state. Their values are in a good agreement with those of Parks *et al.* (1936–163) and are recommended. The results of (1936–442) seem to be doubtful. The measurements reported by McCullough *et al.* (1957–176) were corrected from IPTS–48 to ITS–90 and are listed in Table 12. A comparison of the values of heat capacity and entropy at 298.15 K is as follows (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 133.30, 210.41 (1936–442); 134.93, 179.08 (1936–163); 132.72, 177.90 (1957–176); 132.74, 177.90 (this work).

2-Methylpyridine

Scott *et al.* measured the low-temperature heat capacity from 12 to 369 K by means of adiabatic calorimetry (1963–156). They reported values of enthalpy of fusion ($9724 \text{ J}\cdot\text{mol}^{-1}$) and triple point (206.466 K). The thermodynamic functions calculated by Scott *et al.*, corrected from IPTS–48 to ITS–90, are listed in Table 12. Literature and recommended values of heat capacity and entropy at 298.15 K follow (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 158.41, 217.86 (1963–156); 158.44, 217.85 (this work).

3-Methylpyridine

The low-temperature heat capacity values in the liquid and crystal phases were measured by Scott *et al.* (1963–157) from 12 to 388 K using adiabatic calorimetry. Reported values of the enthalpy of fusion and the triple point are $14180 \text{ J}\cdot\text{mol}^{-1}$ and 255.01 K, respectively (1963–157). The thermodynamic functions updated by Scott *et al.* on the basis of experimental results were adopted after correction from IPTS–48 to ITS–90. Table 12 lists the results. A comparison of our recommended values and literature values of heat capacity and entropy at 298.15 K follow (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 158.70, 216.31 (1963–157); 158.73, 216.30 (this work).

4-Methylpyridine

Messerly *et al.* (1988–93) measured the low temperature heat capacity using an adiabatic calorimeter from 13 to 395 K for two crystal phases (cII and cI) and liquid state. They found a transition between two stable crystal phases with an enthalpy close to zero near 255.00 K. The enthalpy of fusion and triple point from (1988–93) were $12.582 \text{ kJ}\cdot\text{mol}^{-1}$ and 276.818 K correspondingly. Their values were adopted after correction from IPTS–68 to ITS–90. Results are listed in Table 12. Evaluated and initial values are slightly different below 270 K but they coincide at 298.15 K giving a heat capacity of $158.99 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and an entropy of $209.09 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$.

Pyrrolidine

The heat capacity of pyrrolidine at 298.15 K in the liquid state was measured by Patton (1952–573) and by Conti *et al.* (1976–110). McCullough *et al.* (1959–355) and Hildenbrand *et al.* (1959–374) made low-temperature heat capacity measurements from 13 to 360 K and 14 to 300 K respectively. Experimental and calculated values of the thermodynamic functions from these two studies are in excellent agreement. The existence of two crystal phases (cII and cI) was observed in both works. The enthalpy of transition from cII to cI were $540 \text{ J}\cdot\text{mol}^{-1}$ ($T_{\text{tr}} = 207.140 \text{ K}$) and $533 \text{ J}\cdot\text{mol}^{-1}$ ($T_{\text{tr}} = 207.140 \text{ K}$); and the enthalpies of fusion were $8577 \text{ J}\cdot\text{mol}^{-1}$ ($T_{\text{m}} = 215.245 \text{ K}$) and $8592 \text{ J}\cdot\text{mol}^{-1}$ ($T_{\text{m}} = 215.310 \text{ K}$), respectively. The unusual temperature dependence of the heat capacity was explained by either the presence of polymeric complexes formed due to hydrogen bonding (1959–355) or by restricted pseudo-rotation of the ring (1959–374). Thermodynamic functions from (1959–355) were adopted after making correction from IPTS–48 to

ITS–90. Results are listed in Table 12. A comparison of heat capacity and entropy values at 298.15 K follow (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 152.4, – (1952–573); 160.2, – (1976–110); 156.57, 204.09 (1959–374); 156.57, 204.01 (1959–355); 156.60, 204.01 (this work).

Piperidine

The heat capacity in the liquid state measured either over a narrow temperature interval or at a single temperature have been reported by several sources (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 186.1 at 331.6 K (1899–11); 170.7 at 290.15 K (1934–351); 182.76 at 297.39 K (1964–568) and 181.6 at 298.15 K (1976–110). Messerly *et al.* (1988–93) measured the heat capacity in the condensed phases from 13 to 362 K using adiabatic calorimetry. Their value of the enthalpy of fusion coincides with the value reported earlier (1961–350). Thermodynamic functions calculated by Messerly *et al.* were accepted after correction from IPTS–68 to ITS–90 and are listed in Table 12. A comparison of heat capacity and entropy at 298.15 K follows: (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 181.6, – (1976–110); 179.86, 209.97 (1988–93); 179.86, 209.97 (this work).

Indole

No low-temperature thermal measurements have been reported. The only property value reported was melting point: 325.15 K (1910–141); 325.65 K (1936–459); 325.65 K (1955–710); 326.25 K (1958–398).

Quinoline

Radulescu and Jula (1934–351) and Kolossowsky and Udovenko (1934–365 and 1934–408) measured the heat capacity of quinoline in the liquid state near “room” temperature. Parks *et al.* (1936–163) measured the heat capacity from 90 to 240 K for both the crystal and liquid. Results of measurements were extrapolated to 0 K and integrated to obtain the thermodynamic functions. Steele *et al.* (1988–551) measured the low-temperature heat capacities using adiabatic calorimetry from 5 to 445 K. They found a transition between two different crystal phases (cII and cI). Their thermodynamic functions were adopted after correction from IPTS–68 to ITS–90. Corrected and initial values for heat capacity and entropy agree at 298.15 K. The results are listed in Table 12. A comparison of the values of the heat capacity and entropy at 298.15 follows (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 199.28, 217.1 (1936–163); 194.89, 219.72 (1988–551); 194.89, 219.72 (this work). The following enthalpy of fusion values have been reported (in $\text{kJ}\cdot\text{mol}^{-1}$): 10.797 at 258.45 K (1936–163); 10.724 at 257.93 K (1957–551); 10.663 at 258.369 K (1988–551).

Isoquinoline

Low-temperature thermal measurements have been made for isoquinoline in the condensed states by Steele *et al.* (1988–551) using adiabatic calorimetry in the interval of 12 to 390 K. They observed three stable crystal phases (cIII, cII and cI). The enthalpies of transition (cIII to cII) and (cII to cI) were found to be zero.

Temperatures of transition respectively were 221.00 and 275.00 K. The enthalpy of fusion was reported as 13.544 kJ·mol⁻¹ (triple point: 299.620 K). Their calculated values of the thermodynamic functions were adopted after correction from IPTS-68 to ITS-90. The corrected and uncorrected values agree at 298.15 K.

Carbazole

No low-temperature heat capacity measurements have been made. Robinson and Scott (1969-244) found two crystal phases with an enthalpy of transition of 274 J·mol⁻¹ at $T_{tr} = 420$ K. They measured the enthalpy of fusion as 26.903 kJ·mol⁻¹ at $T_m = 519.300$ K.

Acridine

Low-temperature heat capacity values of acridine were measured for the condensed states from 5 to 446 K by Steele *et al.* (1989-76). Thermodynamic functions calculated in this work were accepted after making correction from IPTS-68 to ITS-90. Initial and corrected heat capacity and entropy values at 298.15 K agree (205.07 and 208.03 J·K⁻¹·mol⁻¹ (crystal phase)). It should be noted that the enthalpy of fusion reported by Steele *et al.* (1989-76) is 23.675 kJ·mol⁻¹ at 383.242 K differs significantly from that measured by McEachern *et al.* (1975-228), 18.577 kJ·mol⁻¹ at 384.0 K.

Phenanthridine

Steele *et al.* (1989-76) measured the low-temperature heat capacity from 5 to 440 K using adiabatic calorimetry. They found two crystal phases (cII and cI) with an enthalpy of transition of 20 J·mol⁻¹ ($T_{tr} = 354.00$ K). The enthalpy of fusion was reported as 22.831 kJ·mol⁻¹ at the triple point (379.740 K). Thermodynamic functions obtained by Steele *et al.* (1989-76) were adopted after correction from IPTS-68 to ITS-90. The original and corrected values at 298.15 K agree.

1-Naphthalenamine

No low-temperature heat capacity measurements have been reported. Campetti (1914-155) measured the heat capacity for the crystal and liquid states from 318 to 328 K. The heat capacity of the crystal at 318.15 K is 251.6 J·K⁻¹·mol⁻¹ and the heat capacity of the liquid at 324.85 K is 283.7 J·K⁻¹·mol⁻¹. The enthalpy of fusion reported by Khetarpal *et al.* (1979-205) is in a satisfactory agreement with the value measured by Stillmann and Swain (1899-63): 14.490 kJ·mol⁻¹ at 323.15 K and 15.330 kJ·mol⁻¹ at 323.25 K, respectively.

2-Naphthalenamine

No low-temperature heat capacity measurements have been reported. The enthalpy of fusion reported by Khetarpal *et al.* (1979-205) was 23.610 kJ·mol⁻¹ at 386.15 K.

9-Methylcarbazole

Messerly *et al.*, (1988-93) measured the low-temperature heat capacity in the condensed phase from 13 to

388 K. They also determined the enthalpy of fusion and the triple point temperature. The values of thermodynamic functions calculated by Messerly *et al.* (1988-93) were corrected from IPTS-68 to ITS-90 and the corrected and original heat capacity and entropy values agree at 298.15 K. Recently Callanan *et al.*, (1992-4) measured the low-temperature heat capacity in the solid state from 9 to 344 K by adiabatic calorimetry and from 130 to 340 K by scanning calorimetry and the values obtained using adiabatic calorimetry are slightly greater than those determined by Messerly *et al.* for most temperatures higher than 30 K. These differences could be caused by different thermal histories of the samples used.

3.8. Ideal Gas Thermodynamic Properties

The statistical mechanical methods used for calculating the ideal gas thermodynamic properties in the temperature range 0 to 1500 K at 1 bar are similar to those discussed in previous publications (1986-87, 1990-83), where textbooks and pertinent review articles on statistical mechanical methods are cited.

The evaluation of translational, molecular rotational, and vibrational contributions to the thermodynamic properties of each compound were based on a rigid-rotor and harmonic-oscillator model. The calculations required the molar mass (M), the three principal moments of inertia (I_a , I_b , and I_c) and a complete set of fundamental vibrational frequency assignments. The total number of frequencies required was $3N-3-L$ where N is the number of atoms in each molecule and L is the number of degrees of freedom treated as special inversion or rotational contributions. Contributions from internal rotations of the -NH₂ and the -CH₃ groups, and in the case of 1- and 2-naphthalenamine, contributions from inversion about the nitrogen atom were evaluated separately. Methods for treating inversion have been given by Lister *et al.* (1978-125) and by Wollrab (1967-314).

The contributions of internal rotation and inversion were obtained from direct sums of the partition function with energy levels generated from solutions to the Schrödinger wave equation. The internal rotational potential function used in the Hamiltonian for these calculations was

$$V_{r(\theta)} = \frac{1}{2} V_n (1 - \cos n\theta), \quad (15)$$

where the coefficients V_n are summarized in Table 23, and θ is the angle of internal rotation.

The procedures used for generating the internal rotation energy levels were the same as those employed by Lewis *et al.* (1972-222). Where available, the value of each internal rotational constant (F) was obtained from microwave spectroscopy. If this constant was unavailable, it was calculated from the reduced moment of inertia (I_r) of the rotating group, from

$$F = h/8\pi^2 c I_r, \quad (16)$$

where the value of I_r was calculated from molecular structural parameters. These parameters were either taken from values obtained from spectroscopic measurements or estimated by comparison with those from structurally related molecules. The internal rotation barrier height was usually determined from microwave spectra. Otherwise, it was derived from the observed torsional frequency, $\nu_{\text{tor}}(0 \rightarrow 1)$ (1961–200).

The energy levels for inversion about the nitrogen atom were determined for 1- and 2-naphthalenamines using procedures developed by Laane (1970–13). For 1-butanamine, 2-butanamine, 2-methyl-1-propanamine and 2-methyl-2-propanamine only a simple harmonic-wagging (vibrational) motion was considered.

In the case of piperidine, where vibrational frequency assignments and structural data were available for each rotational conformer (equatorial/axial and twist-boat), the conformers were treated as different species, and the total contributions were taken to be those for the equilibrium mixture. The differences in energy between the conformers and the degeneracy of the configurations were used to determine the composition of the mixture. The thermodynamic properties for the equilibrium mixtures of the conformers were calculated by conventional thermodynamic equilibrium calculations.

Thermodynamic functions of 9-methylcarbazole were calculated by an incremental procedure because of the lack of spectroscopic measurements.

For evaluation of $\Delta_f H_m^\circ(T)$ and $\Delta_f G_m^\circ(T)$, the values of $\Delta_f H_m^\circ(298.15 \text{ K})$ were those of Table 11. The thermal functions for the elements C(graphite), $\text{H}_2(\text{g})$ and $\text{N}_2(\text{g})$ were those listed in the TRC Thermodynamic Tables–Non–Hydrocarbons (1988–192) adopted from the JANAF Thermochemical Tables (1985–249). The calculated heat capacity and entropy values are compared with available experimental results for each substance. They are also compared with other literature values obtained from computational methods. For the comparisons with entropy values obtained from condensed phase heat capacities, values of entropies of vaporization, expansion and recompression were determined with the selected values in this report.

The details of the selection of data required for the calculations for each compound are discussed below.

1-Butanamine

The molecular structure of 1-butanamine has not been determined experimentally. Estimated molecular parameters (1971–155) were used to calculate the values of I_a , I_b , and I_c and reduced moments of inertia I_r for the $-\text{CH}_3$, $-\text{C}_2\text{H}_5$, $-\text{C}_3\text{H}_7$ and $-\text{NH}_2$ rotations (see Table 23). The valence angle of $\text{H}-\text{N}-\text{C}$ was taken as 108° . The symmetry number of the external rotation is one while the symmetry numbers of internal rotation of the $-\text{CH}_3$, $-\text{C}_2\text{H}_5$, $-\text{C}_3\text{H}_7$ and $-\text{NH}_2$ groups are three, one, one, and one, respectively.

Two conformers can be formed by the internal rotation around the C_1-C_2 bond (*trans*- and *gauche*- mutual positions of $-\text{C}_2\text{H}_5$ and $-\text{NH}_2$ groups). Scott (1971–155) could

not find any difference in their stability for 1-propanamine though Profeta and Allinger (1985–281) calculated the *gauche*-isomer to be less stable by $2.72 \text{ kJ}\cdot\text{mol}^{-1}$ using molecular mechanics. The coefficients of the potential function (Table 23) have been calculated using a barrier of $9.54 \text{ kJ}\cdot\text{mol}^{-1}$ for the *trans*-isomer which corresponds to the value reported by Scott (1971–155).

The internal rotation around the C_2-C_3 bond is “butane” like. Therefore we have taken the potential function used by Chen *et al.* (1975–63) for butane which has a more stable *trans*-isomer by $3.18 \text{ kJ}\cdot\text{mol}^{-1}$ with a barrier of $14.64 \text{ kJ}\cdot\text{mol}^{-1}$.

Only one isomer can be formed by rotation around the C_3-C_4 bond. We have used a “butane” like barrier of $15.81 \text{ kJ}\cdot\text{mol}^{-1}$ to obtain the potential for this rotation.

There are two possible conformers for rotation around the C_1-N bond with *trans*- and *gauche*- mutual positions of the $-\text{C}_3\text{H}_7$ group and the unshared pair of electrons in the $-\text{NH}_2$ group. Scott (1971–155) found no evidence from infrared spectroscopy that either form was more stable in 1-propanamine. We have assumed that these two isomers will be equally stable in 1-butanamine on the basis of its similarity with 1-propanamine. The barrier of this rotation was accepted as $7.46 \text{ kJ}\cdot\text{mol}^{-1}$, the value for 1-propanamine.

Krueger and Smith (1967–254) and Stewart (1959–318) have assigned fundamentals for the $\text{N}-\text{H}$ and some $\text{C}-\text{N}$ vibrations. There have been no other investigations of the infrared and Raman spectra of 1-butanamine. Therefore, we included some 30 fundamentals of 1-propanamine (1990–83) and 8 fundamentals for the CH_2 group (the internal rotation mode has already been included); 2950, 2950, 1450, 1350, 1150, 950, 750, 370 cm^{-1} , to calculate the vibrational contribution to the thermodynamic functions. The NH_2 breathing mode was treated as a harmonic oscillation rather than an inversion mode.

The values of the thermodynamic functions for 1-butanamine in the ideal gas state are presented in Table 13. The comparison of our values of $C_{p,m}$ and S_m° at 300 K with values calculated earlier using the statistical mechanics method follows (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 117.24, 331.66 (1968 224); 119.05, 363.76 (1969–147); 119.99, 365.42 (this work).

2-Butanamine

The molecular parameters of 2-butanamine were taken to be the same as for 1-butanamine. The moments of inertia for the external rotation and moments of inertia I_r for the $-\text{C}_2\text{H}_5$, $-\text{NH}_2$, and the two $-\text{CH}_3$ rotations were calculated from these molecular parameters (Table 23). The symmetry number of the external rotation is one and the symmetry number of internal rotation of each $-\text{CH}_3$ group is 3.

Only one conformer can exist for the internal rotation around the C_1-C_2 bond. Earlier we used $17.88 \text{ kJ}\cdot\text{mol}^{-1}$ and $15.09 \text{ kJ}\cdot\text{mol}^{-1}$ as the barriers for rotations around the C_1-C_2 and C_2-C_3 in 2-propanamine (1990–83). Now we use the average of these two values ($16.5 \text{ kJ}\cdot\text{mol}^{-1}$) as

a barrier of internal rotation around the C₁-C₂ bond in 2-butanamine.

There is a possibility that three conformers resulting from the rotation around the C₂-C₃ bond (*gauche-trans*, *trans-gauche* and *gauche-gauche*) coexist. Profeta and Allinger (1985-281) calculated the potential energy of the conformer with the *gauche* position of the CH₃ and NH₂ groups in 1-propanamine (2.72 kJ·mol⁻¹) by molecular mechanics. Chen *et al.* (1975-63) adopted 3.18 kJ·mol⁻¹ for the potential energy of the conformer with a *gauche* position of the two CH₃ groups in butane. We have accepted 5.9 kJ·mol⁻¹ as the potential energy of the *gauche-gauche* conformer for internal rotation in the molecule of 2-butanamine using an approach of additivity of *gauche* interactions. To simplify an expression for the potential function of this rotation we assumed the stability of *gauche-trans* and *trans-gauche* configurations to be equal (considering their relative potential energies as zero). The relative potential energy of the *gauche-gauche* conformer was taken as (2.72 + 3.18)/2 = 2.95 kJ·mol⁻¹. The potential barrier of rotation of this conformer can be considered as "butane" like, that is ~14.6 kJ·mol⁻¹.

Only one isomer can be formed by rotation around the C₃-C₄ bond. We used a "1-propanamine" like barrier of 15.81 kJ·mol⁻¹ to obtain the potential function of this rotation.

There are two energetically different conformers (*gauche-gauche* and *gauche-trans*) for rotation around the C₂-N bond. We accepted the same difference in their stability (1.75 kJ·mol⁻¹) and the same shape of the potential function (a barrier of rotation of the *gauche-trans* conformer of ~11.7 kJ·mol⁻¹) as for 2-propanamine (1990-83).

Stewart (1959-318) has assigned the fundamentals of the -NH₂ bending and C-N stretching modes for 2-butanamine. He showed that the infrared spectrum of 2-butanamine was very similar to that of 2-propanamine. Therefore we have adopted for 2-butanamine the 30 fundamentals of 2-propanamine (1990-83) and the 8 fundamentals for the -CH₂ group (see 1-butanamine). The -NH₂ breathing mode was treated as a wagging vibration.

The thermodynamic functions for 2-butanamine in the ideal gas state are given in Table 13. The comparison of our values of $C_{p,m}$ and S° at 298.15 K with results reported by Stull *et al.* (1969-147) is as follows (in J·K⁻¹·mol⁻¹): 117.14, 351.04 (1969-147); 120.48, 354.19 (this work).

2-Methyl-1-propanamine

The same molecular parameters for 2-methyl-1-propanamine were used as for 1-butanamine. The values of I_a , I_b , and I_c and reduced moments of inertia I_r for *iso*-C₃H₇, -NH₂ and the two -CH₃ groups are summarized in Table 23. The symmetry number of the external rotation is one and the symmetry number of internal rotation of each -CH₃ group is three.

Three conformers can be formed from the internal rotation around the C₁-C₂ bond (*trans-gauche*, *gauche-trans* and *gauche-gauche*). We assumed that the potential

energies of the *trans-gauche* and *gauche-trans* rotamers should be very close and approximately equal to the potential energy of the *gauche*-conformer of 1-propanamine (2.72 kJ·mol⁻¹). The potential energy of the *gauche-gauche* rotamer of 2-methyl-1-propanamine is assumed to approach (2.72) × 2 = 5.44 kJ·mol⁻¹. Consequently the relative potential energies of the *trans-gauche* and *gauche-trans* rotamers can be taken as zero and the potential energy of the *gauche-gauche* form taken as 2.72 kJ·mol⁻¹. The comparison of the barriers of rotation around the C₁-C₂ bond for 2-methylpropane (1975-63) and propane (1973-78) shows that the difference between them is 2.34 kJ·mol⁻¹. We assumed the same difference between the barriers of rotation around the C₁-C₂ bond for 2-methyl-1-propanamine and propanamine. Using the value of the barrier of propanamine from (1990-83) (9.54 kJ·mol⁻¹) we calculated the barrier of rotation of the *gauche-gauche* conformer of 2-methyl-1-propanamine around the C₁-C₂ bond as (9.54 + 2.34 = 11.88) kJ·mol⁻¹.

The internal rotation around the C₂-C₃ bond results in only one conformer. We have assumed that the substitution of a methyl-group by an amino-group will not influence the barrier of this rotation significantly (a comparison of the barriers of rotation around the C₂-C₃ bond for 2-methylpropane and 2-methyl-1-propanamine confirms this assumption (1975-63, 1990-83)). We have used 16.1 kJ·mol⁻¹ as the barrier in 2-methyl-1-propanamine. The same value was used for the barrier for the C₂-C₄ bond.

We considered that the *gauche*- and *trans*- rotamers for rotation around the C₁-N bond to be equally stable. Craven and Bentley (1972-169) observed the torsional wavenumber for this rotation as 225 cm⁻¹ which gives 7.95 kJ·mol⁻¹ as a barrier of rotation.

30 modes of 2-propanamine (1990-83) and 8 modes of the CH₂ group (see 1-butanamine) were adopted as the fundamental wavenumbers of 2-methyl-1-propanamine. Exceptions were made for the C-N stretching and the NH₂ bending vibrations assigned for 2-methyl-1-propanamine by Stewart (1959-318). The inversion of the NH₂ group was considered as a wagging vibration.

The values of the thermodynamic functions for 2-methyl-1-propanamine in the ideal gas state are summarized in Table 13.

2-Methyl-2-propanamine

The same molecular parameters as for the other butanamines were used to calculate the values of I_a , I_b , and I_c and the reduced moments of inertia I_r for the -NH₂ and three -CH₃ rotations (see Table 23). The symmetry number of the external rotation is three and the symmetry number for the internal rotation of each -CH₃ group is three.

Scott and Crowder (1968-227) observed two prominent infrared bands at 279 and 274 cm⁻¹. Scott (1971-155) and Durig *et al.* (1973-288) assigned 279 cm⁻¹ as the A" torsional mode. Scott (1971-155) assigned to the other A" torsion the band at 251 cm⁻¹ in order to obtain consis-

tency between calculated and experimental results. We assumed that both torsions should have the same potential due to symmetry. Therefore we assumed that the second A'' torsion corresponds to the band at 274 cm^{-1} . In this case the average barrier of rotation around the C_1-C_2 and the C_2-C_3 bonds should be $20.46\text{ kJ}\cdot\text{mol}^{-1}$. Scott and Crowder (1968–227) also observed bands at 195 and 200 cm^{-1} . Scott (1971–155) assigned 200 cm^{-1} to the A' torsion while Durig *et al.* (1973–288) preferred 195 cm^{-1} . We have adopted 195 cm^{-1} for this torsion. This assignment gives $10.42\text{ kJ}\cdot\text{mol}^{-1}$ for the barrier of rotation around the C_2-C_4 bond.

Scott (1971–155) assigned the torsion for the $-\text{NH}_2$ group at 253 cm^{-1} but Tsuboi *et al.* (1968–227) and Durig *et al.* (1973–288) proposed the $240\text{--}245\text{ cm}^{-1}$ region for this torsion. Craven and Bentley (1972–169) found that the isotopic shift was too big if the $-\text{NH}_2$ torsion corresponded to 256 cm^{-1} . Thus we have adopted 240 cm^{-1} for this torsion which corresponded to $9.69\text{ kJ}\cdot\text{mol}^{-1}$ for the barrier of rotation around the C_2-N bond.

The far infrared spectra of 2-methyl-2-propanamine was studied by Scott and Crowder (1968–227). Stewart (1959–318) assigned the NH_2 vibrations. Later Scott (1971–155) assigned all the fundamentals by normal coordinate analysis. We used his assignment to calculate the vibrational contributions to the thermodynamic functions of 2-methyl-2-propanamine.

The values of the thermodynamic functions for 2-methyl-2-propanamine in the ideal gas state are presented in Table 13. A comparison of our values of $C_{p,m}$ and S_m° at 298.15 K with those calculated by Scott (1971–155), the experimental results of Finke *et al.* (1972–140) and the experimental results evaluated in this work follows (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 120.5 , 327.6 (1971–155); $-$, 327.73 (1972–140); $-$, 327.65 (experimental evaluated results from this work); 120.44 , 327.58 (our statistical-mechanical calculation).

Pyrrole

Several investigations (1956–652, 1969–107, 1974–232, 1988–154) of the microwave spectra of pyrrole give approximately the same values for the rotational constants. We have calculated the principal central moments of inertia (Table 23) using the experimental results reported by Włodarczak *et al.* (1988–154). Our calculations showed that similar values of I_a , I_b , and I_c can be obtained using the following valence angles: H-C-N , 123.5° ; N-C-C , 107.7° ; and C-C-C , 107.2° . These parameters were used to calculate the moments of inertia of the alkyl-derivatives of pyrrole. The symmetry number for the external rotation is 2.

The assignment of the fundamental vibrational modes for pyrrole has been done by Lord and Miller (1942–328), Morcilio and Orza (1960–372, 1960–373), Scott (1971–76), and Lautie and Novak (1972–297). Later Cataliotti and Paliani (1976–12) and Navarro and Orza (1983–105, 1983–106) made new assignment for the C-H and N-H stretching modes. We have adopted the assignments of Navarro and Orza (1983–105, 1983–106) for the stretch-

ing C-H and N-H modes. All others assignments were adopted from Scott (1971–76).

The values of the thermodynamic functions for pyrrole in the ideal gas state are summarized in Table 13. A comparison of the experimental and calculated values of the entropy for the ideal gas state at 362.11 K and 1 bar reported by Scott *et al.* (1967–116) with our results follow; (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 286.10 (experimental 1967–116); 285.94 (calculated 1967–116); 286.19 (this work). Heat capacities at 388.20 K (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 93.85 (experimental 1967–116); 93.97 (calculated 1967–116); 94.28 (this work). The entropy value at 298.15 K calculated on the basis of experimental data evaluated in this work agrees with the result of our statistical mechanical calculation within the limits of experimental errors (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 270.42 and 270.72 respectively.

1-Methylpyrrole

The structural parameters of 1-methylpyrrole were determined by Vilkov *et al.* (1962–392) from electron diffraction results. Arnold *et al.* (1968–63) reported values of the rotational constants based on microwave spectra. These results were used to calculate the moments of inertia of 1-methylpyrrole (Table 23). The symmetry number for the external rotation is two and the symmetry number of rotation of the CH_3 group is three.

A very small barrier of $\sim 0.5\text{ kJ}\cdot\text{mol}^{-1}$ for the rotation around the C_5-N bond has been determined by Arnold *et al.* (1968–63). We accepted this value for the V_e constant.

Scott (1971–76) made an assignment of the fundamental vibrational modes for 1-methylpyrrole. We modified this assignment (Table 24) to obtain better consistency with the experimental results (1988–93).

The values of the thermodynamic functions for 1-methylpyrrole in the ideal gas state are given in Table 13. A comparison of the results for the entropy at 300 K is given below (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 308.17 (experimental 1988–93); 308.01 (calculated 1971–76); 308.30 (this work). The entropy value at 298.15 K calculated on the basis of experimental data evaluated in this work agrees with the result of our statistical mechanical calculation within the limits of experimental errors (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 307.44 and 307.72 respectively.

2-Methylpyrrole

The values of the valence angles in the pyrrole ring (see discussion on pyrrole above) were used to calculate the moments of inertia of the external rotation and the rotation of the CH_3 group. The length of the C_5-N bond was accepted as $1.49\text{ \AA}$. The symmetry number for the external rotation is one and the symmetry number for the CH_3 rotation is three.

We assumed free rotation around the C_5-N bond in accordance with the very small value of the barrier of internal rotation for 1-methylpyrrole. The assignments of the vibrational modes reported by Scott (1971–76) were adopted in this work and the values of the thermodynamic functions for 2-methylpyrrole in the ideal gas state

are presented in Table 13. There is no other literature values for comparison.

3-Methylpyrrole

The same structural parameters as for 2-methylpyrrole were used to calculate the moments of inertia for the external and internal rotation in 3-methylpyrrole (Table 23). The symmetry number for external rotation is one and the symmetry number of the rotation of the CH_3 group is three.

The model of free internal rotation has been used and the wavenumbers reported by Scott (1971–76) were adopted for the calculation of the vibrational contribution to the thermodynamic functions of 3-methylpyrrole. The values of the thermodynamic functions in the ideal gas state are summarized in Table 13. There is no other literature values available for comparison.

Pyridine

The results of the microwave spectroscopic studies reported by Bak *et al.* (1958–367), Sorensen (1967–294), Sorensen *et al.* (1974–231), Mato *et al.* (1977–40), Heineking *et al.* (1986–222), and Wlodarczak *et al.* (1988–154) are very similar. We have adopted the values of Wlodarczak *et al.* (1988–154) to calculate the moments of inertia of pyridine. The symmetry number for the external rotation is two.

Kline and Turkevich (1944–85) made the first assignment of the fundamentals for pyridine and calculated the thermodynamic properties. Corrsin *et al.* (1953–285 and 1953–708) reassigned the vibrational modes. McCullough *et al.* (1957–176) adjusted the assignment reported by Corrsin *et al.* (1953–285 and 1953–708) to obtain consistency with heat capacity measurements. Wilmshurst and Bernstein (1957–60) presented new assignment of the out-of-plane vibrational modes and the results obtained by Long *et al.* (1963–359), Stidham and DiLella (1979–272 and 1980–201), DiLella and Stidham (1980–115) and DiLella (1980–42) confirmed the assignment reported by Wilmshurst and Bernstein (1957–60). Wong and Colson (1984–273) made high resolution infrared spectral studies to further define the assignment in the C–H region and refine all the normal modes. Wiberg *et al.* (1984–191), Pondor *et al.* (1984–21 and 1985–415), and Walters *et al.* (1986–174) confirmed the assignments made by Wong and Colson (1984–273) which were adopted in this work (Table 24).

The values of the thermodynamic functions for pyridine in the ideal gas state are given in Table 13. Our results coincide with the experimental values within their uncertainties. For example (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$), the entropy at 298.15 K: 284.80 (1957–374), 282.75 (this work); entropy at 346.65 K: 295.73 (1957–176), 295.47 (this work); heat capacity at 374.2 K: 99.54 (1957–176), 98.91 (this work). The results of this work are also in a good agreement with previous statistical calculations. The comparison of the entropy in the ideal gas state at 300 K and 1 bar follow (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 285.02 (1944–85); 284.11 (1957–374); 283.35 (1957–176); 283.02 (1980–42); 283.27 (this work). The entropy value at 298.15 K calcu-

lated on the basis of experimental data evaluated in this work agrees with the result of our statistical mechanical calculation within the limits of experimental errors (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 282.00 and 282.75 respectively.

2-Methylpyridine

Dreizler *et al.* (1970–142) have reported the values of the moments of inertia for the external and internal rotations and the coefficients of the potential function for rotation around the $\text{C}_1\text{--C}_6$ bond based on results of their microwave spectra measurements. Their values were adopted except that the value of the V_6 coefficient was decreased slightly to avoid a small negative potential complicating the calculation of the thermodynamic functions. This is an essentially free internal rotor and confirms our assumption made for 2-methylpyrrole. The symmetry number of external rotation is one and the symmetry number of the CH_3 group is three.

Earlier Scott *et al.* (1963–156), Green *et al.* (1963–274), Pandey and Tripathi (1971–173), and Berezin and Elkin (1972–149) studied the infrared and Raman spectra of 2-methylpyridine. Assignments made initially by Scott *et al.* (1963–156) were changed by Draeger (1983–40) and by Lamba *et al.* (1983–107). We adopted the assignments made by Draeger because they gave better agreement with the thermodynamic measurements compared with those calculated from (1983–107).

The values of the thermodynamic functions for 2-methylpyridine in the ideal gas state are presented in Table 13. Comparison of our results with other sources is given for the entropy at 359.36 K and for the heat capacity at 413.20 K (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 345.97, 137.70 (experimental 1963–156); 345.72, 137.65 (calculated 1963–156); 345.47, 137.50 (this work). Both calculations are in agreement with the experimental results within experimental errors. The entropy value at 298.15 K calculated on the basis of experimental data evaluated in this work agrees with the result of our statistical mechanical calculation within the limits of experimental errors (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 325.51 and 324.93 respectively.

3-Methylpyridine

The molecular parameters of 3-methylpyridine have been estimated on the basis of the structure of the unperturbed pyridine ring, using the following values for the angles and bond lengths: $\text{C}_2\text{--C}_6$ bond length of 1.53 Å, $\text{C}_6\text{--H}$ (in methyl group) bond length of 1.096 Å, and $\text{C}_2\text{--C}_6\text{--H}$ angle of 109.5°. Moments of inertia of the external and internal rotation calculated from these molecular parameters are summarized in Table 23. The symmetry number for the external rotation is one and the symmetry number of the CH_3 group is three.

Prager *et al.* (1978–50) studied the internal rotation in liquid 3-methylpyridine using nuclear magnetic resonance and inelastic neutron scattering methods. The two methods gave conflicting results. For example, the values of coefficients of the potential function for rotation of the CH_3 group determined from inelastic neutron scattering measurements were ($V_3 + V_6$) = 4.54 $\text{kJ}\cdot\text{mol}^{-1}$ while

nuclear magnetic resonance measurements gave $V_3 = 1.90 \text{ kJ}\cdot\text{mol}^{-1}$. These values do not look reasonable compared with barriers in other methylpyridines. Therefore we assumed a free rotation of the CH_3 group in 3-methylpyridine.

Green *et al.* (1963–274), Scott *et al.* (1963–157), Gandolfo and Zarembowitch (1977–120), Draeger (1983–40), and Lamba *et al.* (1983–107) made a complete vibrational analysis of 3-methylpyridine. The results reported by Green *et al.*, Gandolfo and Zarembowitch, and Lamba *et al.* give almost the same thermodynamic results which are slightly different compared to those calculated by Draeger (1983–40). We adopted the wavenumbers by Draeger (1983–40) for the calculation of vibrational terms of the thermodynamic functions.

The values of the thermodynamic functions for 3-methylpyridine in the ideal gas state are summarized in Table 13. Comparison of our results with other sources for the entropy at 372.45 K and for the heat capacity at 404.2 K follow: (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 350.28, 134.47 (experimental 1963–157); 349.87, 134.43 (calculated 1963–157); 350.32, 134.77 (this work). The entropy value at 298.15 K calculated on the basis of experimental data evaluated in this work agrees with the result of our statistical mechanical calculation within the limits of experimental errors (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 325.50 and 325.43 respectively.

4-Methylpyridine

Rudolph *et al.* (1967–165) studied the microwave spectra of 4-methylpyridine. They reported the values of moments of inertia for the external and internal rotations and the barrier for rotation of the CH_3 group. Their values of moments of inertia were accepted in this work (Table 23). Coefficients of the potential function of internal rotation are very small according to (1967–165) ($V_3 = 0$, $V_6 = 0.056 \text{ kJ}\cdot\text{mol}^{-1}$) hence this can be considered as a free rotator. Results of Rudolph *et al.* (1967–165) are in a good agreement with the values reported by Zweers *et al.* (1974–94) and Moffat (1976–66). The symmetry number for the external rotation is 2 while the symmetry number of rotation of the CH_3 group is three.

Earlier partial or total assignments of vibrational modes were made by Green *et al.* (1963–274), Long and George (1963–375), Pandey and Tripathi (1971–173), Berezin and Elkin (1972–149), and Draeger and Scott (1981–46). Comparison of results from the latest assignments, (1983–40) and (1983–107), shows that the assignment made by Draeger (1983–40) leads to an overestimation of the heat capacity compared to the experimental results (1981–44) while the assignment reported by Lamba *et al.* (1983–107) corresponds to an underestimation. The primary difference between these two assignments is in the B_2 modes. Therefore we have adopted the assignments of Draeger (1983–40) but have shifted the wavenumber for the B_2 mode from 969 cm^{-1} to 1053 cm^{-1} to obtain better consistency with experiment. Lamba *et al.* (1983–107) reported this value as 1110 cm^{-1} . Note that Long *et al.* (1963–375) assigned this mode to 1068 cm^{-1} .

Comparison of our entropy values at 298.15 K and heat capacity at 401.15 K with the experimental results (1981–44) and with the results of previous calculations follow: (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 319.4, 133.61 (1981–46); –, 134.02 (1983–40); –, 133.01 (1983–107); 318.6, 133.45 (1981–44); 318.16, – (this work, based on evaluated experimental data); 319.52, 133.57 (this work).

Pyrrolidine

There is conflicting information in the literature regarding the structure of pyrrolidine. Thermodynamic studies (1959–375, 1959–374, 1959–355) indicate a puckered five-membered ring with free or almost free pseudo-rotation. Pitzer and Donath (1959–370) and Profeta and Allinger (1985–281) predict that the twist conformer is the most stable form. From vibrational spectroscopy, Baldock *et al.* (1968–402) considered a mixture of various conformers of similar energy, Krueger and Jan (1970–344) assumed a mixture of two twist conformers, while Tran *et al.* (1973–331) found that the vibrational wavenumbers were not sensitive to the axial or equatorial position of the imino hydrogen. Proton NMR studies (1974–245) did not throw light on the conformation problem. Recently, Pfafferott *et al.* (1985–1415) carried out *ab initio* and electron diffraction studies and found that the envelope conformation with the imino H in the axial position to be the most stable conformer. The *ab initio* calculations predicted a second conformer, with the imino H in the equatorial position. The energy difference between these two conformers is predicted to be about $4.06 \text{ kJ}\cdot\text{mol}^{-1}$ and the barrier to pseudo-rotation to be $6.94 \text{ kJ}\cdot\text{mol}^{-1}$. The low temperature dielectric relaxation study of Gilchrist *et al.* (1988–837) also indicates an envelope structure for pyrrolidine. They reported the pseudo-rotational potential parameters, $V_1 = 4.06 \text{ kJ}\cdot\text{mol}^{-1}$ and $V_2 = 4.69 \text{ kJ}\cdot\text{mol}^{-1}$. The microwave studies of Pfafferott *et al.* (1985–1415) and Ehrlichmann *et al.* (1989–1058) reported the existence of only one conformer, the envelope form with the imino H in the axial position. Pfafferott *et al.* (1985–1415) comment, that if the equatorial conformer exists, its rotational spectrum is very weak and the energy difference between the two isomers could not be estimated. In this work we assume the existence of only axial conformer. The rotational constants reported by Ehrlichmann *et al.* (1989–1058) were used to calculate the moments of inertia (Table 23). The symmetry number of external rotation is one.

The vibrational fundamental wavenumbers reported in the literature (1940–379, 1952–691, 1959–375, 1959–355, 1973–331, 1980–226 and 1983–268) for the axial conformer of pyrrolidine with C_s symmetry were critically analyzed. Pfafferott *et al.* (1985–1415) reported that the ring mode assigned to 290 cm^{-1} (1983–268) is the overtone and not the fundamental wavenumber. In fact, normal coordinate analysis gave 166 cm^{-1} (1973–331) and 174 cm^{-1} (1980–226) for this mode. Earlier, McCullough *et al.* (1959–355) and Evans and Wahr (1959–375) had used 300 cm^{-1} for this mode. The remainder of the

fundamentals adopted here are those reported by McCullough *et al.* except for 980 and 990 cm^{-1} which are replaced by 1136 cm^{-1} and 1171 cm^{-1} which were reported by Evans and Wahr. McCullough *et al.* assumed the latter pair of fundamental wavenumbers to be the combination band with 300 cm^{-1} which is not a fundamental mode. It was found that 50 cm^{-1} for the ring puckering mode gave the best agreement between experimental and calculated $C_{p,m}$ and S_m° . This wavenumber was used to obtain $V_2 = 3.35 \text{ kJ}\cdot\text{mol}^{-1}$ with $I_r = 11.19 \times 10^{-40} \text{ g}\cdot\text{cm}^2$ and these values were used to calculate pseudo-rotational energy levels. The adopted fundamental wavenumbers are given in Table 24.

Assuming only an axial conformer and the pseudo-rotational energy levels, the ideal gas thermodynamic properties were calculated (Table 13). Hildenbrand *et al.* (1959–374) reported only the third law entropies, while McCullough *et al.* (1959–375) reported the vapor heat capacities and the third law entropies. It was found that, if the equatorial conformer was assumed to be present as determined by Pfaferott *et al.* (1985–1415) from their *ab initio* calculations, the calculated heat capacity was too high by about 6 $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and hence the existence of only an axial conformer was assumed. A comparison of the experimental and calculated values presented below for the entropy at 298.15 K and for the heat capacity at 350.2 K (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 309.73, – (1959–374); 309.43, 98.37 (experimental 1959–355); 309.62, 98.28 (calculated 1959–355); 309.74, – (1959–375); 309.40, – (this work, based on evaluated experimental data); 309.21, 98.33 (this work, statistical mechanical calculation).

Piperidine

Various workers have used IR and NMR spectral studies and calculations to show that the equatorial chair conformer is more stable than the axial chair conformer (1968–401, 1968–402, 1968–297, 1970–343, 1970–344, 1971–210, 1975–286, 1976–292, 1976–134, 1976–211, 1977–254, 1981–200, 1983–184 and 1985–1414). The possibility of the existence of a boat form (1971–343) and twist-boat form (1974–320) has been reported. From the structural studies reported in the literature (1968–297, 1969–334, 1976–134, 1981–200, 1983–184 and 1989–1059), we have selected the rotational constants reported by Ehrlichmann *et al.* (1989–1059) to obtain the moments of inertia of the equatorial and axial chair conformers. The twist-boat conformers with three NH orientations (1967–439) were assumed to be present in the equilibrium mixture. The average values of the moments of inertia are given in Table 23. The symmetry number of external rotation is one.

The vibrational wavenumbers available in the literature (1929–352, 1932–332, 1936–443, 1936–464, 1937–515, 1966–583, 1967–438, 1971–210, 1971–343, 1976–211, 1980–227, 1980–228 and 1983–187) were critically evaluated and those reported by Muldagaliev and Ignat'ev (1983–187) were selected for the equatorial and axial conformers. For the twist-boat conformer, the fundamental wavenumbers were transferred from the equatorial as

very little difference was found between the equatorial and axial conformers. The vibrational wavenumbers are presented in Table 24.

Piperidine exists as the mixture of conformers. The conversion between the conformers can take place by inversion of the ring or at the nitrogen atom. As mentioned above, various workers have reported the energy difference between the equatorial and axial conformers. In this work, we have selected $\Delta E_m = 3.07 \text{ kJ}\cdot\text{mol}^{-1}$, obtained from microwave spectral measurement (1981–200). Though experimental evidence for the existence of the twist-boat conformer is not available, some literature sources indicate the possibility of its existence (1967–440 and 1974–320). Scott (1971–210) assumed the existence of a boat form with $\Delta E_m = 23 \text{ kJ}\cdot\text{mol}^{-1}$ which was transferred from cyclohexane. We found that $\Delta E_m = 15 \text{ kJ}\cdot\text{mol}^{-1}$ gave the best agreement between the experimental and calculated $C_{p,m}$ and S_m° values. In the chair conformation only two positions are available for the NH orientation (equatorial and axial), while in the twist-boat conformation three (pseudo-equatorial, pseudo-axial and isoclinal (1967–439 and 1974–320)) positions are available. For all three twist-boat conformers $\Delta E_m = 15 \text{ kJ}\cdot\text{mol}^{-1}$ was adopted.

The ideal gas thermodynamic properties were calculated for the equilibrium mixture of chair-equatorial, chair-axial, twist-boat-equatorial, twist-boat-axial and twist-boat-isoclinal conformers (Table 13). Recently, Hossenlopp and Archer (1988–556) and Messerly *et al.* (1988–93) reported the vapor heat capacities and the third law entropies, respectively. As the ΔE_m for the twist-boat conformers was not available, it was adjusted to obtain the best fit between the experimental and the calculated thermodynamic properties. Earlier, Scott (1971–210) used the same value as for cyclohexane and adjusted the values with an empirical anharmonicity correction. A comparison between calculated and experimental values of the entropy at 298.15 K and the heat capacity at 368.2 K (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$) follows: 315.56, 134.14 (1971–210); 315.23, – (1988–93); –, 134.16 (1988–556); 315.39, – (this work, based on evaluated experimental data); 315.06, 135.45 (this work, statistical mechanical calculation).

Indole

Philips and Levy (1986–783) reported the rotational constants and the possible molecular parameters from the rotationally resolved electronic spectrum in the gas phase. More recently, Suenram *et al.* (1988–552) reported more accurate rotational constants and the molecular parameters from high resolution microwave spectrum.

Indole belongs to the C_s point group with a symmetry number of 1 having 29 A' and 13 A'' vibrational modes. Lautie *et al.* (1980–104) studied the infrared spectra in the gas and solution phase and the Raman spectra in both the liquid and crystal phase of indole and its deuterated species and reported a complete set of vibrational

frequencies. Recently, Harada *et al.* (1986–1113) found that indole gave strong doublet peaks around 1355 to 1332 cm^{-1} and these were assigned as two fundamental vibrations. This was confirmed by the normal coordinate analysis by Takeuchi and Harada (1986–785). Smithson *et al.* (1984–479) published a far-infrared vapor spectrum of indole and Suwaiyan and Zwarich (1986–479) published a crystal phase infrared and Raman study. Recently Collier (1988–553) studied the IR spectra in liquid, vapor, solid and solution phase and the Raman spectra in the liquid and vapor phase and reported the most reliable set of vibrational frequencies which are adopted in this work (Table 24).

The ideal gas thermodynamic properties of indole are reported in Table 13. The third law entropies for indole reported by Collier (1988–553) were obtained by deducting CH_2 -increment from the values for 2-methylindole at 400 and 500 K. The calculated ideal gas thermodynamic properties were reported earlier by Kudchadker and Wilhoit (1982–297). They used the molecular structure and vibrational fundamental wavenumbers of Lautie *et al.* (1980–104). The entropy values at 400 K and at 500 K are compared below (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 374.07, 415.30 (additive 1988–553); 373.82, 414.22 (statistical 1988–553); 368.91, 408.65 (1982–297); 374.07, 414.56 (this work).

Quinoline

Experimental information on the molecular structure of quinoline is not available in the literature. Wait *et al.* (1970–191) calculated the moments of inertia using an assumed molecular structure. However, it seems that they used the wrong conversion factor. Recently, Steele *et al.* (1988–551) used the same molecular structure and recalculated the moments of inertia. Our calculations agree with the latter value of the product of moments of inertia (Table 23). Quinoline has a symmetry number of one.

Steele *et al.* also reported the vapor-phase vibrational wavenumbers which are adopted in this work. Previous studies that have reported partial or complete assignments of the fundamental wavenumbers are: Luther *et al.* (1958–422), Chiorboli and Bertoluzza (1959–395), Deb (1961–73), Wait and McNearney (1970–191), Ghersesti *et al.* (1973–303) and Afifi and Shabana (1985–1397).

The ideal gas thermodynamic properties for quinoline are given in Table 13. Steele *et al.* (1988–551) obtained third law entropies at 300, 400, and 500 K from thermodynamic measurements and their spectroscopically calculated entropy values are in excellent agreement with their experimental values. Earlier Wait and McNearney (1970–191) calculated the ideal gas thermodynamic properties but they used incorrect moments of inertia. The entropy values at 300 K, 400 K, and 500 K are compared as follows: (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 343.80, 387.62, 431.27 (experimental 1988–551); 344.72, 388.37, 431.52 (calculated 1988–551); 344.88, 388.53, 431.77 (this work). The entropy value at 298.15 K calculated on the basis of experimental data evaluated in this work agrees with the result of our statistical mechanical calculation within the

limits of experimental errors (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 342.96 and 344.05 respectively.

Isoquinoline

Neither the molecular structure nor the rotational constants are available for isoquinoline. An assumed molecular structure is reported by Wait *et al.* (1970–191). However, they calculated incorrect moments of inertia. We have assumed that this error was introduced due to a wrong conversion factor of units. Recently, Steele *et al.* (1988–551) have recalculated the moments of inertia using the same structure. Our value of the product of moments of inertia coincides with the value reported by Steele *et al.* (Table 23). Isoquinoline has a symmetry number of one.

Steele *et al.* (1988–551) have also reported the vapor-phase vibrational wavenumbers which are adopted in this work (see Table 24). Previous studies that have reported partial or complete assignments of the fundamental wavenumbers are: Luther *et al.* (1958–422), Chiorboli and Bertoluzza (1959–395), Deb (1961–73), Wait and McNearney (1970–191), Chappell and Ross (1977–235) and Afifi and Shabana (1985–1397).

The ideal gas thermodynamic properties for isoquinoline are given in Table 13. Steele *et al.* (1988–551) have reported the third law entropies at 300 and 400 K. Wait and McNearney (1970–191) calculated the ideal gas thermodynamic properties with their incorrect moments of inertia. The entropy values at 300 K and at 400 K are compared below (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 340.81, 384.79 (experimental 1988–551); 345.13, 388.62 (calculated 1988–551); 345.30, 388.86 (this work). The entropy value at 298.15 K calculated on the basis of experimental data evaluated in this work agrees with the result of our statistical mechanical calculation within the limits of experimental errors (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 340.0 and 344.47 respectively (note that an uncertainty of 1.0 $\text{kJ}\cdot\text{mol}^{-1}$ in the enthalpy of vaporization can cause an uncertainty of 3.4 $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ in the ideal gas entropy at 298.15 K, see Table 10).

Carbazole

Recently, Suenram *et al.* (1988–552) studied the microwave spectrum of carbazole vapor and found the results to be consistent with a planar molecule. They reported the rotational constants which were used to obtain I_a , I_b , and I_c (Table 23). Earlier, the crystal structure was studied by the following: Kuruhashi *et al.* (1966–554), Baskak and Lahiri (1969–310), Kuruhashi *et al.* (1969–310), Robinson and Scott (1969–244), Bel'skii (1985–1398) and Gerkin and Reppart (1986–1112). The symmetry number for the external rotation of carbazole is two.

Bree and Zwarich (1968–349) studied the infrared, Raman and fluorescence spectra of carbazole crystal. Using a crude normal coordinate treatment, the assignments of wavenumbers were made. Danchinov *et al.* (1981–254) studied the infrared and Raman spectra and assigned the planar vibrational wavenumbers while Gastilovich *et al.* (1984–477) made assignments for the

nonplanar vibrational wavenumbers. Later, Danchinov *et al.* (1985–136) restudied the infrared spectrum and reassigned the planar vibrational wavenumbers. We made two statistical mechanical calculations of the thermodynamic properties of carbazole based on the different assignments. In the first case we used the inplane assignments of Danchinov *et al.* (1985–136) and the out of plane assignments of Gastilovich *et al.* (1984–477). In the second case an assignment proposed by Bree and Zwarich (1968–349) was used. The calculated values of the entropy at 298.15 K were then used to calculate the entropy of 9-methylcarbazole by an additive group method and this value was compared with the experimental value (1992–3). Better agreement was obtained from the assignments made by Bree and Zwarich (1968–349). Therefore his assignments were adopted in our work (Table 24).

The thermodynamic properties of carbazole in the ideal gas state are presented in Table 13. No experimental vapor heat capacity or third law entropies are available for comparison. The ideal gas thermodynamic properties were calculated earlier by Viswanath *et al.* (1981–257). However, in these calculations the moments of inertia were obtained from crystal structure results. The values reported in this work are more reliable. The comparison of the entropy values at 300 K follows (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 388.62 (1981–257); 389.40 (this work).

Acridine

The gas phase molecular structure and moments of inertia are not available for acridine. From a crystallography study, Philips *et al.* (1960–378) found that a symmetric unit of acridine consists of two molecules. In this work we used the average values of the weighted mean bond lengths and angles of the two types of molecules in the crystalline form II to calculate the product of the moments of inertia, see Table 23. Acridine belongs to the C_{2v} point group with symmetry number of two.

Brigodiot and Lebas (1972–247) reported a complete vibrational assignment from their infrared spectral measurements on the solid and a suspension and Raman spectral measurements on solutions. Recently, Rodziszewski and Michl (1985–150) made polarized Fourier transform infrared spectral measurements in stretched polyethylene which permitted a complete symmetry assignment for the infrared active vibrations in the 100 to 3200 cm^{-1} region. Using the information given in the above two publications we have tentatively assigned the wavenumbers for acridine, see Table 24. Other references on vibrational spectra are: Perkampus and Baumgarten (1960–379), Lebas and Josien (1962–462) and (1962–461), and Fialkovskaya and Nefedov (1968–350).

Ideal gas thermodynamic properties of acridine are reported in Table 13. Very recently, Steele *et al.* (1989–76) reported the third law entropies from 390 to 500 K. Values calculated in this work are in agreement with these third law entropies. Earlier, Viswanath *et al.* (1981–257) reported calculated ideal gas thermodynamic values

which are slightly different from the present values. The comparison of values of entropies at 400 K is given below (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 455.13 (1989–76); 453.88 (1981–257); 455.55 (this work). The entropy value at 298.15 K calculated on the basis of experimental data evaluated in this work agrees with the result of our statistical mechanical calculation within the limits of experimental errors (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 387.3 and 394.69 respectively (note, that an uncertainty of 4.0 $\text{kJ}\cdot\text{mol}^{-1}$ in the enthalpy of vaporization can cause an uncertainty of 13.4 $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ in the ideal gas entropy at 298.15 K, see Table 10).

Phenanthridine

No vapor phase structural parameters or moments of inertia are available for phenanthridine. However, Chowdhury (1973–305) reported the molecular structure from X-ray crystallographic measurements which are adopted in this work to obtain values for I_a , I_b , and I_c , see Table 23. Phenanthridine has a symmetry number of one.

No complete set of vibrational fundamental wavenumbers are available. It was found that there exists a one to one correspondence between the fundamental wavenumbers of naphthalene and quinoline and anthracene and acridine, so we expect the same to hold between phenanthrene and phenanthridine. Very scanty information is available for this molecule. Coppens and Nasielski (1961–330) reported the C–H out-of-plane fundamental wavenumbers from the infrared spectrum in the region 700–900 cm^{-1} . Klimova *et al.* (1976–261) reported twelve ground state fundamental wavenumbers from the comparative analysis of the quasilinear phosphorescence spectra. Kakas *et al.* (1984–478) reported 24 vibrational wavenumbers from the infrared spectrum and four from the quasilinear phosphorescence spectrum. A complete set of fundamental wavenumbers was obtained by combining the available wavenumbers then comparing them with those of phenanthrene. Missing values were taken from phenanthrene, see Table 24. To check the reliability of this tentative set, the ideal gas entropies were calculated and compared with the third law entropies reported by Steele *et al.* (1989–76). Excellent agreement was obtained at the first trial and hence no adjustment of the values of the fundamental wavenumbers was made.

No ideal gas thermodynamic properties have been reported. The thermodynamic functions for phenanthridine are presented in Table 13. A comparison of the experimental (1989–76) and calculated entropies at 400 K and at 500 K is given below (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 460.29, 520.90 (1989–76); 460.87, 521.56 (this work). The entropy value at 298.15 K calculated on the basis of experimental data evaluated in this work agrees with the result of our statistical mechanical calculation within the limits of experimental errors (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 390.9 and 397.8 respectively (note, that an uncertainty of 4.0 $\text{kJ}\cdot\text{mol}^{-1}$ in the enthalpy of vaporization can cause an uncertainty of 13.4 $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ in the ideal gas entropy at 298.15 K, (see Table 10).

1- and 2-Naphthalenamine

Neither experimental nor calculated thermodynamic properties are available for the 1- and 2-naphthalenamine and very few spectroscopic studies have been made. In this work, the ideal gas thermodynamic properties have been calculated using the available assignments and transferring the other assignments from similar molecules.

The molecular structure and the moments of inertia have not determined for 1- and 2-naphthalenamine. The molecular parameters from naphthalene for the ring contribution (1961–383) and from aniline (1974–79) for the NH_2 group were used to derive the moments of inertia reported in Table 23. Earlier, Sekigawa (1970–345 and 1971–342) reported some of the parameters from theoretical calculations. They found the NH_2 group to be planar while in aniline it is non-planar.

The vibrational spectra for 1-naphthalenamine (1959–412, 1964–147, 1982–261 and 1985–1416) and 2-naphthalenamine (1959–412, 1965–74 and 1982–261) have been reported in the literature. After analyzing the results critically, the sets of vibrational fundamental wavenumbers were selected and are reported in Table 24. The symmetry number for both compounds is one.

The NH_2 torsional wavenumber for 1-naphthalenamine was reported by Singh *et al.* (1982–261) to be 253 cm^{-1} , while Shanker *et al.* (1985–1416) assigned the shoulder at 315 cm^{-1} in the Raman spectrum of the solid as the NH_2 torsional wavenumber. For 2-naphthalenamine, the NH_2 torsional wavenumber has been reported as 225 cm^{-1} by Singh *et al.* (1982–261). By comparison with aniline (1976–13) and the methylanilines (1984–19), we have adopted 253 cm^{-1} as the torsional wavenumber for both 1- and 2-naphthalenamine, and the 225 cm^{-1} wavenumber in 2-naphthalenamine is assigned to the missing out of plane NH_2 deformation mode (1982–261). Using these torsional wavenumber and the reduced moments of inertia, the potential barrier heights were calculated and in turn the internal rotational energy levels were obtained.

As in the case of aniline (1976–13) and the methylanilines (1980–76), instead of using the NH_2 wagging funda-

mental wavenumbers, 660 and 635 cm^{-1} for the 1- and 2-naphthalenamine, respectively, we chose to use the inversional energy levels. For 1- and 2-naphthalenamine these energy levels were transferred from 2-methylaniline and 3-methylaniline, respectively.

The thermodynamic properties of 1-naphthalenamine and 2-naphthalenamine in the ideal gas state are given in Table 13. There are no literature results for comparison.

9-Methylcarbazole

The spectroscopic information necessary to calculate the thermodynamic properties is not available for 9-methylcarbazole. Hence, it was decided to derive the properties by the incremental method. Bickel *et al.* (1988–583) reported the internal rotational parameters ($V_3 = 282.8\text{ cm}^{-1}$, $V_6 = -55.8\text{ cm}^{-1}$, $I_r = 5.19 \times 10^{-40}\text{ g}\cdot\text{cm}^2$) for 1-methylindole based on the rotational spectrum. Arnold (1968–63) suggested that the rotation of methyl group in 1-methylindole is significantly hindered while the methyl rotation is almost free in 1-methylpyrrole. Assuming that this effect should be twice as great in 9-methylcarbazole, a value for V_3 of 566 cm^{-1} was adopted as a barrier of the internal rotation because of the influence of two benzene rings. Kudchadker *et al.* (1991–124) obtained the $-\text{CH}_2$ increments for all the properties from 0 to 1500 K based on the ideal gas functions of pyrrole and 1-methylpyrrole. The properties of 1-methylpyrrole were corrected for this purpose to include the internal rotational levels corresponding to 9-methylcarbazole ($V_3 = 566\text{ cm}^{-1}$, $I_r = 5.39 \times 10^{-40}\text{ g}\cdot\text{cm}^2$). Using the $-\text{CH}_2$ increments and the values for carbazole obtained in this work, the ideal gas thermodynamic properties for 9-methylcarbazole were derived and are presented in Table 13. The difference between entropy values at 298.15 K calculated based on experimental data and the value derived by the incremental method is reasonable taking into account uncertainties of both methods (in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$): 419.21 (1992–3); 419.2 (this work, based on evaluated experimental data); 422.40 (this work, calculation).

TABLE 14. Available freezing and normal boiling temperatures

T_b K	$\sigma(T_b)^a$ K	T_{fus} K	$\sigma(T_{fus})^a$ K	Author(s)	Ref.
1-Butanamine					
336.65	7.0	—	—	Reimer	1870-6
349.45	0.53	—	—	Lieben and Rossi	1871-9
349.65	4.0	—	—	Linnemann	1872-18
336.15	8.0	—	—	Hofmann	1874-11
349.15	2.0	—	—	Werner	1919-57
350.65	1.0	222.65	0.5	Timmermans and Mattaar	1921-17
351.15	2.0	—	—	Erickson	1926-46
350.65	1.0	—	—	Lycan <i>et al.</i>	1931-249
350.96	0.2	—	—	Butler and Ramchandani	1935-366
350.65	2.0	—	—	Brown and Jones	1946-175
349.65	0.09	—	—	Rogers	1947-146
351.15	1.0	—	—	Schuerch and Huntress	1949-167
350.45	0.2	—	—	Few and Smith	1949-482
350.95	0.5	—	—	Arnett <i>et al.</i>	1950-248
350.65	0.6	—	—	Dilke <i>et al.</i>	1950-591
349.65	3.0	—	—	Barcelo <i>et al.</i>	1951-569
350.95	1.0	—	—	James	1952-42
343.15	3.0	—	—	Glaser and Ruland	1957-76
350.15	1.0	—	—	Ross and Finkelstein	1957-212
349.65	0.02	—	—	Evans <i>et al.</i>	1959-313
351.15	1.5	—	—	Holmberg	1962-353
349.55	0.12	—	—	Krichevskii <i>et al.</i>	1962-356
351.15	0.8	—	—	Sudaricov <i>et al.</i>	1963-316
350.65	0.3	—	—	Humphrey and van Winkle	1967-204
351.15	0.3	—	—	Nakanishi <i>et al.</i>	1967-218
349.95	0.5	—	—	Christie and Crisp	1967-324
350.55	0.04	224.05	0.03	Union Carbide Corp.	1968-195
351.05	0.13	—	—	Siedler and Bittrich	1969-2
350.12	0.2	—	—	Letcher and Bayles	1971-42
350.15	0.03	224.05	0.02	TRC - This work	
2-Butanamine					
336.15	2.0	—	—	Sabatier and Mailhe	1909-1
—	—	168.65	0.5	Timmermans and Mattaar	1921-17
336.15	2.0	—	—	Schuerch and Huntress	1949-167
335.65	0.2	—	—	Evans <i>et al.</i>	1959-313
336.15	1.5	—	—	Holmberg	1962-353
335.88	0.03	168.65	0.5	TRC - This work	
2-Methyl-1-propanamine					
341.65	1.5	—	—	Perkin	1889-26
341.15	0.5	187.65	0.5	Timmermans and Mattaar	1921-17
—	—	186.45	0.5	Simon and Huter	1935-278
—	—	188.55	1.5	Simon and Huter	1935-280
341.15	2.0	—	—	Schuerch and Huntress	1949-167
340.15	1.0	—	—	Barcelo <i>et al.</i>	1951-569
340.85	0.3	—	—	Costello and Bowden	1959-218
341.15	1.5	—	—	Holmberg	1962-353
340.718	0.03	—	—	Osborn and Scott	1980-1
340.90	0.01	186.45	0.5	TRC - This work	
2-Methyl-2-propanamine					
316.95	0.4	205.65	0.5	Timmermans and Mattaar	1921-17
318.15	2.0	—	—	Schuerch and Huntress	1949-167
316.90	0.3	—	—	Few and Smith	1949-482
317.15	2.0	—	—	Howk <i>et al.</i>	1954-150
318.15	1.0	—	—	Kornblum <i>et al.</i>	1956-163
317.45	0.2	—	—	Evans <i>et al.</i>	1959-313
317.19	0.03	—	—	Osborn and Douslin	1968-206
—	—	206.197 ^b	0.01	Finke <i>et al.</i>	1972-140
317.19	0.02	206.20	0.01	TRC - This work	

TABLE 14. Available freezing and normal boiling temperatures — Continued

T_b K	$\sigma(T_b)^a$ K	T_{fus} K	$\sigma(T_{fus})^a$ K	Author(s)	Ref.
Pyrrole					
402.85	0.2	—	—	Robles	1939-3
—	—	238.8	0.4	Milazzo	1941-378
402.95	0.2	249.7	0.2	API	1942-300
403.65	3.0	—	—	Yur'ev <i>et al.</i>	1946-260
403.15	0.5	—	—	Lecat	1947-346
403.20	0.15	254.65	2.0	Timmermans <i>et al.</i>	1955-485
403.15	0.07	—	—	Glaser and Ruland	1957-76
—	—	249.747 ^b	0.06	McCullough and Waddington	1957-539
402.914	0.06	—	—	API Project 52	1957-605
402.95	0.3	249.74 ^b	0.03	Helm <i>et al.</i>	1958-216
401.15	2.0	—	—	Patterson and Drenchko	1959-335
401.15	1.5	—	—	Wimette and Linnell	1962-406
402.915	0.03	249.735 ^b	0.07	Scott <i>et al.</i>	1967-116
403.65	1.5	—	—	Anderson and Shimanskaya	1969-163
—	—	250.	0.6	Rosso and Carbonnel	1973-224
402.94	0.01	249.75	0.06	TRC — This work	
1-Methylpyrrole					
—	—	231.200	0.500	Milazzo	1941-378
385.95	0.5	—	—	Lecat	1947-346
385.85	0.3	—	—	API Project 52	1958-417
387.15	4.0	—	—	Vilkov <i>et al.</i>	1962-392
385.893	0.03	—	—	Osborn and Douslin	1968-206
387.65	1.0	—	—	Anderson and Shimanskaya	1969-163
—	—	216.820	0.080	Guanquan <i>et al.</i>	1986-69
—	—	216.911 ^b	0.005	Messerly <i>et al.</i>	1988-93
385.96	0.02	216.91	0.04	TRC — This work	
2-Methylpyrrole					
421.15	1.0	—	—	Knorr and Hess	1912-167
420.65	0.5	—	—	Lecat	1947-346
421.15	2.0	—	—	Rapoport and Baldrige	1952-71
—	—	237.55	0.4	API Project 52	1957-605
—	—	237.55	0.3	Lanum and Morris	1969-51
421.2	1.0	—	—	Cumper and Wood	1971-379
420.65	0.5	237.55	0.3	TRC — This work	
3-Methylpyrrole					
—	—	224.75	0.3	Lanum and Morris	1969-51
416.15	1.0	—	—	Groves <i>et al.</i>	1971-380
416.15	1.0	—	—	Hineman and Theodoropoulos	1976-48dd0
416.15	2.0	—	—	Cornforth and Minh-hui	1990-502
416.	1.0	224.75	0.3	TRC — This work	
Pyridine					
387.65	1.5	—	—	Kahlbaum	1884-15
389.60	1.0	—	—	Perkin	1889-26
388.66	0.4	—	—	Louguinine	1899-11
388.35	0.3	231.15	0.4	Zawidzki	1906-115
—	—	231.15	2.0	Timmermans	1907-128
388.50	0.2	—	—	Hartley <i>et al.</i>	1908-126
388.15	1.0	—	—	Dunstan and Stubbs	1908-127
388.65	0.5	235.15	0.5	Baud	1909-134
388.65	0.35	231.35	0.4	Timmermans	1910-58
388.65	0.3	231.15	0.4	Timmermans	1911-54
388.65	0.3	231.15	0.3	Timmermans	1912-127
388.65	0.5	—	—	Kurnakow and Zemczny	1913-179
—	—	232.45	0.2	Bramley	1916-38
388.70	0.3	235.65	0.3	Hatcher and Skirrow	1917-65

TABLE 14. Available freezing and normal boiling temperatures — Continued

T_b K	$\sigma(T_b)^a$ K	T_{fus} K	$\sigma(T_{fus})^a$ K	Author(s)	Ref.
Pyridine — Continued					
388.45	0.3	—	—	Heap <i>et al.</i>	1921–129
389.20	0.3	—	—	Herz and Neukirch	1923–3
388.65	0.3	—	—	Grimm and Patrick	1923–73
388.50	0.3	—	—	Mathews	1926–71
—	—	233.65	0.7	Arndt and Nachtway	1926–210
388.45	0.4	—	—	Wilkie and Shaw	1927–12
388.45	0.4	—	—	Prentiss	1929–341
389.25	0.4	—	—	Trew and Spencer	1931–278
388.35	0.8	—	—	Meulen and Mann	1931–349
388.55	0.3	—	—	Rau and Narayanaswamy	1934–392
388.15	0.2	—	—	Swearingen	1935–417
—	—	231.15	0.2	Parks <i>et al.</i>	1936–163
388.65	0.3	231.35	0.4	Timmermans and Hennaut-Roland	1937–146
388.15	1.5	—	—	Ewell and Welch	1941–100
388.55	0.2	—	—	Lecat	1943–220
—	—	231.65	0.3	Hoffman and Vander Werf	1946–296
388.55	0.5	—	—	Lecat	1947–346
386.15	1.5	231.35	0.2	Kennard and McCusker	1948–464
388.35	0.5	—	—	Dilke <i>et al.</i>	1950–591
388.25	0.3	—	—	Jones	1950–599
387.63	0.2	—	—	Griffiths	1952–363
—	—	231.44	0.2	Witschonke	1954–24
—	—	231.60	0.06	Biddiscombe <i>et al.</i>	1954–31
388.68	0.2	—	—	Gjaldbaek and Andersen	1954–670
387.70	0.5	—	—	Holland and Smyth	1955–11
388.80	0.2	—	—	Stutchbury	1956–607
388.384	0.03	231.489 ^b	0.05	McCullough <i>et al.</i>	1957–176
388.35	0.3	231.48 ^b	0.03	Helm <i>et al.</i>	1958–216
388.55	0.3	—	—	Zieborak and Wyrzykowska-Stankiewicz	1958–385
388.31	0.1	—	—	Zieborak <i>et al.</i>	1958–388
388.45	0.5	231.15	4.0	Holo <i>et al.</i>	1958–391
388.40	0.1	—	—	Brzostowski and Malanovski	1959–358
388.39	0.2	—	—	Zieborak and Galska-Krajewska	1959–360
388.39	0.2	—	—	Zieborak and Wyrzykowska-Stankiewicz	1959–361
388.45	0.2	—	—	Zieborak and Wyrzykowska-Stankiewicz	1960–333
388.55	0.15	—	—	Findlay	1961–303
388.50	0.1	—	—	Yanyim-Agaev <i>et al.</i>	1961–305
388.39	0.15	—	—	Galska-Krajewska	1961–307
388.15	0.5	—	—	Amaya	1961–308
388.45	0.5	—	—	Jones	1962–97
388.15	1.5	—	—	Wimette and Linnell	1962–406
388.39	0.25	—	—	Galska-Krajewska and Zieborak	1962–411
388.50	0.15	—	—	Yarym-Agaev <i>et al.</i>	1963–379
388.40	0.2	—	—	Maczynska and Zieborak	1963–381
388.40	0.15	—	—	Razniewska	1964–434
388.35	0.25	—	—	Findlay and Kidman	1965–341
388.41	0.05	—	—	Woycicka and Kurtyka	1965–583
—	—	231.15	0.1	Cioffi and Messer	1966–222
388.55	0.2	231.15	0.5	Assal	1966–485
388.35	0.3	—	—	Findlay <i>et al.</i>	1967–319
388.46	0.13	—	—	Fried <i>et al.</i>	1967–320
388.75	0.3	—	—	Waclawek and Hurwic	1967–325
389.05	0.4	—	—	Nakanishi <i>et al.</i>	1968–48
388.55	0.3	—	—	Kind <i>et al.</i>	1968–281
388.27	0.2	—	—	Galska-Krajewska	1970–233
388.70	0.3	—	—	Korchenskaya <i>et al.</i>	1970–239
388.35	0.4	—	—	Paul and Johnny	1971–214
388.65	0.3	—	—	Krupatkin and Rozhentsova	1971–220
388.77	0.3	—	—	Abramov <i>et al.</i>	1972–234
388.75	0.3	—	—	Kanakbaeva	1972–235
388.55	0.25	—	—	Rao and Naidu	1973–222
—	—	231.44	0.05	Goates <i>et al.</i>	1973–225
388.70	0.1	—	—	Kanakbaeva	1974–227

TABLE 14. Available freezing and normal boiling temperatures — Continued

T_b K	$\sigma(T_b)^a$ K	T_{fus} K	$\sigma(T_{fus})^a$ K	Author(s)	Ref.
Pyridine — Continued					
388.725	0.3	—	—	Kanakbaeva <i>et al.</i>	1974–255
388.404	0.2	—	—	Soulie <i>et al.</i>	1975–127
388.55	0.5	—	—	Ezhov <i>et al.</i>	1976–183
388.15	1.0	—	—	Gokavi <i>et al.</i>	1986–2
—	—	231.42	0.08	Guanquan <i>et al.</i>	1986–69
389.15	0.5	—	—	Rajendran <i>et al.</i>	1989–79
388.38	0.01	231.49	0.05	TRC — This work	
2-Methylpyridine					
401.15	1.0	—	—	Bruhl	1895–49
401.15	1.5	203.25	0.3	Timmermans	1921–19
401.15	1.5	—	—	Heap <i>et al.</i>	1921–129
401.45	0.5	—	—	Wilkie and Shaw	1927–12
402.00	0.55	—	—	Riley and Bailey	1929–178
402.25	0.3	—	—	Rau and Narayanaswamy	1934–392
402.55	0.3	206.55	0.5	API Project	1942–300
400.15	1.5	—	—	Herz <i>et al.</i>	1943–29
402.15	1.5	—	—	Hackmann <i>et al.</i>	1943–255
—	—	208.95	0.3	Hoffman and Vander Werf	1946–296
403.85	0.5	—	—	Lecat	1947–346
402.59	0.08	206.60	0.1	Freiser and Glowacki	1948–442
402.15	2.0	—	—	Runge and Hummel	1951–86
402.59	0.2	—	—	Hopke and Sears	1951–314
—	—	206.41	0.06	Biddiscombe <i>et al.</i>	1954–31
402.80	0.2	203.4	0.2	Timmermans and Hennaut-Roland	1955–485
402.588	0.08	—	—	Rostafinska	1955–635
402.95	0.4	—	—	Petro and Smyth	1957–217
—	—	206.44 ^b	0.03	Helm <i>et al.</i>	1958–216
402.45	0.25	—	—	Zieborak and Wyrzykowska-Stankiewicz	1958–387
402.25	0.5	—	—	Ogawa <i>et al.</i>	1958–389
402.62	0.05	—	—	Szafranski	1959–336
402.59	0.06	—	—	Szafranski	1959–337
402.57	0.1	—	—	Brzostowski and Malanowski	1959–358
401.15	1.0	—	—	Terry <i>et al.</i>	1960–9
401.15	2.0	—	—	Farberov <i>et al.</i>	1961–304
401.15	1.5	—	—	Wimette and Linnell	1962–406
402.536	0.03	206.466 ^b	0.05	Scott <i>et al.</i>	1963–156
402.41	0.2	—	—	Razniewska	1964–434
402.45	0.3	—	—	Trabczynski	1964–523
402.35	0.2	207.15	1.0	Assal	1966–485
402.65	1.0	—	—	Waclawek and Hurwic	1967–325
401.95	0.05	203.25	0.03	Union Carbide Corp.	1968–195
402.35	0.3	—	—	Wilson and Worrall	1968–285
—	—	206.29	0.20	Ait-Kaci and Merlin	1979–131
—	—	206.29	0.15	Ait-Kaci and Merlin	1979–132
—	—	206.29	0.15	Ait-Kaci and Merlin	1979–133
—	—	206.29	0.15	Ait-Kaci and Merlin	1979–134
—	—	204.35	0.50	Den Adel <i>et al.</i>	1981–138
402.53	0.02	206.47	0.05	TRC — This work	
3-Methylpyridine					
417.40	0.6	—	—	Bruhl	1895–49
417.05	0.4	—	—	Flaschner	1909–47
416.95	0.3	—	—	Heap <i>et al.</i>	1921–129
416.85	0.4	—	—	Rau and Narayanaswamy	1934–392
416.65	2.0	—	—	Hackmann <i>et al.</i>	1943–255
—	—	254.85	0.3	Hoffman and Vander Werf	1946–296
417.15	0.4	255.45	0.3	Coulson and Jones	1946–308
417.15	0.6	—	—	Lecat	1947–346
416.65	1.0	—	—	Othmer and Savitt	1948–465
416.15	0.3	—	—	Othmer and Savitt	1948–467
416.35	0.5	251.95	0.7	Liplavk and Boliter	1951–184

TABLE 14. Available freezing and normal boiling temperatures — Continued

T_b K	$\sigma(T_b)^a$ K	T_{fus} K	$\sigma(T_{fus})^a$ K	Author(s)	Ref.
3-Methylpyridine					
416.40	0.5	—	—	Hopke and Sears	1951-314
—	—	255.25	0.2	Witschonke	1954-24
—	—	254.95	0.06	Biddiscombe <i>et al.</i>	1954-31
417.25	0.3	—	—	Zieborak <i>et al.</i>	1958-390
417.30	0.1	—	—	Brzostowski <i>et al.</i>	1959-359
417.15	0.3	—	—	Razniewska	1961-306
417.287	0.05	255.01 ^b	0.06	Scott <i>et al.</i>	1963-157
417.25	0.3	—	—	Bylicki and Jankun-Pinska	1964-250
417.25	0.2	—	—	Razniewska	1964-434
416.35	0.2	255.15	1.0	Assal	1966-485
415.15	2.0	—	—	Takata	1966-257
416.45	1.0	—	—	Waclawek and Hurwic	1967-325
417.25	0.3	—	—	Wilson and Worrall	1968-285
—	—	254.85	0.5	Den Adel <i>et al.</i>	1981-138
417.29	0.01	255.01	0.04	TRC — This work	
4-Methylpyridine					
418.23	0.3	—	—	Flaschner	1909-47
419.15	3.0	—	—	Favorskii and Shostakovskii	1943-256
417.15	1.0	—	—	Leis and Curran	1945-205
—	—	276.65	0.3	Hoffman and Vander Werf	1946-296
418.45	0.3	277.45	0.3	Coulson and Jones	1946-308
418.45	0.6	—	—	Lecat	1947-346
417.65	1.0	—	—	Othmer and Savitt	1948-465
417.95	0.3	—	—	Othmer and Savitt	1948-467
416.25	2.0	—	—	Runge and Hummel	1951-86
418.15	0.5	276.15	0.6	Liplavk and Boliter	1951-184
417.90	0.6	—	—	Hopke and Sears	1951-314
—	—	276.85	0.2	Witschonke	1954-24
—	—	276.80	0.06	Biddiscombe <i>et al.</i>	1954-31
417.45	0.3	—	—	Zieborak <i>et al.</i>	1958-390
418.40	0.6	277.4	0.2	Kyte <i>et al.</i>	1960-119
418.25	0.3	—	—	Bylicki and Jankun-Pinska	1964-250
418.05	0.5	276.95	0.3	Assal	1966-485
417.35	1.0	—	—	Waclawek and Hurwic	1967-325
418.55	0.05	276.85	0.03	Union Carbide Corp.	1968-195
418.45	0.3	—	—	Wilson and Worrall	1968-285
418.504	0.03	—	—	Osborn and Douslin	1968-206
—	—	276.95	0.5	Den Adel <i>et al.</i>	1981-138
—	—	276.8 ^b	0.05	Soulard <i>et al.</i>	1986-227
—	—	276.81 ^b	0.03	Messerly <i>et al.</i>	1988-93
418.15	0.09	—	—	Cabezas <i>et al.</i>	1990-77
418.51	0.01	276.81	0.03	TRC — This work	
Pyrrolidine					
358.65	2.	—	—	Yur'ev <i>et al.</i>	1946-260
364.05	0.5	—	—	Lecat	1947-346
359.64	0.4	211.95	0.50	Boord <i>et al.</i>	1950-546
359.71	0.2	—	—	API Project 52	1956-676
359.65	0.15	215.30 ^b	0.03	Helm <i>et al.</i>	1958-216
359.71	0.03	215.31 ^b	0.06	McCullough <i>et al.</i>	1959-355
359.64	0.05	215.31 ^b	0.07	Hildenbrand <i>et al.</i>	1959-374
359.15	1.5	—	—	Anderson and Shimanskaya	1969-163
359.71	0.02	215.31	0.06	TRC — This work	
Piperidine					
379.15	1.5	—	—	Kahlbaum	1884-15
379.2	1.0	—	—	Perkin	1889-26
—	—	256.15	2.0	Altschul and Von Schneider	1895-61
378.91	0.7	—	—	Louguinine	1899-11
379.15	0.6	—	—	Kurnakow and Zemczny	1913-179

TABLE 14. Available freezing and normal boiling temperatures — Continued

T_b K	$\sigma(T_b)^a$ K	T_{fus} K	$\sigma(T_{fus})^a$ K	Author(s)	Ref.
Piperidine — Continued					
—	—	261.15	2.	Pushin and Sladovic	1928–220
379.50	0.5	—	—	Riley and Bailey	1929–178
378.85	0.5	—	—	Semb and McElvain	1931–371
378.95	0.3	—	—	Rau and Narayanaswamy	1934–392
379.55	0.3	262.65	0.2	Timmermans and Hennaut-Roland	1937–146
379.45	0.4	—	—	Magnusson and Schierz	1940–364
379.55	0.7	—	—	Lecat	1947–346
379.65	0.5	—	—	Dilke <i>et al.</i>	1950–591
379.05	0.3	262.12 ^b	0.05	Kalman and Smyth	1960–369
378.15	1.0	—	—	Bedford <i>et al.</i>	1963–357
378.75	0.3	—	—	Moelwyn-Hughes and Thorpe	1964–572
379.37	0.03	—	—	Osborn and Douslin	1968–206
378.45	0.15	—	—	Nakanishi <i>et al.</i>	1975–283
379.15	1.5	264.15	1.5	Vedal <i>et al.</i>	1976–211
—	—	262.12 ^b	0.02	Messerly <i>et al.</i>	1988–93
379.37	0.02	262.12	0.02	TRC — This work	
Indole					
—	—	325.15	3.	Weerman	1910–141
—	—	325.65	0.5	Cowley and Partington	1936–459
526.65	0.6	—	—	Lecat	1947–346
—	—	325.65	0.5	Aihara	1955–710
—	—	326.25	1.	Serpinskii <i>et al.</i>	1958–398
526.65	0.6	325.65	0.5	TRC — This work	
Quinoline					
511.15	2.	—	—	Kahlbaum	1884–15
—	—	253.65	0.5	Altschul and Schneider	1895–61
511.15	0.5	250.55	0.6	Timmermans	1911–54
—	—	253.65	0.2	Bramley	1916–38
509.65	0.6	—	—	Harris and Pope	1922–55
511.15	1.5	—	—	Grimm and Patrick	1923–73
—	—	254.22	0.15	Hammick and Holt	1926–28
—	—	258.15	2.	Pushin and Sladovic	1928–20
511.15	1.	—	—	Earp and Glasstone	1935–428
—	—	258.45	0.3	Parks <i>et al.</i>	1936–163
510.25	0.4	257.55	0.4	Timmermans and Hennaut-Roland	1937–146
510.50	0.4	—	—	Lecat	1943–221
508.15	2.	—	—	Hackmann <i>et al.</i>	1943–255
510.45	0.6	—	—	Lecat	1947–346
509.15	1.5	252.05	0.5	Tschamler and Krischai	1951–444
—	—	257.55	0.5	Timmermans	1952–50
—	—	258.25	0.2	Witschonke	1954–24
—	—	250.75	0.6	Kovalenko and Trifonov	1954–674
—	—	253.65	1.	Holland and Smyth	1955–11
510.85	2.	—	—	Glaser and Ruland	1957–76
—	—	257.93	0.05	Mastrangelo	1957–551
510.78	0.07	—	—	Malanowski	1961–368
—	—	258.15	1.	Mallikarjun and Hill	1965–231
510.57	0.15	—	—	Maczynski and Maczynska	1965–688
510.25	0.6	—	—	Cooper <i>et al.</i>	1967–293
—	—	258.25	0.3	Lanum and Morris	1969–51
510.55	0.4	—	—	Sundaram	1969–243
510.29	0.04	258.37 ^b	0.03	Steele <i>et al.</i>	1988–551
510.31	0.01	258.37	0.03	TRC — This work	
Isoquinoline					
515.65	0.6	297.4	0.5	Harris and Pope	1922–155
515.45	0.4	—	—	Rau and Narayanaswamy	1934–392
514.65	2.	—	—	Hackmann <i>et al.</i>	1943–255
513.45	0.6	—	—	Lecat	1947–346

TABLE 14. Available freezing and normal boiling temperatures — Continued

T_b K	$\sigma(T_b)^a$ K	T_{fus} K	$\sigma(T_{fus})^a$ K	Author(s)	Ref.
Isoquinoline — Continued					
—	—	299.63	0.2	Freiser and Glowacki	1949–545
—	—	297.15	0.5	Kravchenko and Pastukhova	1953–712
—	—	296.65	0.7	Tamres <i>et al.</i>	1953–715
—	—	297.40	0.6	Potashnikov and Gorelo	1957–567
516.39	0.07	—	—	Malanowski	1961–368
—	—	299.15	1.	Mallikarjun and Hill	1965–231
513.65	0.6	—	—	Cooper <i>et al.</i>	1967–293
516.388	0.04	299.62 ^b	0.03	Steele <i>et al.</i>	1988–551
516.37	0.01	299.62	0.03	TRC — This work	
Carbazole					
—	—	511.15	2.	Graeber and Glaser	1872–30
624.65	1.	—	—	Graeber and Glaser	1872–31
—	—	511.15	2.	Tauber	1891–58
—	—	511.15	2.	Borsche	1908–128
—	—	509.15	0.5	Clark	1919–40
624.65	1.	520.15	0.2	Kirby	1921–90
—	—	517.95	0.3	Senseman and Nelson	1923–166
—	—	518.45	0.5	Mortimer and Murphy	1923–167
—	—	513.50	0.3	Burriel	1931–8
—	—	518.15	1.	Cowley and Partington	1936–459
—	—	518.65	0.3	Witschonke	1954–24
—	—	517.65	0.7	Aihara	1955–710
—	—	519.30	0.3	Robinson and Scott	1969–244
—	—	519.35	0.4	Marsh	1987–598
—	—	519.15	1.	NBS Spec. Pub. 260	1988–9
627.84	0.04	519.30	0.5	TRC —* This work	
Acridine					
—	—	382.45	1.	Schuyer <i>et al.</i>	1953–698
—	—	383.55	0.3	Kalman and Smyth	1960–391
—	—	384.15	1.5	Cumper <i>et al.</i>	1962–472
—	—	384.00	2.	McEachern <i>et al.</i>	1975–228
—	—	381.15	3.	Schmitt and Reid	1986–32
618.07	0.03	383.24 ^b	0.01	Steele <i>et al.</i>	1989–76
618.01	0.03	383.24	0.01	TRC — This work	
Phenanthridine					
—	—	372.65	2.	Taylor and Martin	1952–665
—	—	379.65	1.5	Taylor and Kalenda	1954–764
—	—	379.50	1.	Cumper <i>et al.</i>	1962–472
—	—	379.94 ^b	0.02	Steele <i>et al.</i>	1989–76
622.	0.5	379.94	0.02	TRC — This work	
1-Naphthalenamine					
573.15	2.	323.25	0.5	Stillmann and Swain	1899–63
—	—	321.15	0.5	Philip and Smith	1905–101
—	—	324.15	1.5	Buchner	1906–78
—	—	322.65	1.	Beck and Ebbinghaus	1906–123
—	—	322.65	2.	Beck	1907–112
—	—	321.36	1.	Campetti	1914–155
—	—	323.15	0.5	Hammick and Holt	1926–228
—	—	322.35	0.3	Cowley and Partington	1938–372
573.95	1.	323.15	1.5	Stull	1947–83
—	—	321.65	0.7	Bastic and Pushin	1947–406
—	—	317.15	1.5	Snyder <i>et al.</i>	1953–700
—	—	322.35	0.2	Witschonke	1954–24
—	—	322.95	0.3	Assal	1966–514
—	—	323.15	1.5	Khetarpal <i>et al.</i>	1979–205
573.8	0.1	322.35	0.5	TRC — This work	

TABLE 14. Available freezing and normal boiling temperatures — Continued

T_b K	$\sigma(T_b)^a$ K	T_{fus} K	$\sigma(T_{fus})^a$ K	Author(s)	Ref.
2-Naphthalenamine					
—	—	383.15	1	Lee and Jones	1922–161
—	—	382.65	0.3	Skau	1935–435
—	—	383.15	0.4	Cowley and Partington	1938–372
—	—	382.65	5.	Butterworth and Hey	1940–231
579.25	1.	384.55	1.5	Stull	1947–83
—	—	383.15	2.	Bastic and Pushin	1947–406
—	—	381.15	2.	Snyder <i>et al.</i>	1953–700
—	—	385.15	1.	Karyakin <i>et al.</i>	1968–3
—	—	386.15	1.5	Khetarpal <i>et al.</i>	1979–205
579.3	0.1	386.	1.0	TRC — This work	
9-Methylcarbazole					
—	—	361.15	2.	Burton and Gibson	1924–187
—	—	362.49 ^b	0.04	Messerly <i>et al.</i>	1988–93
616.97	0.006	—	—	Steele <i>et al.</i>	1992–3
616.79	0.02	362.49	0.04	TRC — This work	

^aSee Sec. 1.6.^bTriple point temperature.

TABLE 15. Measured and estimated critical properties

T_c K	$\sigma(T_c)^a$ K	P_c MPa	$\sigma(P_c)^a$ MPa	V_c cm ³ ·mol ⁻¹	$\sigma(V_c)^a$ cm ³ ·mol ⁻¹	Author(s)	Ref.
1-Butanamine							
524.2	1	4.15	0.05	—	—	Glasser and Rüland	1957–76
530 ^b	—	3.981 ^b	0.02	—	—	ESDU	1976–328
531.9	1	4.20	0.05	275	—	Toczylkin and Young	1980–25
531.9	1	4.25 ^c	0.02 ^c	277 ^d	2 ^d	TRC — this work	
2-Butanamine							
511 ^b	1	3.97 ^b	0.02	—	—	ESDU	1976–328
514.3	1	5.0	1.	—	—	Toczylkin and Young	1980–25
514.3	1	4.16 ^c	0.05 ^c	278 ^d	4 ^d	TRC — this work	
2-Methyl-1-propanamine							
519 ^b	1	4.073 ^b	—	—	—	ESDU	1976–328
5192	—	4.07 ^b	0.08 ^b	278 ^d	4 ^d	TRC — this work	
2-Methyl-2-propanamine							
483.9	1	3.84	0.01	293	2	Kobe and Mathews	1970–5
483.9 ^b	1	3.85 ^b	0.02 ^b	—	—	ESDU	1976–328
483.9	1	3.84 ^b	0.02 ^b	292 ^d	5 ^d	TRC — this work	
Pyrrole							
625	5	5.67	0.05	—	—	Glasser and Rüland	1957–76
639.7	1	—	—	—	—	Cheng <i>et al.</i>	1962–230
639.8 ^b	1	7.25 ^b	0.02	—	—	ESDU	1980–255
639.7	1	6.34 ^c	0.02 ^c	200 ^d	2 ^d	TRC — this work	
1-Methylpyrrole							
596.0 ^b	1	4.85 ^b	—	—	—	ESDU	1980–255
596.0	1	4.86 ^b	0.20 ^b	271 ^d	2 ^d	TRC — this work	
2-Methylpyrrole							
654. ^b	5	5.08 ^b	0.1 ^b	266 ^b	4 ^b	TRC — this work	
3-Methylpyrrole							
647. ^b	5	5.08 ^b	0.1 ^b	266 ^b	4 ^b	TRC — this work	

TABLE 15. Measured and estimated critical properties — Continued

T_c K	$\sigma(T_c)^a$ K	p_c MPa	$\sigma(p_c)^a$ MPa	V_c $\text{cm}^3\text{mol}^{-1}$	$\sigma(V_c)^a$ $\text{cm}^3\text{mol}^{-1}$	Author(s)	Ref.
Pyridine							
617.4	3	—	—	—	—	Radice	1899-59
620	6	—	—	—	—	Livingston <i>et al.</i>	1908-112
—	—	6.0	0.4	—	—	Herz and Neukrich	1923-3
618 ^b	2 ^b	—	—	—	—	Kreglewski	1954-36
618	4	—	—	—	—	Swietoslowski and Kreglewski	1954-736
620.2	2	5.63	0.03	254	2	Kobe <i>et al.</i>	1956-9
620	2	—	—	—	—	Ambrose and Grant	1957-423
620.0 ^b	2	5.645 ^b	0.02	—	—	ESDU	1980-255
620	2	5.66	0.06	—	—	Brunner	1987-588
620	2	5.67 ^c	0.02 ^c	243 ^d	5 ^d	TRC — this work	
2-Methylpyridine							
621	2	—	—	—	—	Ambrose and Grant	1957-423
621.1	1	4.6	0.1	335	5	Kobe and Mathews	1970-5
621.0 ^b	2	4.60 ^b	0.02	—	—	ESDU	1980-255
621.0	1	4.60 ^c	0.02 ^c	292 ^d	4 ^d	TRC — this work	
3-Methylpyridine							
645	2	—	—	—	—	Ambrose and Grant	1957-423
645.0 ^b	2	4.65 ^b	0.02	—	—	ESDU	1980-255
645	2	4.65 ^c	0.1 ^c	288 ^d	5 ^d	TRC — this work	
4-Methylpyridine							
645.7	2	—	—	—	—	Ambrose and Grant	1957-423
646.3	0.5	4.66	0.05	325	3	Kobe and Mathews	1970-5
646.0 ^b	2	4.60 ^b	0.02	—	—	ESDU	1980-255
645.7	2	4.70 ^c	0.02 ^c	292 ^d	5 ^d	TRC — this work	
Pyrrolidine							
570.2	1	5.70	0.05	249	5	Kobe <i>et al.</i>	1956-9
568.2	1	—	—	—	—	Cheng <i>et al.</i>	1962-230
568.6 ^b	2	5.60 ^b	0.02	—	—	ESDU	1980-255
568.2	1	5.60	0.05	238 ^d	5 ^d	TRC — this work	
Piperidine							
—	—	4.65 ^b	0.20 ^b	—	—	Guye and Mallet	1902-64
594.0	1	—	—	—	—	Cheng <i>et al.</i>	1962-230
594.1	1	—	—	—	—	Ambrose	1963-213
594.0	1	4.94 ^c	0.20 ^c	288 ^d	5 ^d	TRC — this work	
Indole							
794 ^b	4 ^b	4.8 ^b	0.1 ^b	356 ^b	5 ^b	TRC — this work	
Quinoline							
794	5	—	—	—	—	Livingston <i>et al.</i>	1908-112
800	5	5.78	0.05	—	—	Glasser and Rüland	1957-76
782	2	—	—	—	—	Ambrose	1963-213
782 ^b	2 ^b	3.80 ^b	0.02	—	—	ESDU	1980-255
782	2	4.86 ^c	0.05 ^c	371 ^d	5 ^d	TRC — this work	
Isoquinoline							
803	3	—	—	—	—	Ambrose	1963-213
803 ^b	3	4.60 ^b	0.02 ^b	—	—	ESDU	1980-255
803	3	5.10 ^c	0.02 ^c	374 ^d	5 ^d	TRC — this work	
Carbazole							
901.8 ^b	2 ^b	3.13 ^b	0.02	—	—	Sivaraman <i>et al.</i>	1985 185
901.8	2	3.13	0.02 ^b	454 ^d	5 ^d	TRC — this work	
Acridine							
891.1 ^b	2 ^b	3.21 ^b	0.02 ^b	—	—	Sivaraman <i>et al.</i>	1983 189
891.1	—	3.21	0.02	548 ^b	5 ^b	TRC — this work	

TABLE 15. Measured and estimated critical properties — Continued

T_c K	$\sigma(T_c)^a$ K	p_c MPa	$\sigma(p_c)^a$ MPa	V_c $\text{cm}^3\text{mol}^{-1}$	$\sigma(V_c)^a$ $\text{cm}^3\text{mol}^{-1}$	Author(s)	Ref.
895 ^b	3	3.63 ^b	0.05 ^b	Phenanthridine 548 ^b	5 ^b	TRC — this work	
850 ^b	3	5.00 ^b	0.02 ^b	1-Naphthalenamine —	—	ESDU	1981–100
850	3	5.00	0.05	438 ^b	5 ^b	TRC — this work	
850 ^b	3	4.90 ^b	0.05	2-Naphthalenamine —	—	ESDU	1981–100
850	3	4.90	0.05 ^b	438 ^b	5 ^b	TRC — this work	
890	1	3.38	0.05	9-Methylcarbazole 572 ^b	4 ^b	Steele <i>et al.</i>	1992–3
890	1	3.39 ^c	0.05 ^c	572	4	TRC — this work	

^aSee Sec. 1.6.^bEstimated values.^cFrom Cox vapor pressure equation with selected T_c in Table 1.^dFrom fit to rectilinear diameter line with selected T_c in Table 1.

TABLE 16. Available vapor pressure data

Range K	$\sigma(T)^a$ K	Range kPa	$\sigma_c(p_{sat})^a$ kPa	$10^3 \cdot \sigma_r(p_{sat})^a$	sl ^b	Meth. ^c	Author(s)	Ref.
1-Butanamine								
348–349	0.5	99–101	0.1	1.5	0	U	Lieben and Rossi	1871–9
277–305	0.05	3–14	0.1	2.0	0	U	Copley <i>et al.</i>	1941–101
349–350	0.05	100–101	0.05	1.5	0	U	Rogers	1947–146
343–522	0.5	101–4053	0.05	1.5	1	S	Glaser and Ruland	1957–76
216–350	0.05	6–101	0.05	1.0	0	S	Krichevskii <i>et al.</i>	1962–356
293–351	0.1	10–16	0.1	1.0	0	S	Siedler and Bittrich	1969–2
318–338	0.05	30–65	0.05	1.0	0	S	Pradhan	1979–77
297–349	0.01	12–98	0.02	0.2	1	D	Majer <i>et al.</i>	1979–78
2-Butanamine								
278–305	0.5	7–38	0.1	2.0	1	U	Copley <i>et al.</i>	1941–101
300–335	0.01	25–99	0.02	0.2	1	D	Majer <i>et al.</i>	1979–78
2-Methyl-1-propanamine								
236–347	0.01	0.3–123	0.01	2.0	1	S	Simon and Huter	1935–278
278–305	0.5	6–26	0.1	2.0	0	U	Copley <i>et al.</i>	1941–101
297–340	0.01	18–98	0.02	0.2	1	D	Majer <i>et al.</i>	1979–78
289–374	0.001	12–270	0.01	0.1	1	E	Osborn and Scott	1980–1
2-Methyl-2-propanamine								
292–348	0.001	39–270	0.001	0.15	1	E	Osborn and Douslin	1968–206
293–313	0.01	40–88	0.05	0.5	0	S	Valero <i>et al.</i>	1979–80
Pyrrole								
242–290	0.1	0.02–0.9	0.001	1.0	1	S	Milazzo	1941–378
450–544	0.005	19–101	0.01	1.5	0	S	Kobe <i>et al.</i>	1956–9
403–615	0.5	101–5066	0.05	2.0	1	S	Glaser and Ruland	1957–76
339–439	0.001	10–270	0.001	0.2	1	E	Scott <i>et al.</i>	1967–116
333–373	0.02	8–42	0.01	1.0	0	S	Eon <i>et al.</i>	1971–47
1-Methylpyrrole								
231–291	0.1	0.02–2	0.001	1.0	1	S	Milazzo	1941–378
322–423	0.001	10–270	0.001	0.15	1	E	Osborn and Douslin	1968–206
333–373	0.02	16–71	0.01	1.0	0	S	Eon <i>et al.</i>	1971–47
Pyridine								
388–389	1.0	99–100	0.1	3.0	0	U	Bruhhl	1895–49
387–390	0.5	98–99	0.1	5.0	0	U	Kahlenberg	1901–63

TABLE 16. Available vapor pressure data — Continued

Range K	$\sigma(T)^a$ K	Range kPa	$\sigma_c(p_{sat})^a$ kPa	$10^3 \sigma_f(p_{sat})^a$	sl ^b	Meth. ^c	Author(s)	Ref.
387–388	0.05	99–100	0.05	2.0	0	U	Arndt and Nachtway	1926–210
253–393	0.1	0.1–116	0.02	1.0	0	S	van der Meulen and Mann	1931–349
290–389	0.1	1.5–101	0.1	1.5	0	U	Hieber and Woerner	1934–26
363–387	0.05	54–99	0.1	2.0	0	U	Bratton	1935–418
320–389	0.005	8.5–102	0.01	1.0	1	D	Herington and Martin	1953–518
323–353	0.05	10–100	0.01	1.5	0	S	Ibl <i>et al.</i>	1954–757
303–323	0.05	3–10	0.01	1.5	0	S	Ibl <i>et al.</i>	1956–615
450–616	0.005	462–5433	0.01	1.5	1	S	Kobe <i>et al.</i>	1956–9
340–426	0.001	20–270	0.01	0.15	1	E	McCullough <i>et al.</i>	1957–176
343–363	0.1	16–342	0.05	1.5	0	S	Andon <i>et al.</i>	1957–537
341–374	0.01	8.5–102	0.01	0.5	0	S	Maczynska	1963–382
323–337	0.05	9.5–17	0.05	1.0	0	S	Findlay and Kenyon	1969–224
338–363	0.05	18–46	0.05	1.0	0	S	Findlay and Copp	1969–226
293–313	0.1	2–6	0.02	0.2	1	D	Kanakbaeva <i>et al.</i>	1974–227
298–318	0.05	3–8	0.05	1.0	0	S	Nakanishi <i>et al.</i>	1976–132
296–349	0.01	2–27	0.01	0.1	1	E	Chan and Van Hook	1976–182
298–318	0.05	3–8	0.05	1.0	0	S	Abe <i>et al.</i>	1978–131
299–354	0.005	3–33	0.1	0.5	0	S	Weclawski and Bylicki	1983–11
273–298	0.5	0.6–3	0.005	1.5	0	S	Gardener and Day	1984–49
336–443.3	0.05	16–434	0.05	1.0	0	S	Oscarson <i>et al.</i>	1987–835
2-Methylpyridine								
289–402	0.05	0.8–101	0.01	1.5	1	S	Riley and Bailey	1929–178
338–403	0.005	11–103	0.01	1.0	1	D	Herington and Martin	1953–518
353–441	0.001	20–270	0.01	0.15	1	E	Scott <i>et al.</i>	1963–156
298–318	0.05	1.6–4.5	0.01	1.0	0	S	Nakanishi <i>et al.</i>	1976–132
298–318	0.05	1.6–4.5	0.05	1.0	0	S	Abe <i>et al.</i>	1978–131
3-Methylpyridine								
360–417	0.1	16–101	0.1	1.5	0	U	Coulson and Jones	1946–308
373–416	1.0	27–101	0.05	1.0	0	S	Othmer and Savitt	1948–467
288–407	0.1	1.7–83	0.001	1.0	0	S	Liplavk and Boliter	1951–184
354–418	0.005	13–104	0.01	1.0	1	D	Herington and Martin	1953–518
343–363	0.1	16–342	0.05	1.5	0	S	Andon <i>et al.</i>	1957–537
347–458	0.001	10–270	0.01	0.2	1	S	Scott <i>et al.</i>	1963–157
298–308	0.05	0.9–1.7	0.01	1.0	0	S	Abe <i>et al.</i>	1978–131
338–348	0.02	7–26	0.05	0.5	0	S	Semeniuk <i>et al.</i>	1988–1133
4-Methylpyridine								
360–418	0.1	16–101	0.1	2.0	0	U	Coulson and Jones	1946–308
375–418	0.1	27–101	0.05	1.0	0	S	Othmer and Savitt	1948–467
289–408	0.1	2–79	0.01	1.0	0	S	Liplavk and Boliter	1951–184
350–419	0.001	10–102	0.01	1.0	1	D	Herington and Martin	1953–518
343–363	0.1	6–13	0.05	1.5	0	S	Andon <i>et al.</i>	1957–537
348–459	0.001	10–270	0.01	0.15	1	E	Osborn and Douslin	1968–206
298–338	0.05	0.8–1.5	0.01	1.0	0	S	Abe <i>et al.</i>	1978–131
338–348	0.02	7–9	0.05	0.5	0	S	Semeniuk <i>et al.</i>	1988–1133
Pyrrolidine								
359–566	0.005	100–5461	0.01	1.5	0	S	Kobe <i>et al.</i>	1956–9
316–394	0.001	20–270	0.01	0.15	1	E	McCullough <i>et al.</i>	1959–355
293–361	0.05	6.5–104	0.01	1.5	0	D	Hildenbrand <i>et al.</i>	1959–374
313–358		17–95			1		Wu <i>et al.</i>	1990–32
Piperidine								
280–380	0.05	1.3–101	0.01	1.5	0	S	Riley and Bailey	1929–178
315–417	0.001	9.6–270	0.001	0.15	1	E	Osborn and Douslin	1968–206
298–318	0.01	4–11	0.1	1.0	0	S	Nakanishi <i>et al.</i>	1975–283
Indole (Crystal)								
283–301	0.1	0.0004–0.002	0.0	1.5	1	S	Aihara	1955–710
292–319	0.1	0.0008–0.011	0.0	1.5	1	e	Serpinskii <i>et al.</i>	1958–398

TABLE 16. Available vapor pressure data — Continued

Range K	$\sigma(T)^a$ K	Range kPa	$\sigma_c(p_{\text{sat}})^a$ kPa	$10^3 \cdot \sigma_f(p_{\text{sat}})^a$	sl ^b	Meth. ^c	Author(s)	Ref.
Quinoline								
348–511	0.1	0.3–101	0.01	1.5	0	S	Young	1889–25
511–735	0.5	101–3040	0.05	1.5	1	S	Glaser and Ruland	1957–76
438–511	0.02	15–102	0.01	1.0	0	E	Malanowski	1961–32
377–506		1.6–100			0			1962–471
286–309	0.01	0.004–0.02	0.1	0.15	0	D	Van De Rostyne and Prausnitz	1980–6
433–503	0.01	12–74	0.1	0.15	0	S	Krevor <i>et al.</i>	1986–24
450–548	0.05	23–223	0.15	1.5	0	S	Klara <i>et al.</i>	1987–21
523–598	0.1	135–520	0.15	1.5	0	D	Niesen and Yesavage	1988–70
298–559	0.0001	0.01–270	0.1	0.15	1	E	Steele <i>et al.</i>	1988–551
544–644	0.1	206–1034	0.1	1.5	0	E	Flanigan <i>et al.</i>	1988–555
Isoquinoline								
440–517	0.02	13–102	0.01	1.0	0	E	Malanowski	1961–32
313–566	0.0001	0.03–270	0.1	0.15	1	E	Steele <i>et al.</i>	1988–551
Carbazole (Crystal)								
342–362	0.1	0.00009–0.0005	0.0	1.5	1	U	Aihara	1955–710
347–364		0.00006–0.0003			1	e	Jimenez <i>et al.</i>	1990–65
Carbazole (Liquid)								
526–631	0.05	9–108	0.01	1.0	0	S	Senseman and Nelson	1923–166
518–625	0.1	7–99	0.1	1.5	0	S	Mortimer and Murphy	1923–167
522–642	0.01	9–133	0.01	0.15	1	S	Sivaraman <i>et al.</i>	1983–185
Acridine (Crystal)								
281–389	0.1	0.0000007–0.000002	0.0	1.5	1	F	McEchern <i>et al.</i>	1975–228
Acridine (Liquid)								
424–621	0.01	0.4–108	0.1	1.0	0	S	Sivaraman and Kobayashi	1983–189
383–637	0.0001	0.04–143	0.1	0.15	1	E	Steele <i>et al.</i>	1989–76
Phenanthridine (Crystal)								
288–323	0.1	0.0000008–0.00006	0.0	1.5	1	F	McEchern <i>et al.</i>	1975–229
Phenanthridine (Liquid)								
383–473	0.0001	0.03–1.9	0.1	0.15	1	E	Steele <i>et al.</i>	1989–76
1-Naphthalenamine (Liquid)								
377–574	0.05	0.13–101.3	0.0	1.5	1	U	Stull	1947–83
2-Naphthalenamine (Crystal)								
283–323	0.1	0.000001–0.00004	1	e			Karykin <i>et al.</i>	1986–3
2-Naphthalenamine (Liquid)								
381–579	0.05	0.13–101.3	0.0	1.5	1	U	Stull	1947–83
9-Methylcarbazole (Crystal)								
313–333		0.00005–0.0005			1	e	Jimenez <i>et al.</i>	1990–65
9-Methylcarbazole (Liquid)								
373–674	0.001	0.016–270	.0005	0.5	1	E	Steele <i>et al.</i>	1992–3

*See Sec. 1.6.

^b1 for data selected and 0 for data not selected for least squares fit.^cMethod of measurement: S, static; E, ebulliometric; F, molecular flow; G, gas saturation; e, effusion; and U, unspecified.

TABLE 17. Available saturated liquid density data

Range K	$\sigma(T)^a$ K	Range kg·m ⁻³	$\sigma(\rho)^a$ kg·m ⁻³	sl ^b	N ^c	Author(s)	Ref.
1-Butanamine							
273–299	0.5	755–730	0.5	0	2	Lieben and Rossi	1871–21
292–346	0.5	713–689	0.3	0	6	Freind and Hageaves	1944–125
293–335	0.5	741–702	0.5	0	3	Vogel	1948–262
213–433	0.5	814–597	0.45	1	12	Costello and Bowden	1959–218
293–313	0.5	741–723	1.5	0	3	Zhigunov and Ampeloga	1972–237
303–313	0.3	735–725	0.3	1	2	Sreenivasulu and Naidu	1978–77
298–313	0.3	737–725	0.3	0	3	Sreenivasulu and Naidu	1979–96
298–313	0.3	737–725	0.3	0	3	Sreenivasulu and Naidu	1979–209
2-Butanamine							
290–293	0.5	727–723	0.5	1	2	Bruhl	1895–49
293–314	0.5	724–705	0.5	1	2	Vogel	1948–262
2-Methyl-1-propanamine							
277–298	0.3	746–726	0.3	0	5	Perkin	1889–26
290–293	0.3	736–733	0.5	0	2	Bruhl	1895–49
293–333	0.1	734–695	0.5	1	3	Vogel	1948–262
213–433	0.2	804–580	0.45	1	12	Costello and Bowden	1959–218
2-Methyl-2-propanamine							
291–293	0.01	698–696	0.6	0	2	Bruhl	1897–43
278–313	0.5	707–672	0.5	1	4	Krishnaji and Mansingh	1965–387
293–303	0.2	696–684	0.2	1	2	Otin <i>et al.</i>	1973–148
273–288	0.2	715–700	0.6	1	2	Whitmer and Cyvin	1978–36
Pyrrole							
898–293	0.2	958–953	0.4	0	2	Dezelic	1937–487
274–333	0.3	985–935	0.3	0	4	Holland and Smyth	1955–11
273–303	0.02	987–961	0.15	1	4	Timmermans <i>et al.</i>	1955–485
293–303	0.02	970–961	0.2	1	3	Helm <i>et al.</i>	1958–216
1-Methylpyrrole							
289–293	0.3	911–907	0.5	0	2	Auwers and Kohlhas	1924–198
293–303	0.2	910–900	0.4	1	3	API Project 52	1958–417
298.15	0.005	904.69	0.04	1	1	Good	1972–41
2-Methylpyrrole							
288.2	0.2	944.6	0.6	0	1	Pictet	1904–106
293.2	0.2	942.6	0.5	0	1	Mikhaleva <i>et al.</i>	1979–333
Pyridine							
292–294	0.02	982–981	0.5	0	6	Bruhl	1895–49
237–274	0.03	1039–1003	0.5	0	2	Timmermans	1907–128
284–347	0.03	991–927	2.0	0	4	Livingston <i>et al.</i>	1908–112
273–298	0.02	1003–978	0.3	0	4	Timmermans	1910–58
273–383	0.01	1001–890	0.4	0	8	Bramley	1916–37
293–298	0.01	982–976	0.5	0	2	Arndt and Nachtway	1926–210
273–363	0.04	1003–911	0.3	1	19	Muller and Brenneis	1932–322
298–363	0.04	977–912	0.45	0	2	Bratton <i>et al.</i>	1935–418
273–303	0.02	1003–973	0.15	0	3	Timmermans <i>et al.</i>	1937–146
293–298	0.01	983–979	0.3	0	2	Leis and Curran	1945–205
271–308	0.01	985–969	0.4	0	6	Hatem	1949–43
283–323	0.01	994–953	0.3	1	5	Lagemann <i>et al.</i>	1949–264
273–333	0.02	1000–943	0.5	0	5	Naumova	1953–615
293–303	0.02	983–972	0.1	0	2	Biddiscombe <i>et al.</i>	1954–31
274–333	0.3	995–942	0.3	0	4	Holland and Smyth	1955–11
293–333	0.01	983–943	0.5	1	3	Toropov	1956–639
293–303	0.01	983–973	0.25	1	3	Helm <i>et al.</i>	1958–216
288–303	0.01	988–973	0.5	1	4	Mato and Sanchez	1967–321
298–308	0.03	978–968	0.3	1	2	Deshpande <i>et al.</i>	1971–130
293–318	0.03	968–958	0.5	1	4	Meyer <i>et al.</i>	1971–213
303–313	0.03	973–963	0.4	1	2	Rao and Naidu	1973–222
293–323	0.02	983–953	0.1	0	4	Malanowski <i>et al.</i>	1979–207
303–333	0.03	973–943	0.4	1	2	Pikkarainen	1980–121

TABLE 17. Available saturated liquid density data — Continued

Range K	$\sigma(T)^a$ K	Range kg·m ⁻³	$\sigma(\rho)^a$ kg·m ⁻³	sl ^b	N ^c	Author(s)	Ref.
298–328	0.03	981–962	1.5	0	5	Gokavi <i>et al.</i>	1986–2
2-Methylpyridine							
290–296	0.2	951–943	0.5	0	6	Bruhl	1895–49
293–353	0.03	944–887	0.1	1	7	Freiser and Glowacki	1948–442
293–303	0.5	944–935	0.1	0	2	Biddiscombe <i>et al.</i>	1954–31
273–303	0.02	963–925	0.15	0	4	Timmermans <i>et al.</i>	1955–485
293–333	0.05	942–905	0.5	0	3	Totopov	1956–639
293–303	0.1	944–935	0.25	0	3	Helm <i>et al.</i>	1958–216
293–358	0.02	944–885	0.4	0	6	Kyte <i>et al.</i>	1960–119
293–318	0.05	944–921	0.4	1	4	Meyer <i>et al.</i>	1971–213
273–353	0.03	963–889	0.3	1	13	Minana Aznar <i>et al.</i>	1984–95
3-Methylpyridine							
293–297	0.2	958–954	0.5	0	2	Bruhl	1895–49
293–303	0.5	957–947	0.1	1	2	Biddiscombe <i>et al.</i>	1954–31
293–358	0.02	957–900	0.4	1	4	Kyte <i>et al.</i>	1960–119
4-Methylpyridine							
293–303	0.5	955–946	0.1	1	2	Biddiscombe <i>et al.</i>	1954–31
274–333	0.3	971–917	0.3	0	4	Holland and Smyth	1955–11
293–358	0.02	954–896	0.4	1	7	Kyte <i>et al.</i>	1960–119
293–318	0.05	955–932	0.4	1	4	Meyer <i>et al.</i>	1971–213
298.15	0.005	950.37	0.04	1	1	Good	1972–41
Pyrrolidine							
274–333	0.3	887–829	0.3	0	4	Holland and Smyth	1955–11
293–303	0.1	859–849	0.25	1	3	Helm <i>et al.</i>	1958–216
Piperidine							
277–298	0.3	876–857	0.3	1	5	Perkin	1889–26
298–353	0.5	856–803	0.3	0	3	Kurnakow and Zemczuny	1913–179
273–303	0.02	880–852	0.1	1	3	Timmermans and Hennaut-Roland	1937–146
287–368	0.3	883–806	0.3	0	6	Friend and Hargreaves	1944–126
273–348	0.1	881–811	0.2	1	4	Teitelbaum <i>et al.</i>	1947–402
293–303	0.05	861–852	0.15	1	3	1960–369	
Quinoline							
288–493	0.3	1098–931	0.3	0	7	Lumsden	1907–64
304–338	0.5	1085–1058	0.5	0	3	Livingston <i>et al.</i>	1908–112
281–347	0.1	1103–1051	0.3	0	4	Schwers	1911–44
273–423	0.2	1108–988	0.2	0	9	Bramley	1916–37
273–303	0.02	1110–1086	0.15	0	3	Timmermans and Hennaut-Roland	1937–146
291–308	0.2	1097–1084	0.3	0	6	Hatem	1949–43
298–313	0.3	1086–1069	0.5	0	2	Tschamler and Krischai	1951–444
293–363	0.3	1094–1039	0.3	0	3	Kovalenko and Trifonov	1954–674
274–333	0.3	1108–1062	0.5	0	4	Holland and Smyth	1955–11
243–323	0.05	1138–1075	0.5	1	9	Mallikarjun and Hill	1965–231
298–318	0.3	1089–1074	0.4	0	4	Irwin <i>et al.</i>	1984–246
298–358	0.2	1088–1041	0.5	0	4	Oshmyansky <i>et al.</i>	1986–86
298–424	0.01	1090–988	0.15	1	6	Steele <i>et al.</i>	1988–551
Isoquinoline							
303–473	0.1	1091–953	0.2	1	11	Freiser and Glowacki	1949–545
298–333	0.3	1094–1066	0.3	0	3	Holland and Smyth	1955–11
298–323	0.3	1095–1075	0.5	0	4	Mallikarjun and Hill	1965–231
300–373	0.05	1093–1035	0.15	1	4	Steele <i>et al.</i>	1988–551
Carbazole							
520–524	0.3	1000–997	0.3	0	2	Burriel	1931–8
523–583	0.1	1004–960	0.5	1	4	Gurevich and Bednov	1972–326
Acridine							
392	0.05	1080	1.	0	1	Steele <i>et al.</i>	1989–76

TABLE 19. Available enthalpy of vaporization data at 298.15 K — Continued

x^a	T K	ΔH_m kJ·mol ⁻¹	$\sigma(\Delta H_m)^b$ kJ·mol ⁻¹	Method	sl ^c	Author(s)	Ref.
1	368.15	36.25	0.10	Calorimetry	0	Majer <i>et al.</i>	1984-94
1	298.15	40.23	0.20	Vapor press.	0	TRC — this work	
2-Methylpyridine							
1	402.15	35.36	0.20	Calorimetry	0	Kahlenberg	1901-64
1	400.88	36.12	0.40	Calorimetry	0	Constan and White	1903-66
1	359.35	38.84	0.10	Calorimetry	0	Scott <i>et al.</i>	1963-156
1	379.48	37.66	0.10	Calorimetry	0	Scott <i>et al.</i>	1963-156
1	402.54	36.21	0.10	Calorimetry	0	Scott <i>et al.</i>	1963-156
1	298.15	42.51	0.10	Calorimetry	1	Majer <i>et al.</i>	1984-94
1	313.15	41.61	0.10	Calorimetry	0	Majer <i>et al.</i>	1984-94
1	328.15	40.74	0.10	Calorimetry	0	Majer <i>et al.</i>	1984-94
1	343.15	39.83	0.10	Calorimetry	0	Majer <i>et al.</i>	1984-94
1	358.15	38.93	0.10	Calorimetry	0	Majer <i>et al.</i>	1984-94
1	368.15	38.27	0.10	Calorimetry	0	Majer <i>et al.</i>	1984-94
1	298.15	42.42	0.50	Vapor press.	1	TRC — this work	
3-Methylpyridine							
1	414.84	36.95	2.10	Calorimetry	0	Constan and White	1903-66
1	372.45	40.16	0.10	Calorimetry	0	Scott <i>et al.</i>	1963-157
1	393.36	38.89	0.10	Calorimetry	0	Scott <i>et al.</i>	1963-157
1	417.29	37.31	0.10	Calorimetry	0	Scott <i>et al.</i>	1963-157
1	298.15	44.83	0.10	Calorimetry	1	Kusano and Saito	1976-127
1	298.15	44.64	0.10	Calorimetry	1	Majer <i>et al.</i>	1984-94
1	313.15	43.63	0.10	Calorimetry	0	Majer <i>et al.</i>	1984-94
1	328.15	42.74	0.10	Calorimetry	0	Majer <i>et al.</i>	1984-94
1	343.15	41.98	0.10	Calorimetry	0	Majer <i>et al.</i>	1984-94
1	358.15	40.96	0.10	Calorimetry	0	Majer <i>et al.</i>	1984-94
1	368.15	40.38	0.10	Calorimetry	0	Majer <i>et al.</i>	1984-94
1	298.15	44.01	0.20	Vapor press.	1	TRC — this work	
4-Methylpyridine							
1	298.15	44.56	0.20	Vapor press.	0	Good	1972-41
1	298.15	45.74	0.10	Calorimetry	0	Kusano and Saito	1976-127
1	355.04	41.38	0.10	Calorimetry	0	Hossenlopp and Scott	1981-44
1	365.58	40.75	0.10	Calorimetry	0	Hossenlopp and Scott	1981-44
1	373.53	40.27	0.10	Calorimetry	0	Hossenlopp and Scott	1981-44
1	385.47	39.55	0.10	Calorimetry	0	Hossenlopp and Scott	1981-44
1	394.51	39.01	0.10	Calorimetry	0	Hossenlopp and Scott	1981-44
1	418.52	37.52	0.10	Calorimetry	0	Hossenlopp and Scott	1981-44
1	434.26	36.52	0.10	Calorimetry	0	Hossenlopp and Scott	1981-44
1	298.15	44.56	0.10	Calorimetry	1	Majer <i>et al.</i>	1984-94
1	313.15	43.85	0.10	Calorimetry	0	Majer <i>et al.</i>	1984-94
1	328.15	42.93	0.10	Calorimetry	0	Majer <i>et al.</i>	1984-94
1	343.15	42.09	0.10	Calorimetry	0	Majer <i>et al.</i>	1984-94
1	358.15	41.15	0.10	Calorimetry	0	Majer <i>et al.</i>	1984-94
1	368.15	40.56	0.10	Calorimetry	0	Majer <i>et al.</i>	1984-94
1	298.15	44.64	0.20	Vapor press.	0	TRC — this work	
Pyrrolidine							
1	298.15	37.61	0.13	Calorimetry	0	Hildenbrand <i>et al.</i>	1959-374
1	321.90	35.75	0.10	Calorimetry	0	McCullough <i>et al.</i>	1959-355
1	339.50	34.48	0.10	Calorimetry	0	McCullough <i>et al.</i>	1959-355
1	359.72	33.01	0.10	Calorimetry	0	McCullough <i>et al.</i>	1959-355
1	298.15	37.52	0.10	Calorimetry	1	Majer and Svoboda	1985-23
1	298.15	37.69	0.10	Vapor press.	0	TRC — this work	
Piperidine							
1	378.91	31.68	0.20	Calorimetry	0	Louguinine	1899-11
1	298.15	39.29	0.20	Vapor press.	1	Good	1972-41
1	338.34	36.58	0.02	Calorimetry	0	Hossenlopp and Archer	1988-556
1	357.42	35.25	0.02	Calorimetry	0	Hossenlopp and Archer	1988-556
1	379.36	33.75	0.03	Calorimetry	0	Hossenlopp and Archer	1988-556
1	298.15	39.44	0.20	Vapor press.	0	TRC — this work	

TABLE 19. Available enthalpy of vaporization data at 298.15 K – Continued

x^a	T K	ΔH_m kJ·mol ⁻¹	$\sigma(\Delta H_m)^b$ kJ·mol ⁻¹	Method	sl ^c	Author(s)	Ref.
Indole							
cr	298.15	69.9	1.0	Vapor press.	1	Aihara	1955–710
cr	298.15	77.8	2.5	Vapor press.	0	Arshadi	1974–238
cr	298.15	68.5	1.0	Vapor press.	0	TRC – this work	
Quinoline							
l	544.00	55.0	0.8	Calorimetry	0	Flanigan <i>et al.</i>	1988–555
l	595.80	39.42	0.85	Calorimetry	0	Flanigan <i>et al.</i>	1988–555
l	617.80	37.64	0.92	Calorimetry	0	Flanigan <i>et al.</i>	1988–555
l	644.20	35.58	0.96	Calorimetry	0	Flanigan <i>et al.</i>	1988–555
l	260.00	61.78	0.48	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	280.00	60.48	0.31	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	298.15	59.31	0.20	Vapor press.	1	Steele <i>et al.</i>	1988–551
l	300.00	59.20	0.19	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	320.00	57.93	0.12	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	340.00	56.69	0.07	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	360.00	55.46	0.03	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	380.00	54.26	0.02	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	400.00	53.08	0.03	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	420.00	51.92	0.06	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	440.00	50.75	0.08	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	460.00	49.60	0.12	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	480.00	48.43	0.18	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	500.00	47.25	0.26	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	520.00	46.05	0.35	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	540.00	44.81	0.46	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	560.00	43.53	0.60	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	580.00	42.20	0.76	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	600.00	40.80	0.94	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	298.15	59.45	0.20	Vapor press.	0	TRC – this work	
Isoquinoline							
l	298.15	60.26	0.12	Vapor press.	1	Steele <i>et al.</i>	1988–551
l	300.00	60.15	0.11	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	320.00	58.89	0.07	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	340.00	57.65	0.04	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	360.00	56.43	0.02	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	380.00	55.43	0.02	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	400.00	54.06	0.02	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	420.00	52.89	0.05	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	440.00	51.73	0.07	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	460.00	49.60	0.12	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	480.00	48.43	0.18	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	500.00	47.25	0.26	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	520.00	46.05	0.35	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	540.00	44.81	0.46	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	560.00	43.53	0.60	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	580.00	42.20	0.76	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	600.00	40.80	0.94	Vapor press.	0	Steele <i>et al.</i>	1988–551
l	298.15	60.08	0.50	Vapor press.	0	TRC – this work	
Acridine							
cr	300.00	91.63	2.0	Vapor press.	0	McEachern <i>et al.</i>	1975–228
cr	298.15	94.5	4.0	Vapor press.	1	Steele <i>et al.</i>	1989–76
l	380.00	72.94	0.23	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	400.00	71.59	0.23	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	420.00	70.26	0.23	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	440.00	68.94	0.23	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	460.00	67.65	0.23	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	480.00	66.37	0.23	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	500.00	65.09	0.22	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	520.00	63.83	0.22	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	540.00	62.56	0.22	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	560.00	61.27	0.22	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	580.00	59.96	0.22	Vapor press.	0	Steele <i>et al.</i>	1989–76

TABLE 19. Available enthalpy of vaporization data at 298.15 K – Continued

x^a	T K	ΔH_m kJ·mol ⁻¹	$\sigma(\Delta H_m)^b$ kJ·mol ⁻¹	Method	sl ^c	Author(s)	Ref.
Acridine – Continued							
l	600.00	58.62	0.27	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	620.00	57.24	0.30	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	640.00	55.82	0.35	Vapor press.	0	Steele <i>et al.</i>	1989–76
cr	298.15	94.2	4.0	Vapor press.	0	TRC – this work	
Carbazole							
cr	298.15	99.0	4.0	Vapor press.	1	Aihara	1955–710
cr	355.27	117.	2.0	Vapor press.	0	Jimenez <i>et al.</i>	1990–65
cr	298.15	98.2	4.0	Vapor press.	0	TRC – this work	
Phenanthridine							
cr	298.15	98.6	4.0	Vapor press.	1	Steele <i>et al.</i>	1989–76
l	380.00	74.31	0.22	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	400.00	72.93	0.24	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	420.00	71.59	0.24	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	440.00	70.26	0.24	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	460.00	68.95	0.24	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	480.00	67.67	0.28	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	500.00	66.40	0.30	Vapor press.	0	Steele <i>et al.</i>	1989–76
l	520.00	65.14	0.32	Vapor press.	0	Steele <i>et al.</i>	1989–76
cr	298.15	100.	4.0	Vapor press.	0	TRC – this work	
1-Naphthalenamine							
cr	298.15	65.0	4.0	Estimated	1	TRC – this work	
2-Naphthalenamine							
cr	303.15	74.1	4.0	Vapor Press.	1	Karyakin <i>et al.</i>	1968–3
9-Methylcarbazole							
cr	322.69	95.0	1.0	Vapor press.	0	Jimenez <i>et al.</i>	1990–65
l	380.00	74.89	0.02	Vapor press.	0	Steele <i>et al.</i>	1992–3
l	400.00	73.41	0.02	Vapor press.	0	Steele <i>et al.</i>	1992–3
l	420.00	71.95	0.01	Vapor press.	0	Steele <i>et al.</i>	1992–3
l	440.00	70.52	0.01	Vapor press.	0	Steele <i>et al.</i>	1992–3
l	460.00	69.12	0.02	Vapor press.	0	Steele <i>et al.</i>	1992–3
l	480.00	76.73	0.02	Vapor press.	0	Steele <i>et al.</i>	1992–3
l	500.00	66.35	0.03	Vapor press.	0	Steele <i>et al.</i>	1992–3
l	520.00	64.96	0.06	Vapor press.	0	Steele <i>et al.</i>	1992–3
l	540.00	63.56	0.08	Vapor press.	0	Steele <i>et al.</i>	1992–3
l	560.00	62.13	0.12	Vapor press.	0	Steele <i>et al.</i>	1992–3
l	580.00	60.66	0.16	Vapor press.	0	Steele <i>et al.</i>	1992–3
l	600.00	59.15	0.21	Vapor press.	0	Steele <i>et al.</i>	1992–3
cr	298.15	95.5	4.0	Vapor press.	1	TRC – this work	

^aDesignation for condensed phase (x).^bSee Sec. 1.6.^c1 for data selected and 0 for data not selected.

TABLE 20. Available enthalpy of combustion data referred to 298.15 K

ph ^a	$\Delta_c U^\circ/M$ kJ·g ⁻¹	$2\sigma(\Delta_c U^\circ/M)^b$ kJ·g ⁻¹	$\Delta_c H^\circ$ kJ·mol ⁻¹	$2\sigma(\Delta_c H^\circ)^b$ kJ·mol ⁻¹	Author(s)	Ref.
1-Butanamine						
1	-40.8	0.2	-2989	20	Lemoult	1907-116
1	-40.6	0.2	-2974	20	Swietoslawski and Popov	1925-236
1	-41.1951	0.0077	-3018.46	1.13	Evans <i>et al.</i>	1959-313
2-Butanamine						
1	-40.7	0.2	-2984	20	Lemoult	1907-116
1	-41.0606	0.0061	-3008.63	0.92	Evans <i>et al.</i>	1959-313
2-Methyl-1-propanamine						
1	-40.8	0.2	-2987	20	Lemoult	1907-116
1	-41.1266	0.0009	-3013.52	0.42	Good and Moore	1970-167
2-Methyl-2-propanamine						
1	-41.0	0.2	-3001	20	Lemoult	1907-116
1	-40.8	0.2	-2986	20	Swietoslawski and Popov	1925-236
1	-40.885	0.0075	-2995.79	1.13	Evans <i>et al.</i>	1959-313
1	-40.8798	0.0007	-2995.49	0.42	Smith and Good	1967-60
Pyrrole						
1	-35.4	0.4	-2377	25	Berthelot and Andre	1899-60
1	-35.0247	0.0012	-2351.68	0.67	Scott <i>et al.</i>	1967-116
1-Methylpyrrole						
1	-37.3189	0.0012	-3030.35	0.42	Good	1972-41
2-Methylpyrrole						
1	-36.83	0.02	-2991	2	TRC - this work ^c	
3-Methylpyrrole						
1	-36.84	0.02	-2988	2	TRC - this work ^c	
Pyridine						
1	-35.15	0.03	-2782	3	Delepine	1898-41
1	-34.8	0.4	-2756	30	Constam and White	1903-66
1	-35.17	0.03	-2784	3	Swietoslawski	1909-138
1	-35.152	0.019	-2782	3	Cox <i>et al.</i>	1954-514
1	-35.1497	0.0015	-2782.28	0.42	Hubbard <i>et al.</i>	1961-295
2-Methylpyridine						
1	-36.6	0.4	-3412	30	Constam and White	1903-66
1	-36.695	0.0013	-3420.5	2.6	Cox <i>et al.</i>	1954-514
1	-36.6705	0.0023	-3418.16	0.67	Scott <i>et al.</i>	1963-156
3-Methylpyridine						
1	-36.5	0.4	-3399	30	Constam and White	1903-66
1	-36.795	0.001	-3429.8	2.0	Cox <i>et al.</i>	1954-514
1	-36.7267	0.0018	-3423.39	0.50	Scott <i>et al.</i>	1963-156
4-Methylpyridine						
1	-36.6	0.4	-3414	30	Constam and White	1903-66
1	-36.674	0.015	-3418.3	1.3	Cox <i>et al.</i>	1954-514
1	-36.6969	0.0054	-3420.63	0.84	Good	1972-41
Pyrrolidine						
1	-39.5785	0.0008	-2819.30	0.84	Hildenbrand <i>et al.</i>	1959-116
1	-39.5741	0.0046	-2819.17	0.75	McCullough <i>et al.</i>	1959-353
Piperidine						
1	-40.6	0.2	-3458	20	Delepine	1898-42
1	-40.6	0.2	-3458	20	Delepine	1899-62
1	-40.47	0.03	-3451.5	2.3	Bedford <i>et al.</i>	1963-357
1	-40.4892	0.0059	-3453.18	0.83	Good	1972-41

TABLE 20. Available enthalpy of combustion data referred to 298.15 K

ph ^a	$\frac{\Delta_c U^\circ/M}{\text{kJ}\cdot\text{g}^{-1}}$	$\frac{2\sigma(\Delta_c U^\circ/M)^b}{\text{kJ}\cdot\text{g}^{-1}}$	$\frac{\Delta_c H^\circ}{\text{kJ}\cdot\text{mol}^{-1}}$	$\frac{2\sigma(\Delta_c H^\circ)^b}{\text{kJ}\cdot\text{mol}^{-1}}$	Author(s)	Ref.
Indole						
cr	-36.5	0.3	-4278	30	Berthelot and Andre	1899-60
cr	-36.5	0.3	-4278	30	Berthelot and Andre	1899-61
cr	-36.38	0.04	-4265.2	4.2	Stern and Klebs	1932-334
cr	-36.1249	0.0058	-4235.13	0.63	Good	1972-41
Quinoline						
l	-36.4	0.2	-4702	20	Delepine	1898-42
l	-36.4	0.2	-4702	20	Delepine	1899-62
l	-36.2342	0.0016	-4683.21	0.80	Steele <i>et al.</i>	1988-551
Isoquinoline						
l	-36.1	0.2	-4688	20	Delepine	1898-42
l	-36.1	0.2	-4688	20	Delepine	1899-62
l	-36.2595	0.0058	-4686.5	0.75	Good	1972-41
Acridine						
cr	-36.82	0.04	-6602.8	6.7	Albert and Willis	1946-316
cr	-36.82	0.04	-6602.8	6.7	Willis	1947-404
cr	-36.6972	0.0005	-6581.27	0.90	Steele <i>et al.</i>	1989-76
Carbazole						
cr	-36.9	0.2	-6173	40	Berthelot and Andre	1899-60
cr	-36.9	0.2	-6173	40	Berthelot and Andre	1899-61
cr	-36.66	0.02	-6133.5	3.6	Tavernier and Lamouroux	1957-593
cr	-36.5160	0.0036	-6110.1	2.3	Jimenez <i>et al.</i>	1990-65
Phenanthridine						
cr	-36.4825	0.0023	-6542.79	1.22	Steele <i>et al.</i>	1989-76
1-Naphthalenamine						
cr	-37.1	0.2	-5316	25	Lemoult	1907-116
cr	-36.9	0.2	-5289	25	Swietoslawski and Popov	1925-236
cr	-36.91	0.04	-5289.0	5.4	Milone and Rossignoli	1932-52
2-Naphthalenamine						
cr	-37.0	0.2	-5306	25	Lemoult	1907-116
s	-36.8	0.2	-5279	25	Swietoslawski and Popov	1925-236
cr	-36.87	0.04	-5284.0	5.4	Milone and Rossignoli	1932-52
cr	-36.84	0.03	-5279.0	4.6	Willis	1947-384
9-Methylcarbazole						
cr	-37.4513	0.0045	-6793.18	0.83	Good	1972-41
cr	-37.4418	0.0093	-6791.4	1.7	Jimenez <i>et al.</i>	1990-65

^aPhase of substances for which measurements were made.^bSee Sec. 1.6.^cEstimated.

TABLE 21. Enthalpies of formation of auxiliary substances at 298.15 K

Compound	Phase	$\Delta_f H^\circ/\text{kJ}\cdot\text{mol}^{-1}$ ^a	Ref.
Carbon dioxide	g	-393.51 ± 0.13	1978-115
Water	g	-241.814 ± 0.042	1978-115
Water	l	-285.830 ± 0.042	1978-115

^aUncertainties are two standard errors, see Sec. 1.6.

TABLE 22. Available heat capacity and phase transition data for the condensed phases

ph.	Range K	Heat Capacity		$\sigma_f(C_{sat})^a$	Pts.	Trans.	Phase Transition		$\sigma(\Delta_{tr}H)^a$ J·mol ⁻¹	Author(s)	Ref.
		$\sigma(T)^a$ K	$\sigma_c(C_{sat})^a$ R				T K	$\frac{\Delta_{tr}H}{J·mol^{-1}}$			
1-Butanamine											
l	—	—	—	—	—	cr $\rightleftharpoons$ l	222.65	—	—	Timmermans and Mattaar	1921–17
	—	—	—	—	—	cr $\rightleftharpoons$ l	224.05	—	—	Anonymous	1968–195
	298.15	—	—	0.005	1	—	—	—	—	Konicek and Wadsö	1971–11
2-Butanamine											
—	—	—	—	—	—	cr $\rightleftharpoons$ l	168.65	—	—	Timmermans and Mattaar	1921–17
2-Methyl-1-propanamine											
l	—	—	—	—	—	cr $\rightleftharpoons$ l	187.65	—	—	Timmermans and Mattaar	1921–17
	—	—	—	—	—	cr $\rightleftharpoons$ l	186.45	—	—	Simon and Huter	1935–278
	—	—	—	—	—	cr $\rightleftharpoons$ l	188.55	—	—	Simon and Huter	1935–280
	298.15	—	—	0.005	1	—	—	—	—	Konicek and Wadsö	1971–11
2-Methyl-2-propanamine											
l	298.15	—	—	0.001	1	—	—	—	—	Smith and Good	1967–60
l	298.15	—	—	0.005	1	—	—	—	—	Konicek and Wadslapos' o	1971–11
crIII	11.8–91.3	0.002	0.035	0.005 ^c	42	crIII $\rightleftharpoons$ crII	91.30	113.51	0.05	Finke <i>et al.</i>	1972–140
crII	91.51–196.41	0.002	0	0.005 ^c	24	crII $\rightleftharpoons$ crI	202.27	6052.6	0.5		
crI	202.99–204.98	0.002	0	0.005 ^c	4	crI $\rightleftharpoons$ l	206.19	882	1		
l	209.78–332.49	0.002	0	0.001	20	—	—	—	—		
Pyrrole											
crII,I	—	—	—	—	—	cr $\rightleftharpoons$ l	—	7908	25	Anonymous	1956–676
	11.48–238.03	0.002	0.020	0.005 ^c	84	crII $\rightleftharpoons$ crI	65.5	< 1.5	—	Scott <i>et al.</i>	1967–116
l	—	—	—	—	—	crI $\rightleftharpoons$ l	249.735	7908	4		
l	256.15–359.74	0.002	0	0.001	20	—	—	—	—		
1-Methylpyrrole											
cr	—	—	—	—	—	cr $\rightleftharpoons$ l	—	7828	42	Anonymous	1960–369
	11.369–201.574	0.002	0.025	0.005 ^c	73	cr $\rightleftharpoons$ l	216.912	7825	3	Messerly <i>et al.</i>	1988–93
l	221.181–364.655	0.002	0	0.001	37	—	—	—	—		
2-Methylpyrrole											
—	—	—	—	—	—	cr $\rightleftharpoons$ l	237.55	—	—	Anonymous	1957–605
	—	—	—	—	—	cr $\rightleftharpoons$ l	237.55	—	—	Lanum and Morris	1969–51
3-Methylpyrrole											
—	—	—	—	—	—	cr $\rightleftharpoons$ l	224.75	—	—	Lanum and Morris	1969–51

TABLE 22. Available heat capacity and phase transition data for the condensed phases — Continued

ph.	Range K	Heat Capacity		$\sigma_f(C_{sat})^a$	Pts.	Trans.	Phase Transition		$\sigma(\Delta_{tr}H)^a$ J·mol ⁻¹	Author(s)	Ref.
		$\sigma(T)^a$ K	$\sigma_c(C_{sat})^a$ R				$\frac{T}{K}$	$\frac{\Delta_{tr}H}{J·mol^{-1}}$			
Pyridine											
l	294.6–380.7	—	—	0.05	1		—	—	—	Louguinine	1899–11
l	327.75–371.46	—	—	0.05	1		—	—	—	Constam and White	1903–66
l	293.15	—	—	0.05	1		—	—	—	Timofeev	1905–94
l	273.15–293.15	—	—	0.05	1		—	—	—	Bramley	1916–244
l	294.15	—	—	0.05	1		—	—	—	Mathews <i>et al.</i>	1917–66
l	300.15	0.1	0	0.05	1		—	—	—	Swietoslawski <i>et al.</i>	1931–362
l	289.15	—	—	0.02	1		—	—	—	Radulescu and Jula	1934–351
cr	90–220	0.15	0.07	0.01 ^c	14	cr $\rightleftharpoons$ l	231.15	8270	30	Parks <i>et al.</i>	1936–163
l	230–300	0.15	0	0.01	8		—	—	—		
cr	90.0–223.1	0.15	0.08	0.01 ^c	15	cr $\rightleftharpoons$ l	230.38	3100	—	Pearce and Bakke	1936–442
l	233.1–298.1	0.15	0	0.01	8		—	—	—		
cr	13.080–223.74	0.002	0.034	0.005 ^c	101	cr $\rightleftharpoons$ l	231.489	8278	8	McCullough <i>et al.</i>	1957–176
l	239.7–346.69	0.002	0	0.001	13		—	—	—		
l	294.85–369.45	0.1	0	0.01	1		—	—	—	Swietoslawski and Zielenkiewicz	1958–69
l	293.15–373.15	0.01	0	0.01	5		—	—	—	Rastorguev and Ganiev	1967–37
2-Methylpyridine											
cr	12.37–188.56	0.002	0.031	0.005 ^c	60	cr $\rightleftharpoons$ l	206.466	9724	6	Scott <i>et al.</i>	1963–156
l	209.9–369.01	0.002	0	0.001	18		—	—	—		
cr	1.5–90.0	0.002	—	— ^b	~100	—	—	—	—	den Adel <i>et al.</i>	1981–138
3-Methylpyridine											
cr	11.94–242.35	0.002	0.025	0.005 ^c	58	cr $\rightleftharpoons$ l	255.01	14180	4	Scott <i>et al.</i>	1963–157
l	257.52–387.93	0.002	0	0.001	16	—	—	—	—		
cr	1.5–90.0	0.002	—	— ^b	~100	—	—	—	—	den Adel <i>et al.</i>	1981–138
4-Methylpyridine											
cr	1.5–90.0	0.002	—	— ^b	~100	—	—	—	—	den Adel <i>et al.</i>	1981–138
crII	13.198–252.094	0.002	0.089	0.005 ^c	64	crII $\rightleftharpoons$ crI	255.00	0	3	Messerly <i>et al.</i>	1988–93
crI	256.26–270.168	0.002	0	0.005 ^c	7	crI $\rightleftharpoons$ l	276.818	12582	2		
l	233.155–394.846	0.002	0	0.001	16	—	—	—	—		
Pyrrolidine											
l	298.15	0.01	0	0.01	1		—	—	—	Patton	1952–573
crII	13.050–204.240	0.002	0.032	0.005 ^c	63	crII $\rightleftharpoons$ crI	207.140	540	2	McCullough <i>et al.</i>	1959–355
crI	209.17–211.56	0.002	0	0.005 ^c	9	crI $\rightleftharpoons$ l	215.45	8577	6		
l	218.35–359.729	0.002	0	0.001	40	—	—	—	—		
crII	13.80–206.92	0.002	0.033	0.005 ^c	82	crII $\rightleftharpoons$ crI	207.140	533	13	Hildenbrand <i>et al.</i>	1959–374
crI	207.91–210.30	0.002	0	0.005 ^c	6	crI $\rightleftharpoons$ l	215.310	8592	8		
l	218.73–300.00	0.002	0	0.001	46	—	—	—	—		
l	298.15	—	—	0.01	1	—	—	—	—	Conti <i>et al.</i>	1976–110

TABLE 22. Available heat capacity and phase transition data for the condensed phases — Continued

ph.	Range K	Heat Capacity		$\sigma_r(C_{\text{sat}})^a$	Pts.	Trans.	Phase Transition		$\sigma(\Delta_{\text{tr}}H)^a$ J·mol ⁻¹	Author(s)	Ref.
		$\sigma(T)^a$ K	$\sigma_c(C_{\text{sat}})^a$ R				$\frac{T}{K}$	$\frac{\Delta_{\text{tr}}H}{\text{J·mol}^{-1}}$			
Piperidine											
l	292.6–370.6	—	—	0.05	1		—	—	—	Louguinine	1899–11
l	290.15	—	—	0.02	1		—	—	—	Radulescu and Jula	1934–351
	—	—	—	—	—	cr $\rightleftharpoons$ l	—	14854	4	Anonymous	1961–350
l	297.39	0.02	0	0.01	1		—	—	—	Moelwyn-Hughes and Thorpe	1964–568
l	298.15	—	—	0.01	1		—	—	—	Conti <i>et al.</i>	1976–110
cr	13.141–247.268	0.002	0.027	0.005 ^c	57	cr $\rightleftharpoons$ l	262.124	14854	12	Messerly <i>et al.</i>	
l	267.309–361.969	0.002	0	0.001	17		—	—	—		
Indole											
	—	—	—	—	—	cr $\rightleftharpoons$ l	325.15	—	—	Weerman	1910–141
	—	—	—	—	—	cr $\rightleftharpoons$ l	325.65	—	—	Cowley and Partington	1936–459
	—	—	—	—	—	cr $\rightleftharpoons$ l	325.65	—	—	Aihara	1955–710
	—	—	—	—	—	cr $\rightleftharpoons$ l	326.25	—	—	Serpinskii <i>et al.</i>	1958–398
Quinoline											
l	289.65	—	—	0.02	1		—	—	—	Radulescu and Jula	1934–351
l	302.4–302.6	—	0	0.005	1		—	—	—	Kolossowsky and Udovenko	1934–365
l	302.4–302.6	—	0	0.005	1		—	—	—	Kolossowskii and Udovenko	1934–408
cr	90–240	0.15	0.05	0.01 ^c	25	cr $\rightleftharpoons$ l	258.45	10797	30	Parks <i>et al.</i>	1936–163
l	260–300	0.15	0	0.01	10		—	—	—		
	—	—	—	—	—	cr $\rightleftharpoons$ l	257.93	10724	84	Mastrangelo	1957–551
crII	4.813–225.081	0.002	0.004	0.005 ^c	50	crII $\rightleftharpoons$ crI	200.0	27	2	Steele <i>et al.</i>	1988–551
crI	225.276–255.119	0.002	0	0.005 ^c	9	crI $\rightleftharpoons$ l	258.369	10663	5		
l	261.176–445.401	0.002	0	0.001	22		—	—	—		
Isoquinoline											
crIII	11.574–219.118	0.002	0.005	0.005 ^c	51	crIII $\rightleftharpoons$ crII	221.00	0	0	Steele <i>et al.</i>	1988–551
crII	221.608–273.366	0.002	0	0.005 ^c	11	crII $\rightleftharpoons$ crI	275.00	0	0		
crI	280.015–294.984	0.002	0	0.005 ^c	6	crI $\rightleftharpoons$ l	299.620	13544	5		
l	304.946–389.889	0.002	0	0.001	11		—	—	—		
Carbazole											
	—	—	—	—	—	crII $\rightleftharpoons$ crI	420	274	42	Robinson and Scott	1969–244
	—	—	—	—	—	crI $\rightleftharpoons$ l	519.300	26903	251		
Acridine											
cr	—	—	—	—	—	cr $\rightleftharpoons$ l	384.0	18577	628	McEachern <i>et al.</i>	1975–228
cr	4.858–354.928	0.002	0.003	0.005 ^c	58	cr $\rightleftharpoons$ l	383.242	23675	2	Steele <i>et al.</i>	1989–76
l	391.913–445.550	0.002	0	0.001	9		—	—	—		

TABLE 22. Available heat capacity and phase transition data for the condensed phases — Continued

ph.	Range K	Heat Capacity		$\sigma_f(C_{\text{sat}})^a$	Pts.	Trans.	Phase Transition		$\sigma(\Delta_{\text{tr}}H)^a$ J·mol ⁻¹	Author(s)	Ref.
		$\sigma(T)^a$ K	$\frac{\sigma_c(C_{\text{sat}})^a}{R}$				$\frac{T}{\text{K}}$	$\frac{\Delta_{\text{tr}}H}{\text{J}\cdot\text{mol}^{-1}}$			
Phenanthridine											
crII	4.766–346.684	0.002	0.003	0.005 ^c	64	crII $\rightleftharpoons$ crI	354.00	20	4	Steele <i>et al.</i>	1989–76
crI	359.429–369.254	0.002	0	0.005 ^c	4	crI $\rightleftharpoons$ l	379.740	22831	4		
l	377.077–439.623	0.002	0	0.001	9		–	–	–		
1-Naphthalenamine											
cr l	–	–	–	–	–	cr $\rightleftharpoons$ l	323.25	15330	126	Stillman and Swain Campetti	1899–63 1914–155
	318.15–321.15	–	–	–	4		–	–	–		
		324.85–327.85	–	–	–	2		–	–	–	Khetarpal <i>et al.</i>
	–	–	–	–	–	cr $\rightleftharpoons$ l	323.15	14490	200		
2-Naphthalenamine											
	–	–	–	–	–	cr $\rightleftharpoons$ l	386.15	23610	300	Khetarpal <i>et al.</i>	1979–205
9-Methylcarbazole											
cr	12.946–355.490	0.002	0.093	0.005 ^c	65	cr $\rightleftharpoons$ l	362.490	17154	1	Messerly <i>et al.</i>	1988–93
l	366.154–388.416	0.002	0	0.001	8		–	–	–		
cr	9.41–344.26	0.002	0.10	0.005 ^c	88		–	–	–		

^aSee Sec. 1.6.^bData reported graphically.^cValues for solid within 20 K of phase transition temperature is three times as large.

TABLE 23. Molar mass, product of moments of inertia, internal rotation

Molecule	M^a	$I_a I_b I_c^b$	σ_{total}^c	E_0	Bond	Internal rotation ^e								
						I_r	$\nu(0 \leftarrow 1)$	m	V_m	n	V_n	k	V_k	V_0
1-Butanamine	73.139	8855.2	3	—	C ₁ —C ₂	17.502	104.0	1	3.670	3	8.590	—	—	—
					C ₂ —C ₃	23.314	112.0	1	4.799	2	−0.490	3	13.790	—
					C ₃ —C ₄	4.445	259.0	3	15.807	—	—	—	—	—
					C ₁ —N	2.866	210.0	3	7.456	—	—	—	—	—
2-Butanamine (d,l)	73.139	7889.0	9	—	C ₁ —C ₂	5.251	245.0	3	16.506	—	—	—	—	—
					C ₂ —C ₃	27.299	104.0	1	−3.879	3	15.573	—	—	2.929
					C ₃ —C ₄	4.678	252.0	3	15.807	—	—	—	—	—
					C ₂ —N	3.027	264.0	3	11.799	—	—	—	—	—
2-Methyl-1-propanamine	73.139	7859.1	9	—	C ₁ —C ₂	26.984	94.0	1	−3.598	3	12.761	—	—	2.720
					C ₂ —C ₃	5.046	246.0	3	11.924	—	—	—	—	—
					C ₂ —C ₄	5.171	243.0	3	16.108	—	—	—	—	—
					C ₁ —N	2.747	225.0	3	7.950	—	—	—	—	—
2-Methyl-2-propanamine	73.139	6097.7	81	—	C ₁ —C ₂	5.095	279.0	3	20.460	—	—	—	—	—
					C ₂ —C ₃	5.252	274.0	3	20.460	—	—	—	—	—
					C ₂ —C ₄	5.100	195.0	3	10.418	—	—	—	—	—
					C ₂ —N	2.989	240.0	3	9.686	—	—	—	—	—
Pyrrole	67.091	1586.5	2	—	—	—	—	—	—	—	—	—	—	—
1-Methylpyrrole	81.117	7455.8	6	—	C ₅ —N	5.098	61.5	6	0.536	—	—	—	—	—
2-Methylpyrrole	81.117	7964.5	3	—	C ₁ —C ₅	5.015	0.0	—	—	—	—	—	—	—
3-Methylpyrrole	81.117	8219.5	3	—	C ₂ —C ₅	5.015	0.0	—	—	—	—	—	—	—
Pyridine	79.101	5696.6	2	—	—	—	—	—	—	—	—	—	—	—
2-Methylpyridine	93.128	21653.8	3	—	C ₁ —C ₆	5.164	44.6	3	1.081	6	−0.377	—	—	0.033
3-Methylpyridine	93.128	22385.5	3	—	C ₂ —C ₆	5.164	0.0	—	—	—	—	—	—	—
4-Methylpyridine	93.128	22408.2	6	—	C ₃ —C ₆	5.114	0.0	—	—	—	—	—	—	—
Pyrrolidine	71.122	3330.5	1	—	Pseudo	11.192	50.0	2	3.350	—	—	—	—	—
Piperidine (equatorial)	85.149	11569.3	1	0.0	—	—	—	—	—	—	—	—	—	—
Piperidine (axial)	85.149	11799.5	1	3.07	—	—	—	—	—	—	—	—	—	—
Piperidine (twist-boat)	85.149	11684.4	1	15.0	—	—	—	—	—	—	—	—	—	—
Indole	117.150	80998.5	1	—	—	—	—	—	—	—	—	—	—	—
Quinoline	129.161	159000.4	1	—	—	—	—	—	—	—	—	—	—	—

TABLE 23. Molar mass, product of moments of inertia, internal rotation - Continued

Molecule	M^a	$I_a I_b I_c^b$	σ_{total}^c	E_0	Internal rotation ^e									
					Bond	I_r	$\nu(0 \leftarrow 1)$	m	V_m	n	V_n	k	V_k	V_0
Isoquinoline	129.161	160900.4	1	—	—	—	—	—	—	—	—	—	—	—
Carbazole	167.210	938534.8	2	—	—	—	—	—	—	—	—	—	—	—
Acridine	179.221	1456147.2	2	—	—	—	—	—	—	—	—	—	—	—
Phenanthridine	179.221	1612079.0	2	—	—	—	—	—	—	—	—	—	—	—
1-Naphthalenamine ^f	143.188	37632.3	1	—	C ₁ -N	2.524	253.0	2	19.04	—	—	—	—	—
2-Naphthalenamine ^f	143.188	39038.9	1	—	C ₂ -N	2.524	253.0	2	19.04	—	—	—	—	—

^a M = molar mass, g·mol⁻¹.^b $I_a I_b I_c$ = product of the three principal moments of inertia, 10⁻¹¹⁷ g³·cm⁶.^c σ_{total} = total symmetry number.^d E_0 = energy of lowest state relative to ground state, kJ·mol⁻¹.^eBond is the axis of relative rotation and the subscripts denote carbon numbers; I_r = reduced moment of inertia, 10⁻⁴⁰ g·cm²; $\nu(0 \leftarrow 1)$ = torsional wavenumber, cm⁻¹; V_m , V_n , V_k and V_0 in kJ·mol⁻¹ for the internal rotation potential function: $V_r = \frac{1}{2}[V_m(1 - \cos m\theta) + V_n(1 - \cos n\theta) + V_k(1 - \cos k\theta)] + V_0$ with θ = angle of internal rotation.^fNH₂ inversion was taken into account separately.

TABLE 24. Fundamental vibrational wavenumbers

Compound	Fundamental vibrational wavenumber (cm ⁻¹)
1-Butanamine	3347, 3244, 2972, 2954, 2954, 2950, 2950, 2943, 2902, 2892, 2885, 1626, 1475, 1466, 1460, 1450, 1437, 1400, 1354, 1350, 1316, 1302, 1275, 1220, 1150, 1142, 1087, 1077, 1023, 950, 887, 878, 775, 750, 722, 454, 370, 323
2-Butanamine	3411, 3342, 2968, 2965, 2950, 2950, 2950, 2945, 2932, 2878, 2860, 1618, 1469, 1469, 1460, 1450, 1449, 1375, 1360, 1350, 1343, 1245, 1240, 1170, 1150, 1130, 1029, 976, 950, 942, 919, 819, 785, 750, 472, 404, 370, 369
2-Methyl-1-propanamine	3411, 3342, 2968, 2965, 2950, 2950, 2950, 2945, 2932, 2878, 2860, 1618, 1469, 1469, 1460, 1450, 1449, 1375, 1360, 1350, 1343, 1245, 1240, 1170, 1150, 1130, 1068, 976, 950, 942, 919, 773, 755, 750, 472, 404, 370, 369
2-Methyl-2-propanamine	3320, 3240, 2975, 2975, 2975, 2975, 2975, 2915, 2915, 1635, 1492, 1477, 1477, 1460, 1460, 1460, 1390, 1379, 1379, 1329, 1312, 1234, 1111, 1033, 1033, 1000, 942, 921, 910, 812, 743, 456, 456, 446, 346, 337
Pyrrole	3527, 3148, 3140, 3125, 3116, 1530, 1467, 1422, 1382, 1287, 1144, 1134, 1074, 1048, 1016, 881, 869, 865, 826, 721, 710, 618, 601, 474
1-Methylpyrrole	3024, 3024, 3024, 3024, 3024, 3024, 1525, 1525, 1450, 1450, 1450, 1382, 1382, 1250, 1250, 1047, 1047, 1047, 1047, 1047, 966, 847, 847, 847, 720, 675, 675, 605, 605, 354, 186
2-Methylpyrrole	3532, 3156, 3120, 3120, 2918, 2918, 2865, 1571, 1469, 1450, 1450, 1435, 1412, 1380, 1266, 1232, 1116, 1091, 1037, 1025, 973, 950, 882, 855, 783, 711, 648, 630, 607, 468, 338, 257
3-Methylpyrrole	3532, 3130, 3130, 3094, 2923, 2923, 2866, 1563, 1486, 1453, 1453, 1431, 1385, 1371, 1279, 1258, 1139, 1061, 1047, 1043, 982, 954, 887, 840, 774, 706, 647, 638, 618, 466, 327, 266
Pyridine	3094.2, 3086.9, 3072.8, 3042.4, 3030.1, 1583.9, 1580.5, 1483.4, 1441.9, 1362.3, 1227.0, 1218.0, 1143.3, 1079.0, 1071.9, 1031.7, 1007.0, 991.4, 980.0, 936.6, 880.0, 744.0, 700.3, 652.0, 601.4, 403.3, 373.0
2-Methylpyridine	3082, 3064, 3046, 3027, 2950, 2950, 2925, 1594, 1565, 1468, 1451, 1436, 1436, 1385, 1299, 1246, 1176, 1148, 1095, 1052, 1041, 1036, 972, 972, 928, 883, 803, 781, 729, 628, 548, 470, 401, 355, 194
3-Methylpyridine	3085, 3054, 3054, 3030, 2941, 2941, 2923, 1595, 1581, 1472, 1452, 1419, 1381, 1316, 1247, 1193, 1165, 1111, 1035, 1035, 1023, 984, 941, 923, 909, 810, 782, 711, 630, 536, 455, 399, 337, 206
4-Methylpyridine	3070, 3070, 3038, 3038, 2937, 2937, 2910, 1603, 1575, 1501, 1447, 1445, 1420, 1383, 1279, 1228, 1208, 1157, 1112, 1066, 1053, 1039, 996, 969, 870, 870, 800, 800, 727, 668, 512, 482, 385, 344, 203
Pyrrolidine	3367, 2970, 2970, 2882, 2882, 2882, 2882, 2818, 2818, 1480, 1480, 1468, 1468, 1418, 1348, 1299, 1284, 1239, 1220, 1205, 1171, 1136, 1105, 1080, 1053, 1025, 980, 925, 909, 872, 844, 792, 612, 570, 145
Piperidine (equatorial)	3341, 2947, 2940, 2931, 2917, 2902, 2892, 2850, 2850, 2803, 2730, 1476, 1468, 1452, 1444, 1440, 1386, 1365, 1346, 1322, 1318, 1313, 1285, 1266, 1258, 1191, 1164, 1146, 1121, 1052, 1045, 1006, 964, 906, 898, 860, 822, 743, 743, 560, 445, 427, 401, 254, 246
Piperidine (axial)	3309, 2947, 2947, 2940, 2917, 2892, 2892, 2850, 2850, 2850, 1476, 1468, 1452, 1444, 1440, 1386, 1365, 1346, 1322, 1318, 1313, 1285, 1268, 1266, 1191, 1164, 1146, 1115, 1052, 1035, 992, 964, 906, 898, 859, 822, 743, 743, 542, 445, 432, 390, 254, 246
Indole	3520, 3140, 3083, 3083, 3068, 3068, 3068, 1617, 1578, 1510, 1489, 1458, 1410, 1348, 1300, 1275, 1245, 1205, 1150, 1122, 1082, 1068, 1015, 968, 930, 900, 869, 860, 800, 762, 761, 738, 715, 625, 608, 575, 544, 428, 400, 400, 240, 208
Quinoline	3074, 3062, 3048, 3035, 3017, 3006, 2980, 1619, 1595, 1568, 1500, 1469, 1431, 1391, 1370, 1312, 1253, 1216, 1189, 1140, 1117, 1093, 1032, 1012, 976, 968, 952, 938, 903, 864, 802, 785, 785, 759, 733, 627, 611, 521, 505, 476, 467, 389, 377, 181, 168
Isoquinoline	3089, 3060, 3055, 3055, 3025, 3008, 2990, 1627, 1587, 1552, 1497, 1460, 1432, 1381, 1377, 1315, 1273, 1255, 1179, 1140, 1118, 1095, 1034, 1013, 985, 970, 959, 942, 930, 831, 823, 800, 778, 765, 740, 637, 610, 522, 504, 479, 460, 375, 354, 180, 169
Carbazole	3421, 3094, 3084, 3077, 3055, 3050, 3039, 3030, 2940, 1625, 1594, 1576, 1490, 1481, 1452, 1449, 1380, 1334, 1320, 1288, 1233, 1205, 1204, 1158, 1152, 1136, 1118, 1107, 1022, 1012, 995, 989, 939, 926, 910, 893, 880, 856, 835, 771, 747, 741, 737, 722, 691, 658, 616, 566, 548, 505, 467, 445, 425, 410, 310, 299, 222, 220, 139, 104
Acridine	3085, 3085, 3075, 3055, 3055, 3037, 3037, 3014, 3014, 1627, 1622, 1578, 1556, 1516, 1480, 1464, 1441, 1402, 1397, 1373, 1360, 1317, 1274, 1266, 1232, 1168, 1158, 1140, 1121, 1009, 1009, 1009, 999, 974, 965, 955, 939, 939, 905, 901, 861, 851, 814, 785, 762, 744, 735, 712, 655, 617, 600, 581, 523, 477, 469, 417, 401, 275, 240, 217, 156, 139, 106
Phenanthridine	3082, 3072, 3064, 3057, 3047, 3037, 3034, 3019, 3002, 1615, 1600, 1587, 1575, 1525, 1485, 1455, 1445, 1425, 1405, 1390, 1345, 1290, 1245, 1227, 1190, 1173, 1163, 1135, 1110, 1094, 1046, 1035, 1001, 970, 943, 895, 876, 874, 832, 819, 791, 775, 750, 725, 713, 712, 711, 620, 576, 548, 536, 505, 494, 460, 435, 415, 408, 395, 279, 240, 234, 170, 108
1-Naphthalenamine	3455, 3370, 3100, 3075, 3075, 3050, 3030, 3010, 2970, 1620, 1615, 1593, 1576, 1514, 1460, 1450, 1405, 1385, 1360, 1285, 1248, 1215, 1176, 1164, 1140, 1125, 1086, 1026, 1012, 970, 953, 943, 876, 858, 810, 788, 768, 715, 670, 625, 566, 530, 508, 478, 452, 412, 397, 358, 312, 266, 185, 165
2-Naphthalenamine	3470, 3390, 3085, 3065, 3050, 3020, 2995, 2970, 2950, 1626, 1612, 1596, 1572, 1509, 1466, 1446, 1383, 1362, 1282, 1260, 1250, 1220, 1180, 1151, 1122, 1062, 1013, 1000, 962, 953, 951, 936, 852, 840, 810, 765, 748, 740, 700, 618, 580, 523, 478, 470, 450, 393, 380, 366, 340, 225, 196, 165

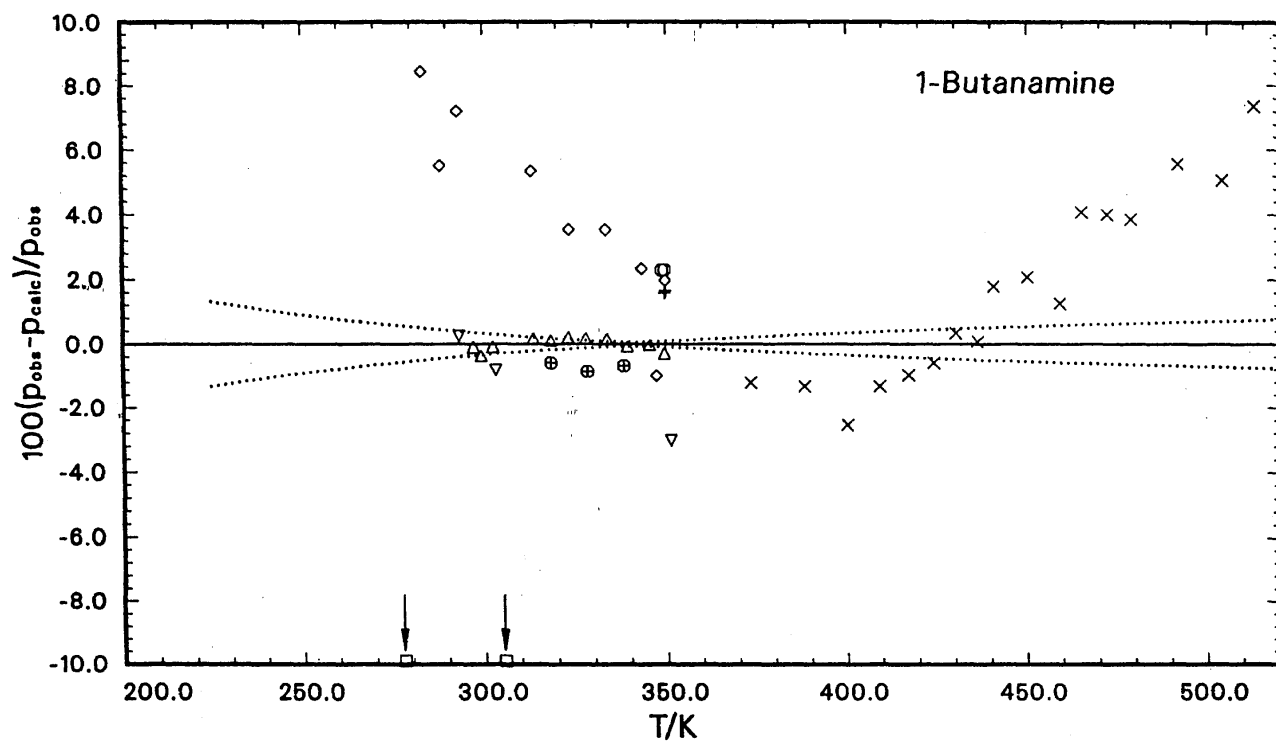


FIG. 1. Percent deviation of experimental vapor pressures for 1-butanamine from the Cox equation. $\circ$ (1871-9); $\square$ (1941-101); $+$ (1947-146); $\times$ (1957-76)*; $\diamond$ (1962-356); ∇ (1969-2); $\oplus$ (1979-77); $\triangle$ (1979-78); * data from this reference used in the evaluation.

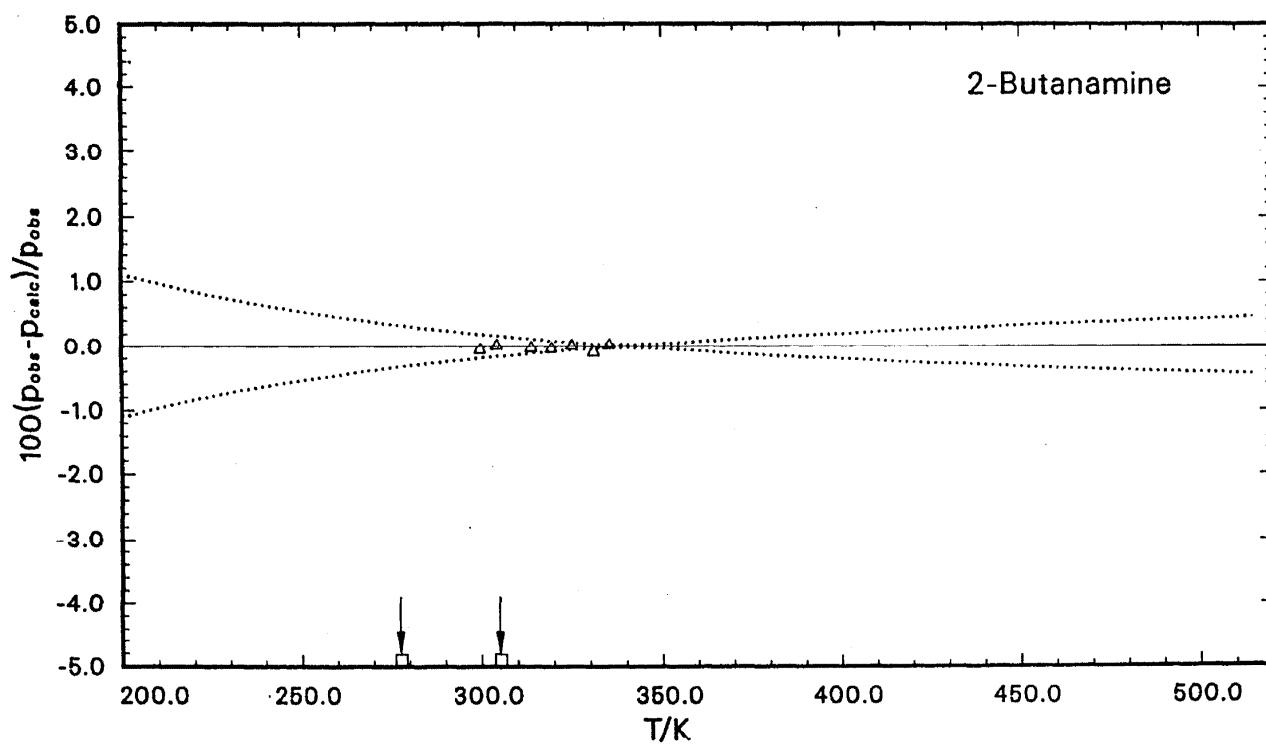


FIG. 2. Percent deviation of experimental vapor pressures for 2-butanamine from the Cox equation. $\circ$ (1941-101); $\triangle$ (1979-78)*; * data from this reference used in the evaluation.

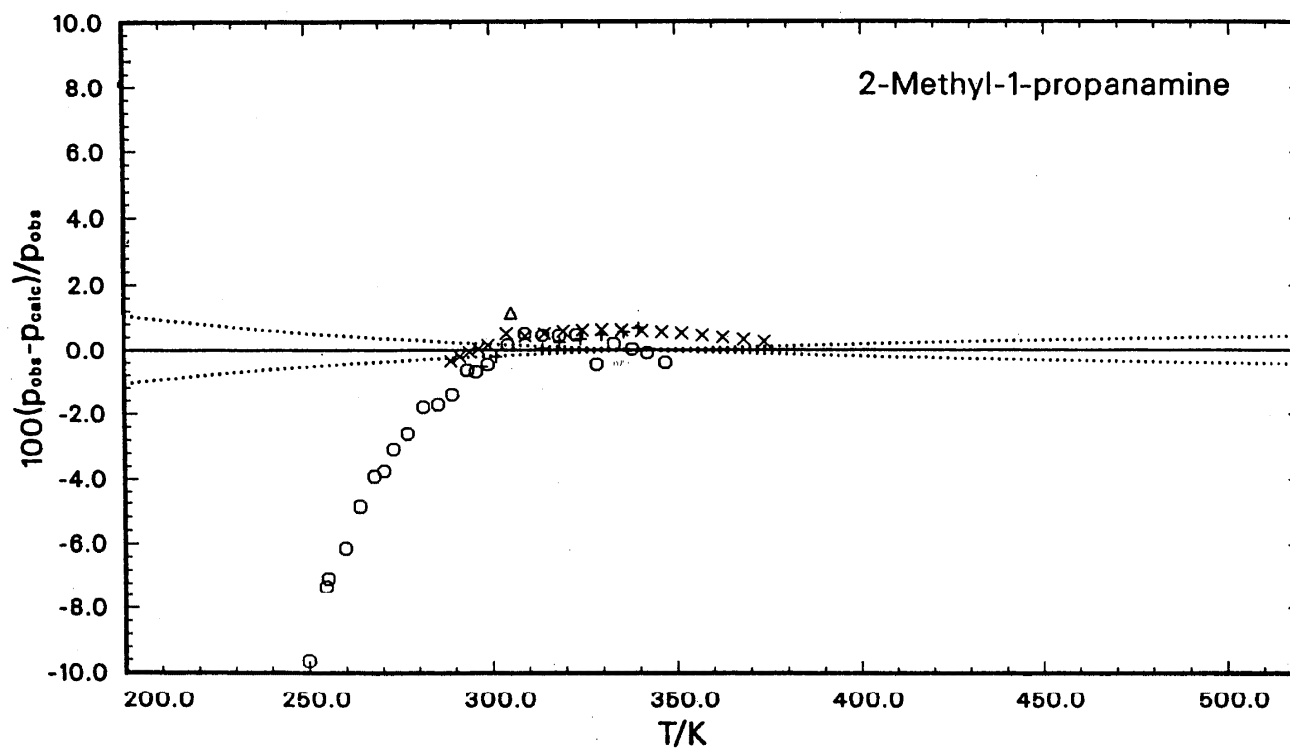


FIG. 3. Percent deviation of experimental vapor pressures for 2-methyl-1-propanamine from the Cox equation. $\circ$ (1935-278)*; Δ (1941-101); + (1979-78)*; $\times$ (1980-1)*; * data from this reference used in the evaluation.

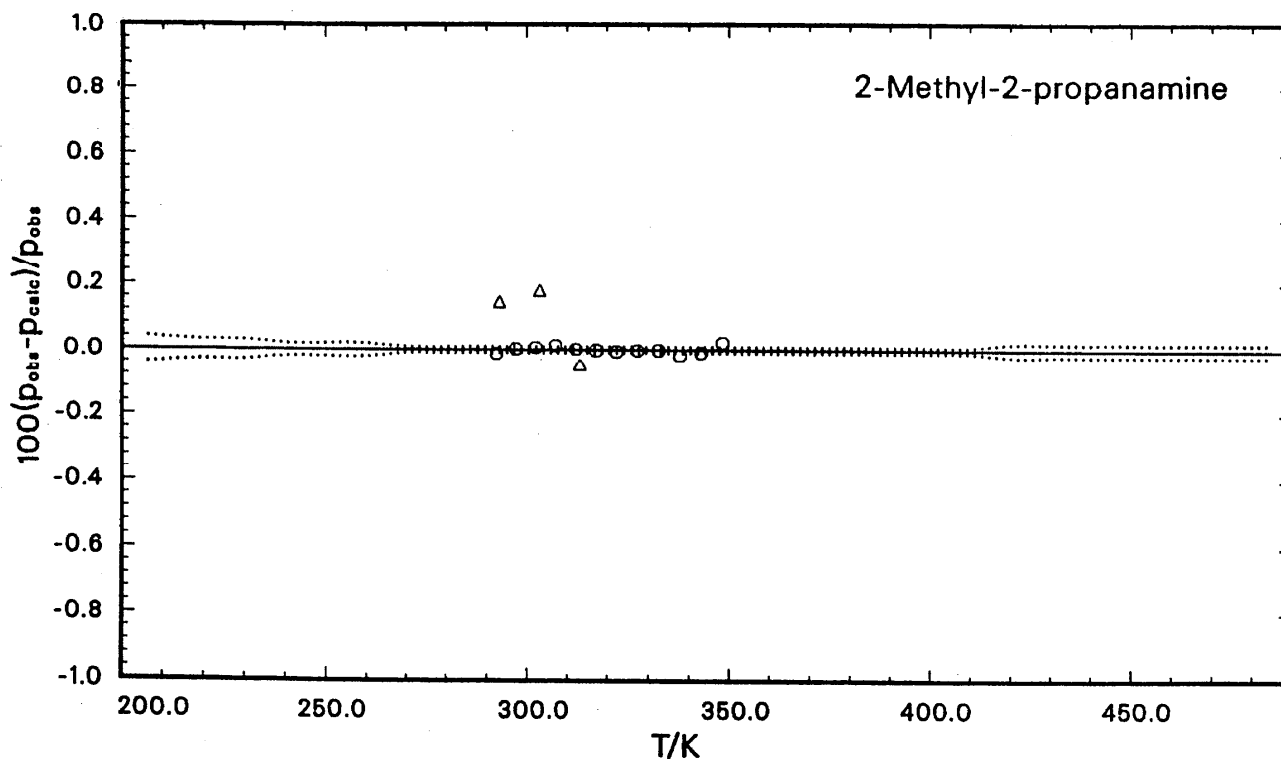


FIG. 4. Percent deviation of experimental vapor pressures for 2-methyl-2-propanamine from the Cox equation. $\circ$ (1968-206)*; Δ (1979-80); * data from this reference used in the evaluation.

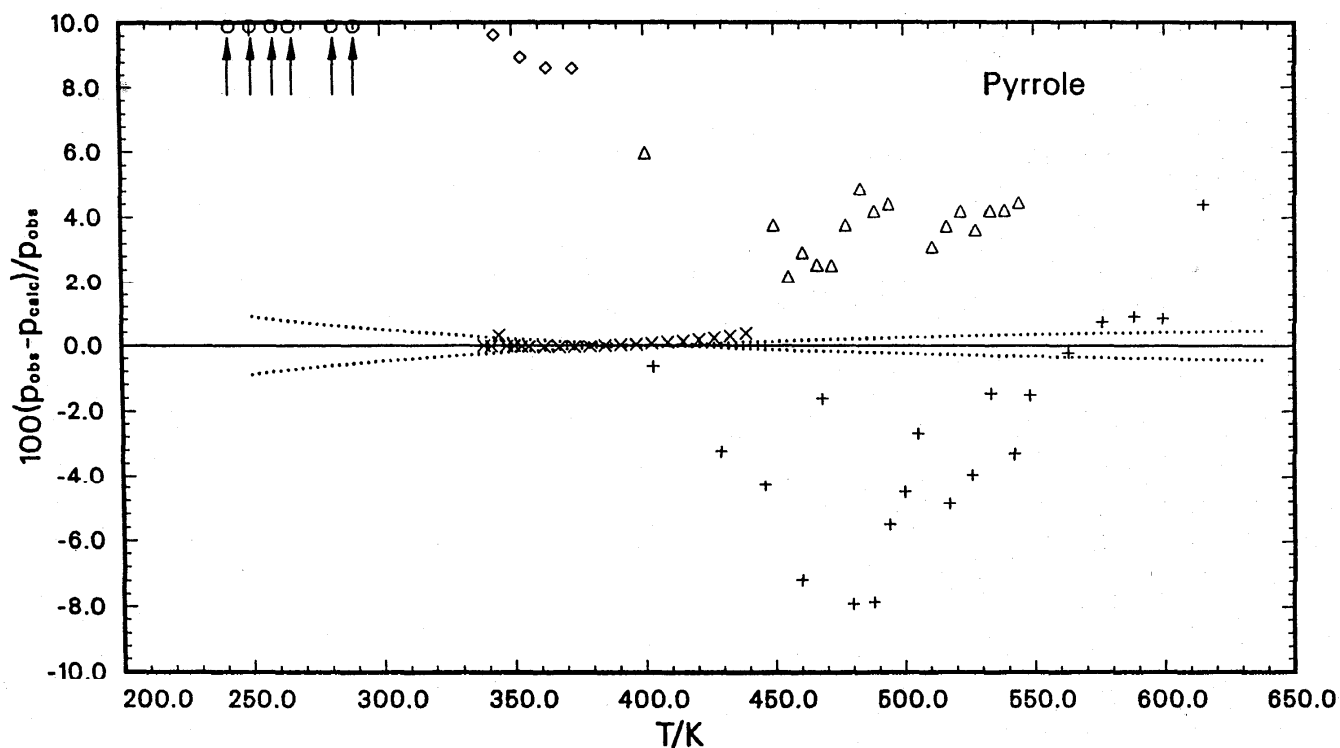


FIG. 5. Percent deviation of experimental vapor pressures for pyrrole from the Cox equation. $\circ$ (1941-378); $\triangle$ (1956-9); + (1957-76)*; $\times$ (1967-116)*; $\diamond$ (1971-47); * data from this reference used in the evaluation.

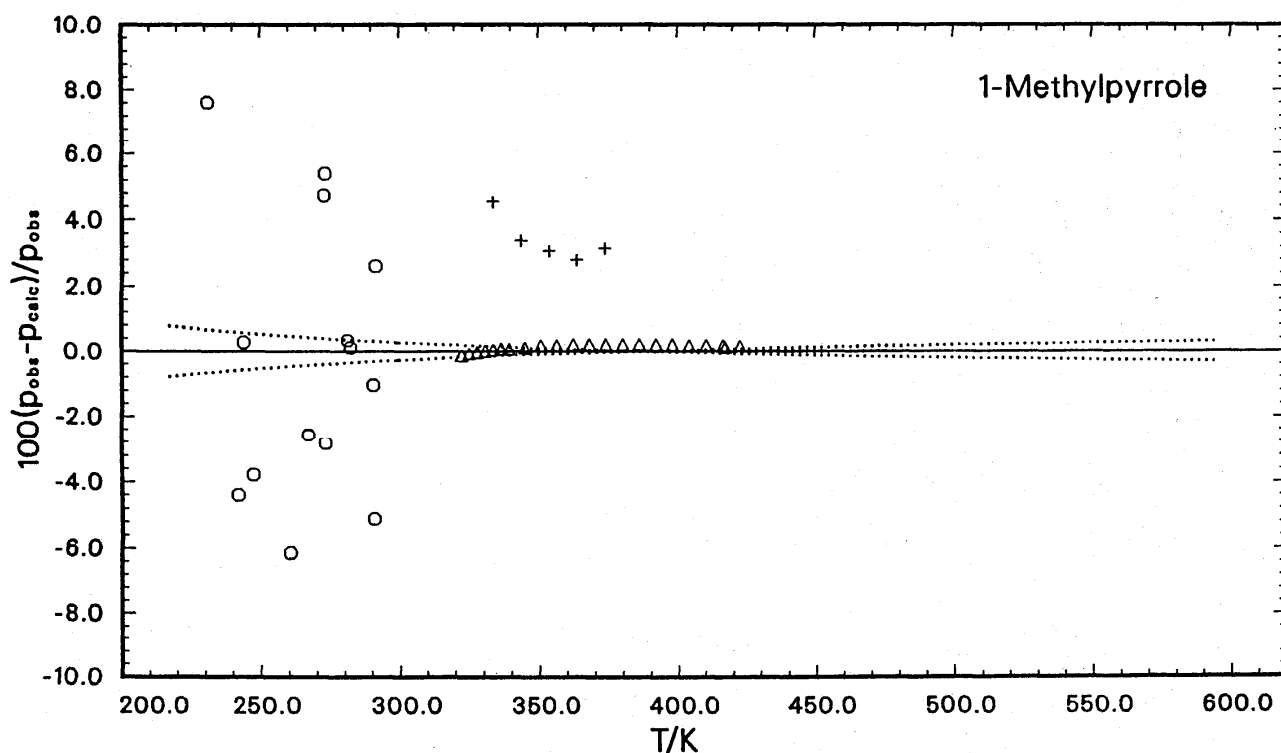


FIG. 6. Percent deviation of experimental vapor pressures for 1-methylpyrrole from the Cox equation. $\circ$ (1941-378)*; $\triangle$ (1968-206)*; + (1971-47); * data from this reference used in the evaluation.

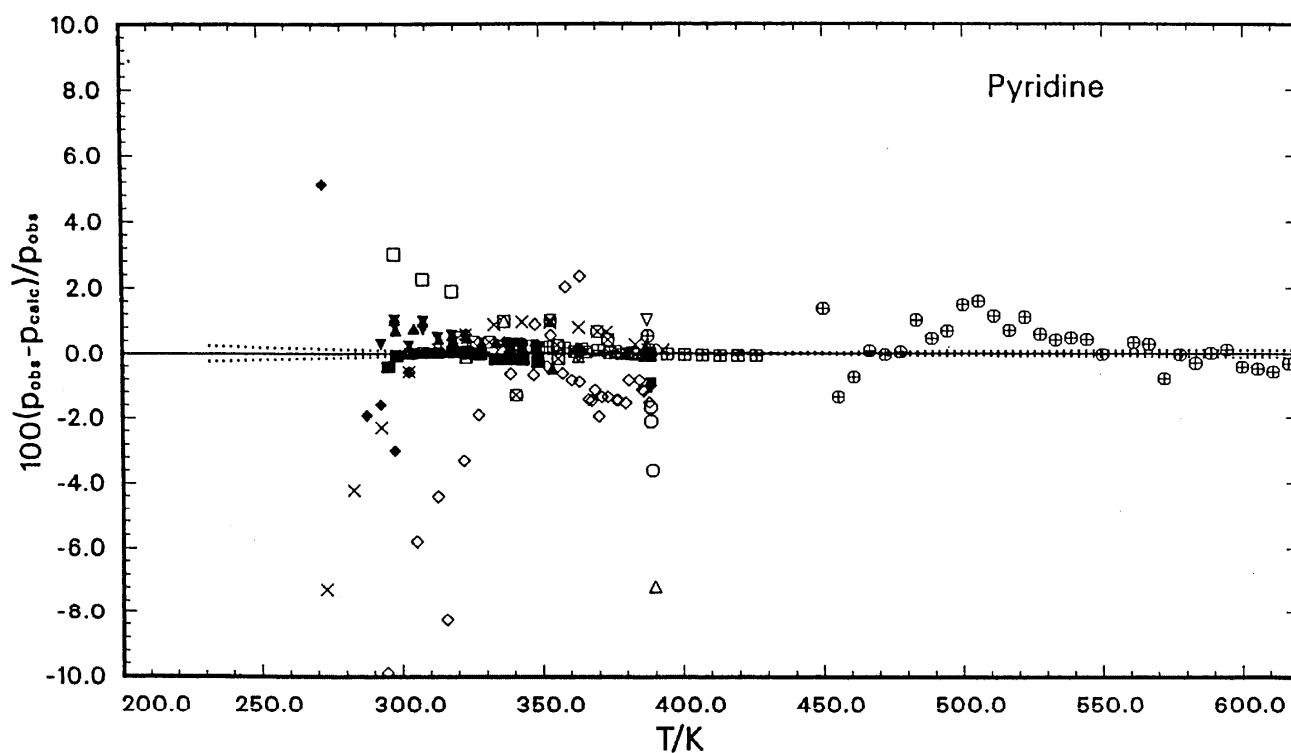


FIG. 7. Percent deviation of experimental vapor pressures for pyridine from the Cox equation. $\circ$ (1895–49); $\triangle$ (1901–63); $+$ (1926–210); $\times$ (1931–349); $\diamond$ (1934–26); ∇ (1935–418); $\boxtimes$ (1953–518)*; $\ast$ (1954–757); $\diamond$ (1956–615); $\boxtimes$ (1957–537); $\otimes$ (1963–382); $\boxplus$ (1969–224); $\oplus$ (1956–9)*; $\boxplus$ (1957–176)*; $\bullet$ (1969–226); ∇ (1974–227)*; $\blacksquare$ (1976–132); $\blacksquare$ (1976–182)*; $\blacktriangledown$ (1978–131); $\blacktriangle$ (1983–11); $\blacklozenge$ (1984–49); * data from this reference used in the evaluation.

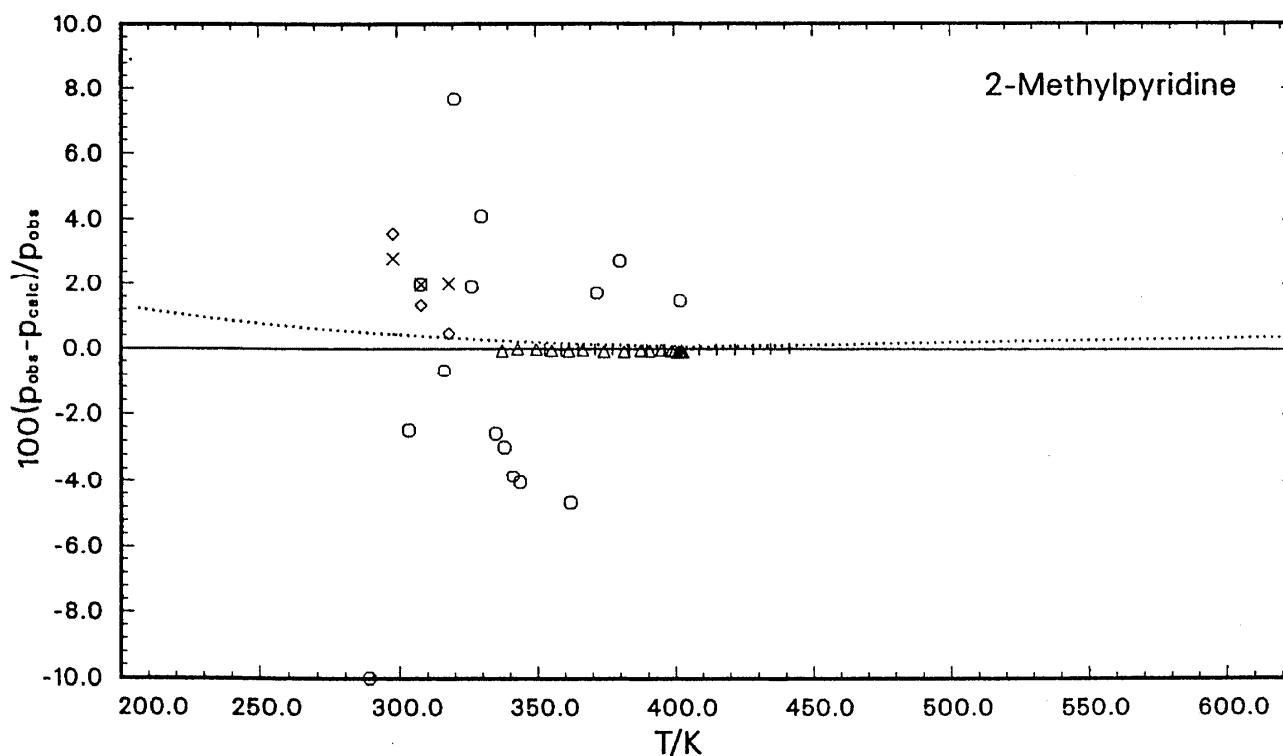


FIG. 8. Percent deviation of experimental vapor pressures for 2-methylpyridine from the Cox equation. $\circ$ (1929–178); $\triangle$ (1953–518)*; $+$ (1963–156)*; $\times$ (1976–132); $\diamond$ (1978–131); * data from this reference used in the evaluation.

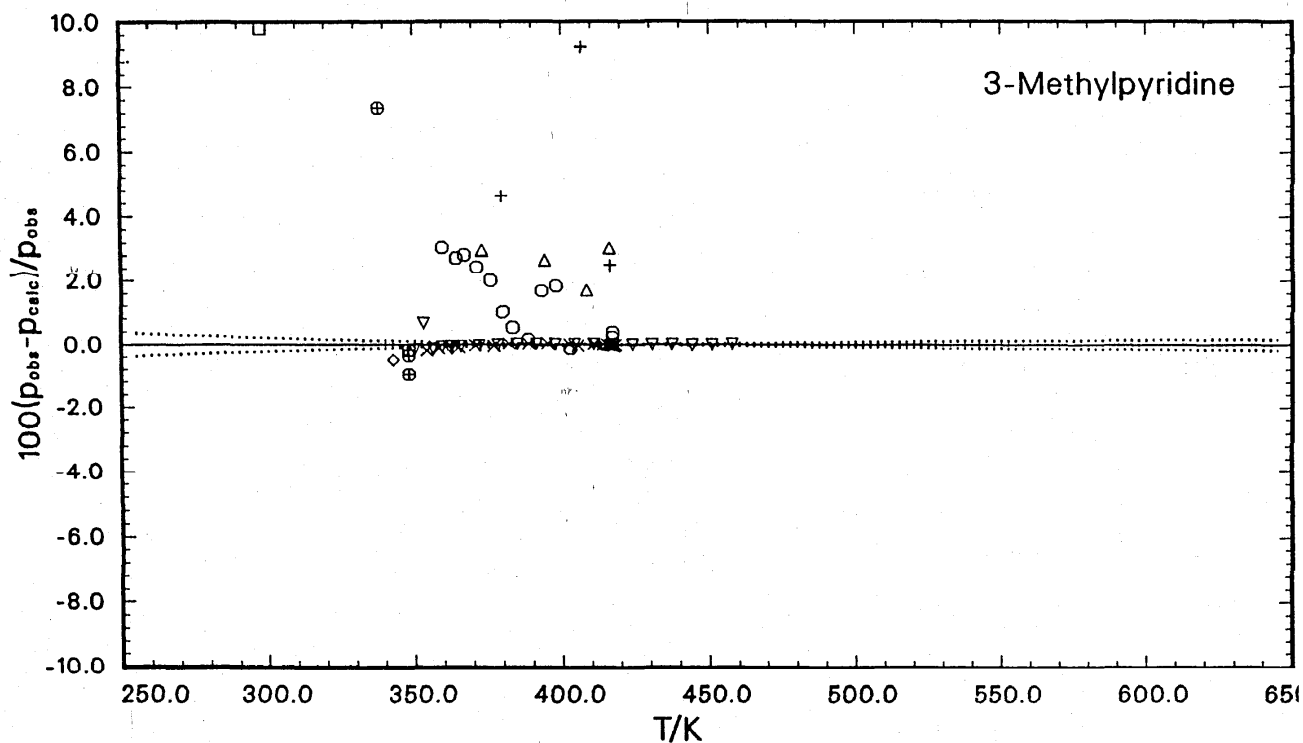


FIG. 9. Percent deviation of experimental vapor pressures for 3-methylpyridine from the Cox equation. ○ (1946–308); △ (1948–467); + (1951–184); × (1953–518)*; ◇ (1957–537); ▽ (1963–157)*; □ (1978–131); ⊕ (1988–1133); * data from this reference used in the evaluation.

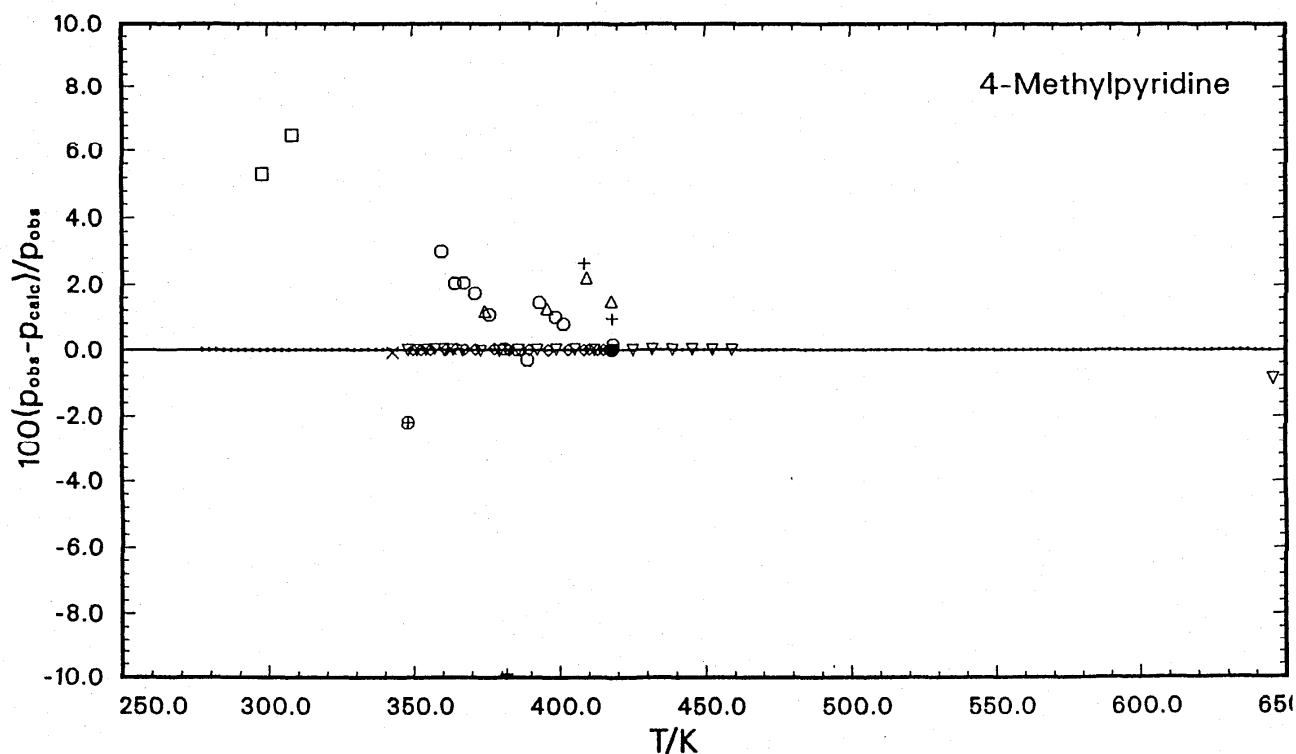


FIG. 10. Percent deviation of experimental vapor pressures for 4-methylpyridine from the Cox equation. ○ (1946–308); △ (1948–467); + (1951–184); ◇ (1953–518)*; × (1957–537); ▽ (1968–206)*; □ (1978–131); ⊕ (1988–1133); * data from this reference used in the evaluation.

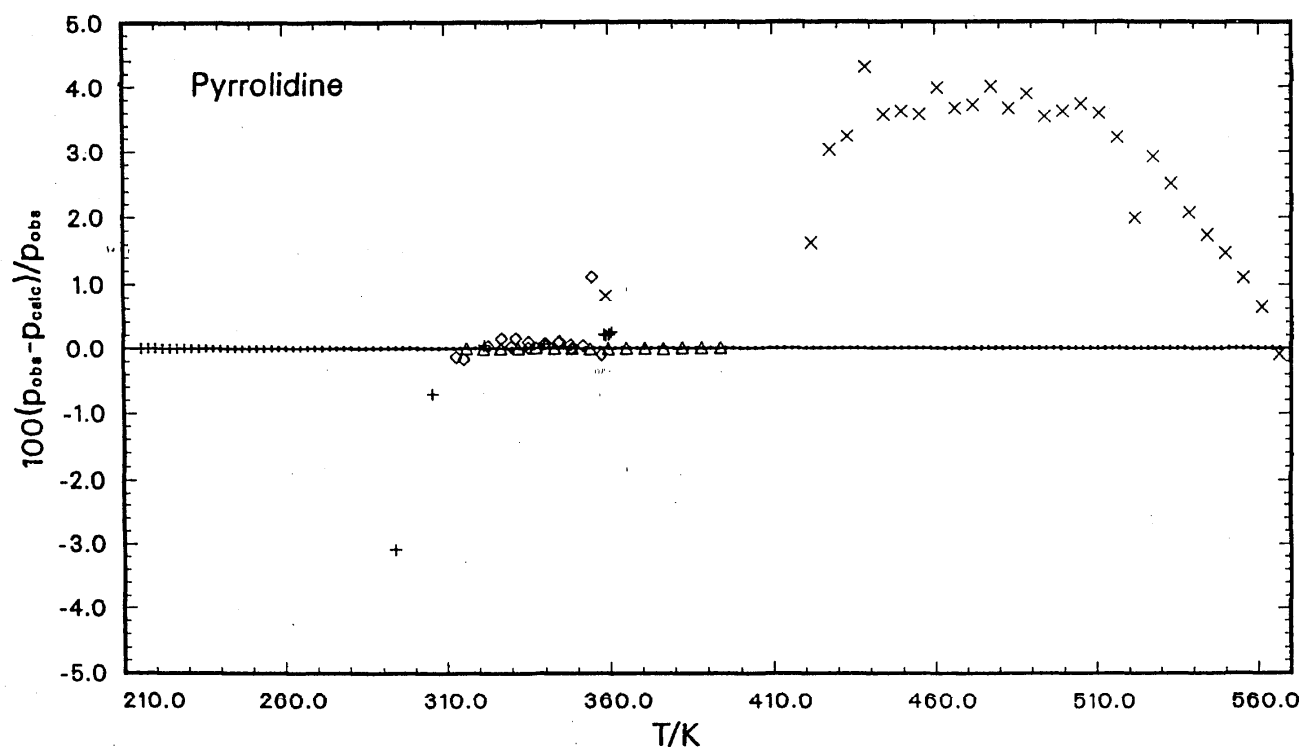


FIG. 11. Percent deviation of experimental vapor pressures for pyrrolidine from the Cox equation. $\times$ (1956-9); Δ (1959-355)*; + (1959-374); $\diamond$ (1990-32)*; * data from this reference used in the evaluation.

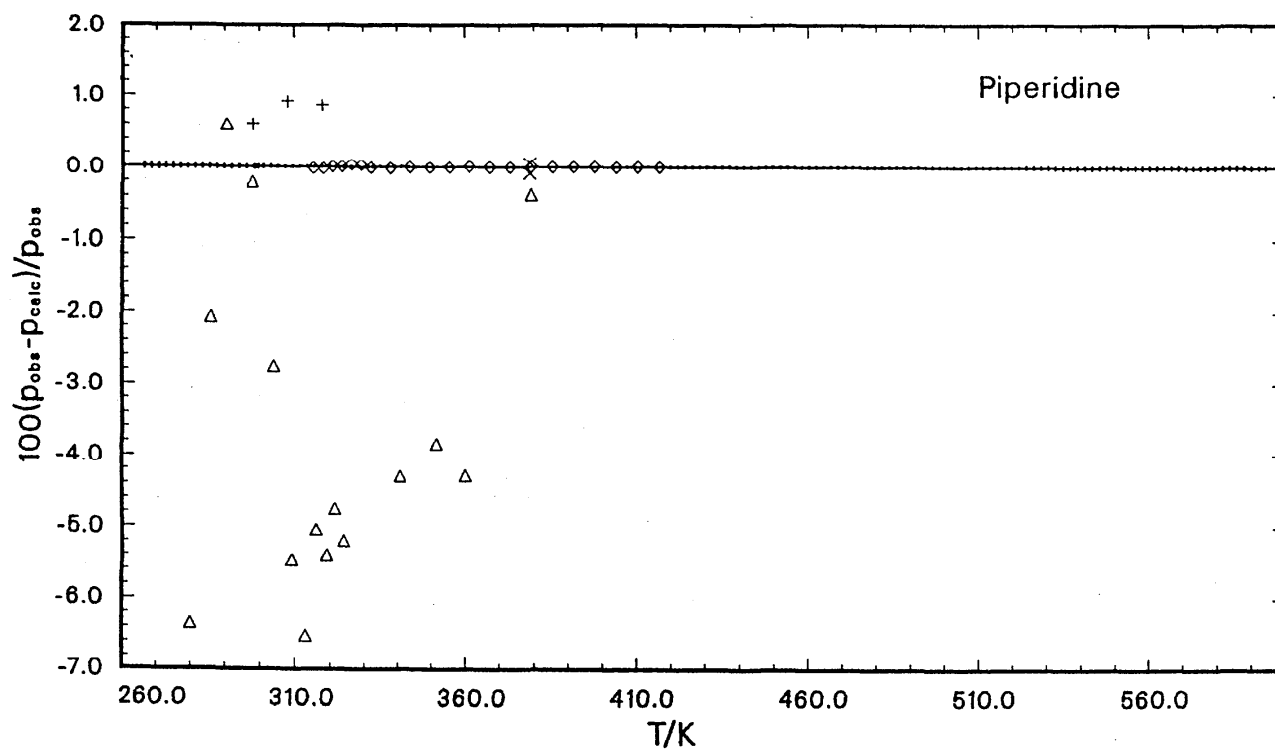


FIG. 12. Percent deviation of experimental vapor pressures for piperidine from the Cox equation. Δ (1929-178); $\times$ (1937-261); $\diamond$ (1968-206)*; + (1975-283); * data from this reference used in the evaluation.

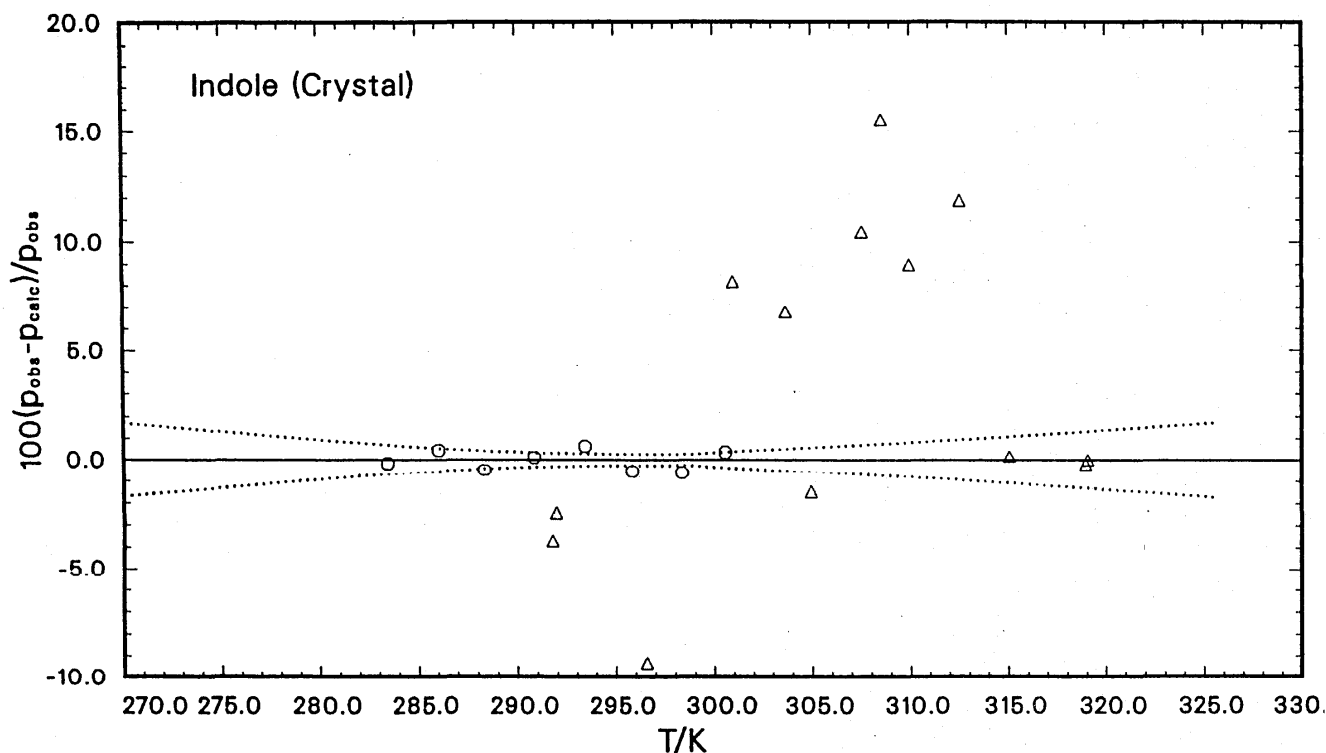


FIG. 13. Percent deviation of experimental vapor pressures for indole (crystal) from the Antoine equation. $\circ$ (1955-710)*; $\triangle$ (1958-398); * data from this reference used in the evaluation.

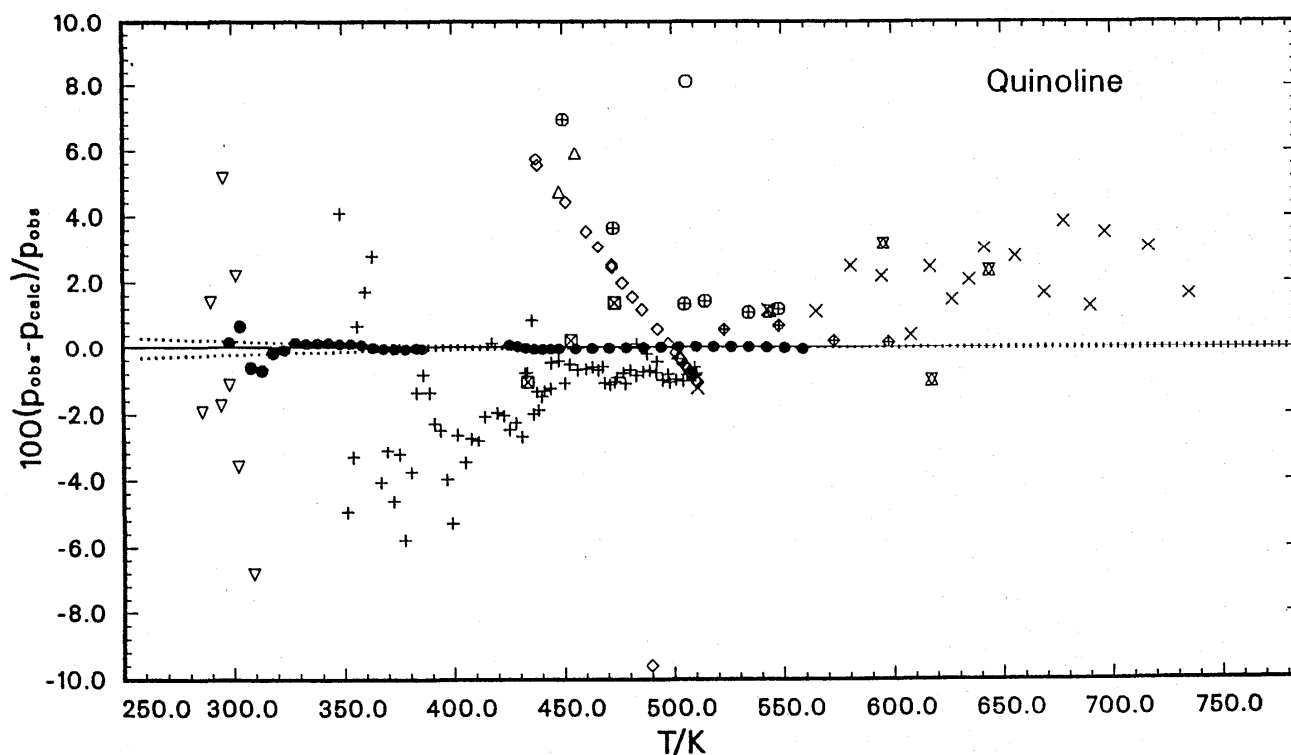


FIG. 14. Percent deviation of experimental vapor pressures for quinoline from the Cox equation. + (1889-25); $\times$ (1957-76); $\diamond$ (1961-32); $\circ$ (1962-471); $\triangle$ (1963-438); ∇ (1980-6); $\square$ (1986-24); $\oplus$ (1987-21); $\diamond$ (1988-70); $\bullet$ (1988-551)*; $\square$ (1988-555); * data from this reference used in the evaluation.

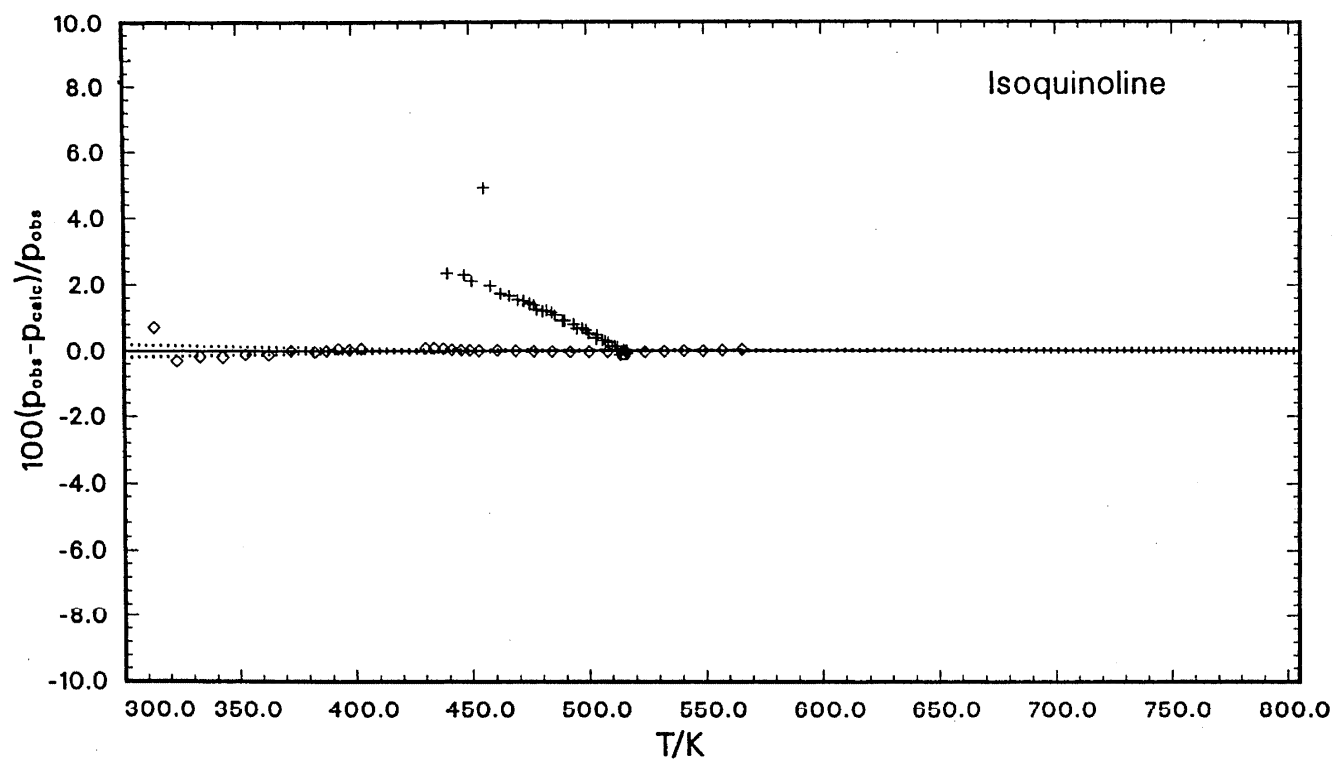


FIG. 15. Percent deviation of experimental vapor pressures for isoquinoline from the Cox equation. $\circ$ (1949-545); $+$ (1961-32); $\diamond$ (1988-551)*; * data from this reference used in the evaluation.

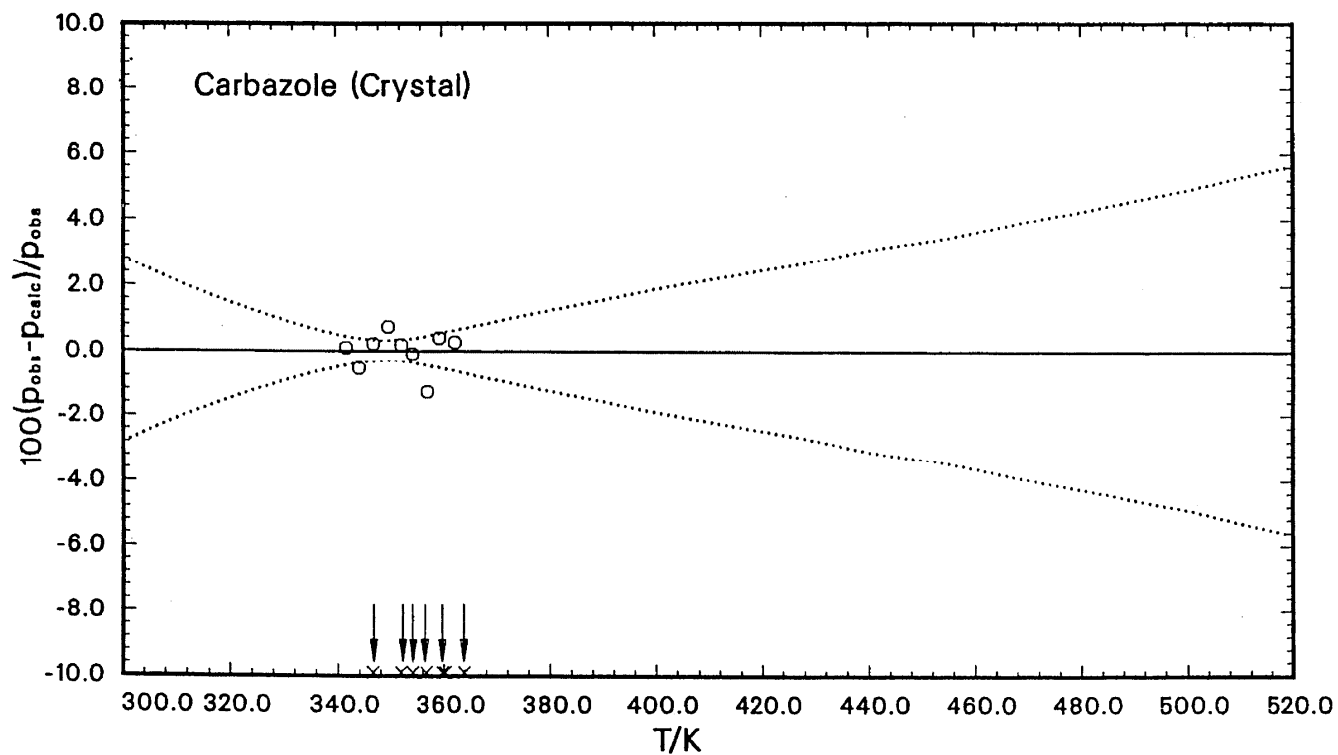


FIG. 16. Percent deviation of experimental vapor pressures for carbazole (crystal) from the Antoine equation. $\circ$ (1955-710)*; $\times$ (1990-65); * data from this reference used in the evaluation.

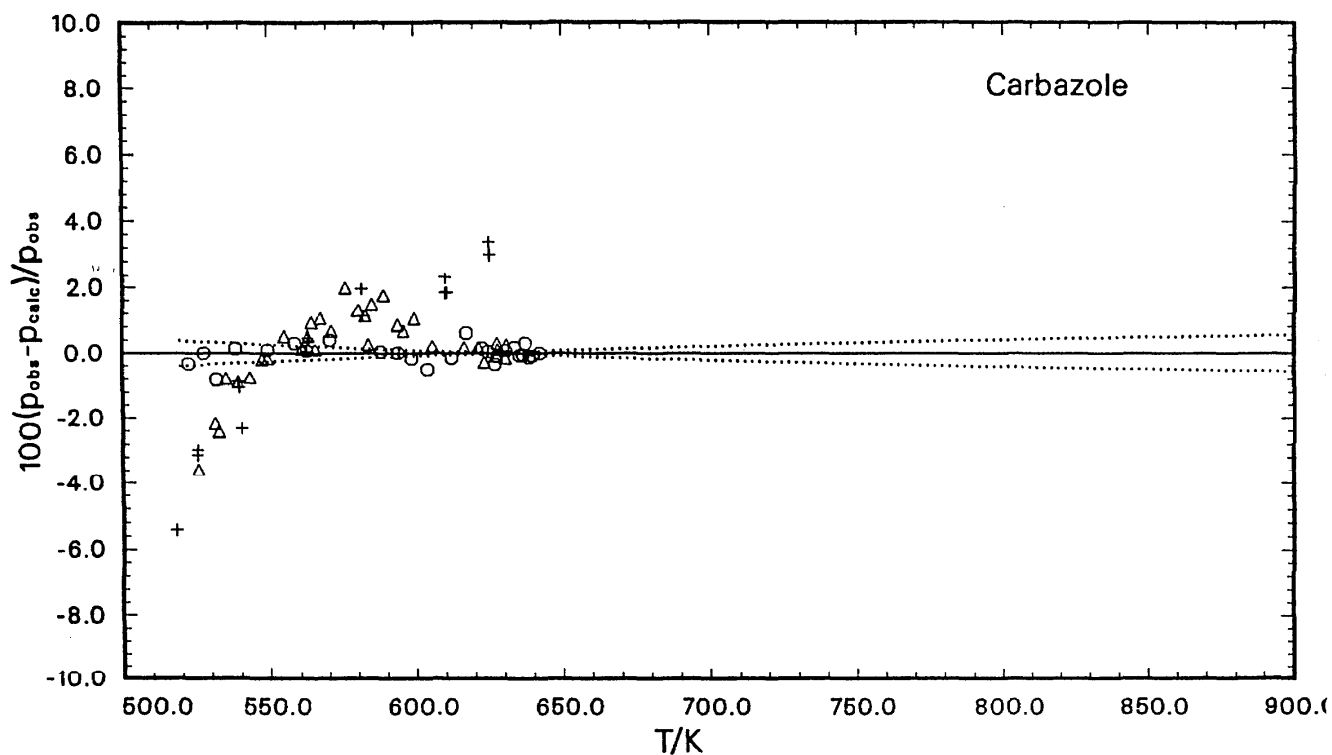


FIG. 17. Percent deviation of experimental vapor pressures for carbazole (liquid) from the Cox equation. Δ (1923-166); + (1923-167); $\circ$ (1983-185)*; * data from this reference used in the evaluation.

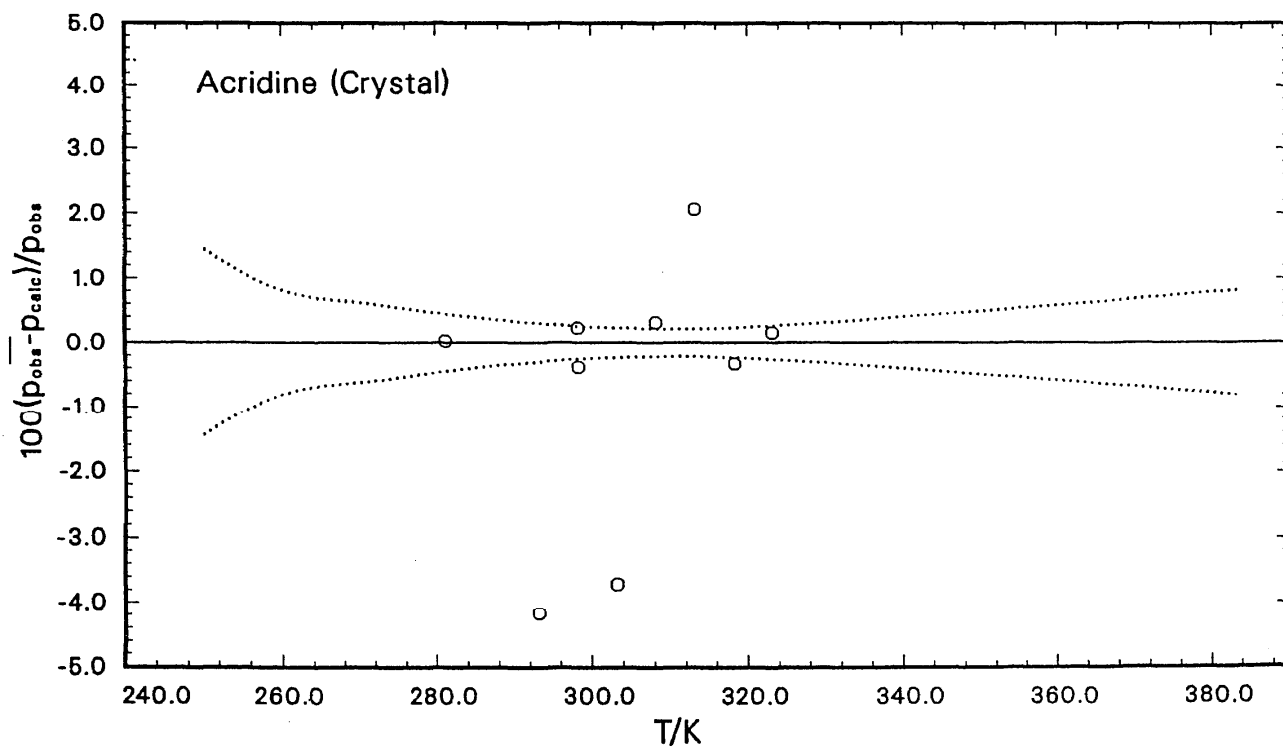


FIG. 18. Percent deviation of experimental vapor pressures for acridine (crystal) from the Antoine equation. $\circ$ (1975-228)*; * data from this reference used in the evaluation.

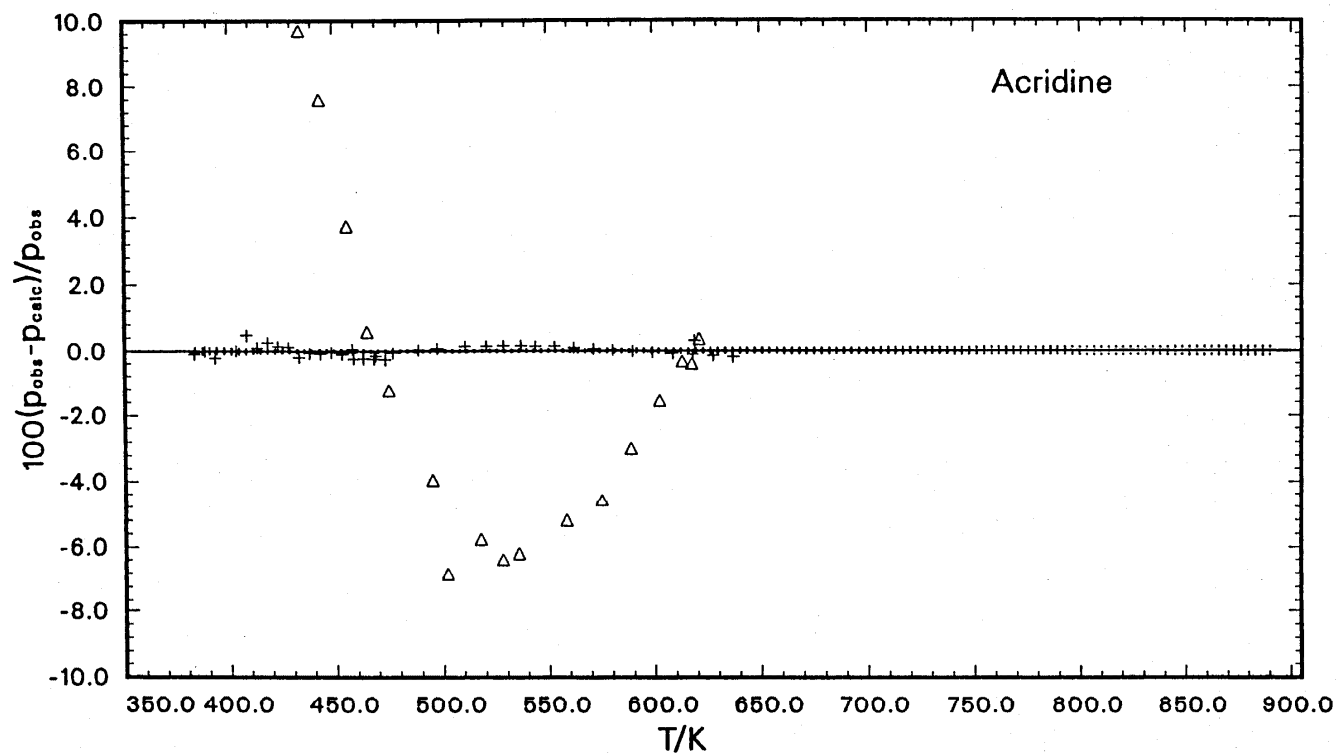


FIG. 19. Percent deviation of experimental vapor pressures for acridine (liquid) from the Cox equation. Δ (1983-189); + (1989-76)*; * data from this reference used in the evaluation.

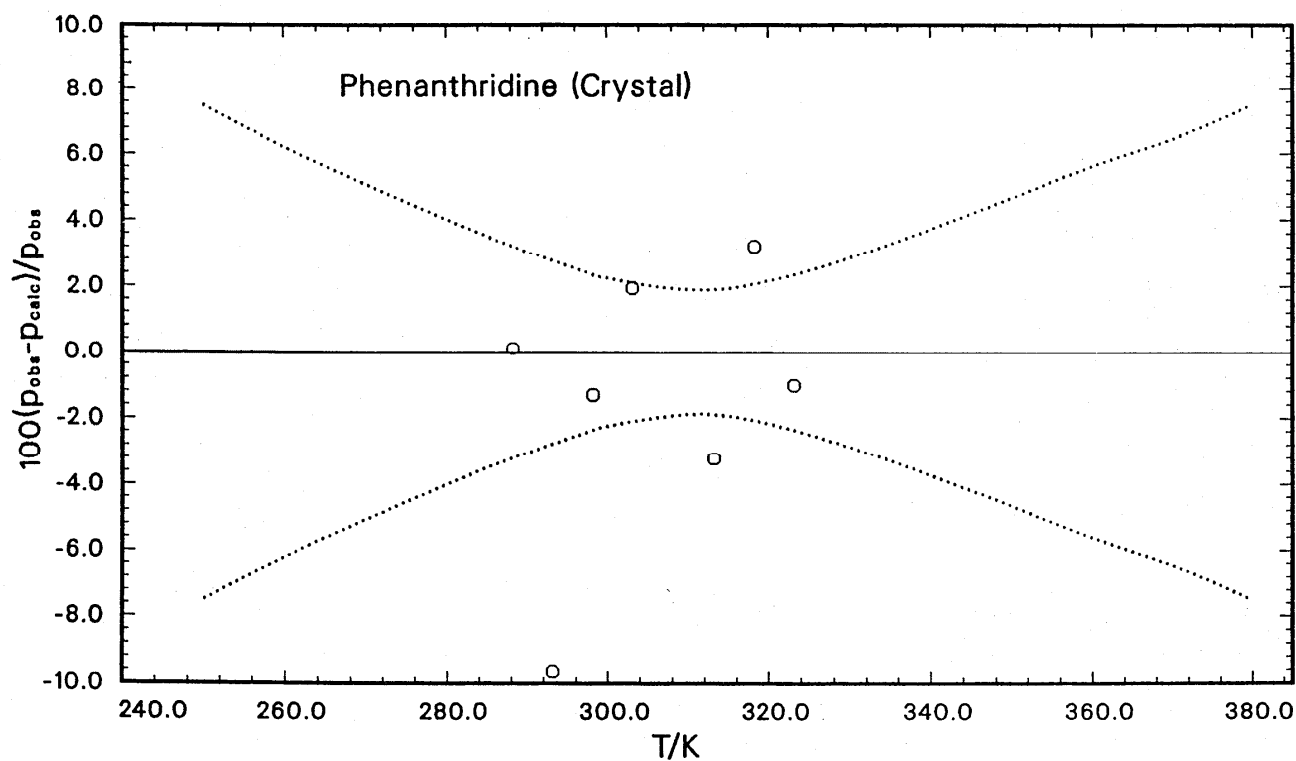


FIG. 20. Percent deviation of experimental vapor pressures for phenanthridine (crystal) from the Antoine equation. $\circ$ (1975-228)*; * data from this reference used in the evaluation.

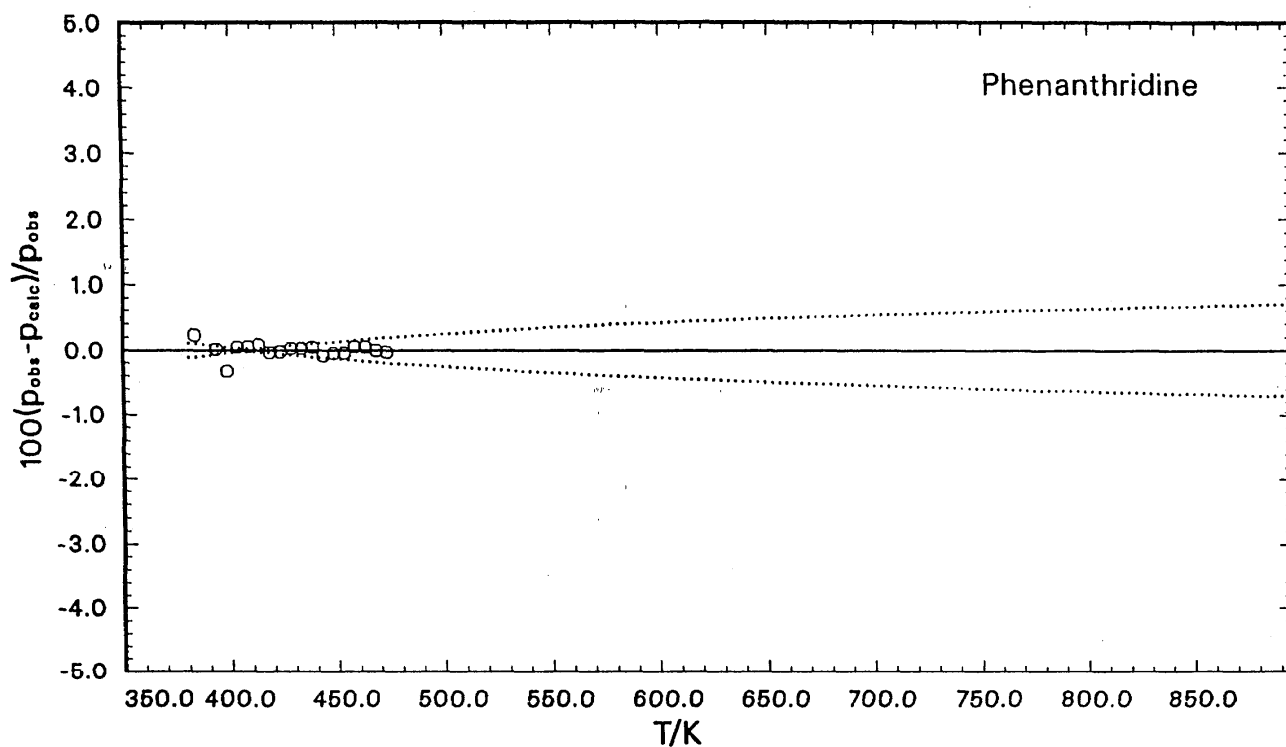


FIG. 21. Percent deviation of experimental vapor pressures for phenanthridine (liquid) from the Cox equation. $\circ$ (1989-76)*; * data from this reference used in the evaluation.

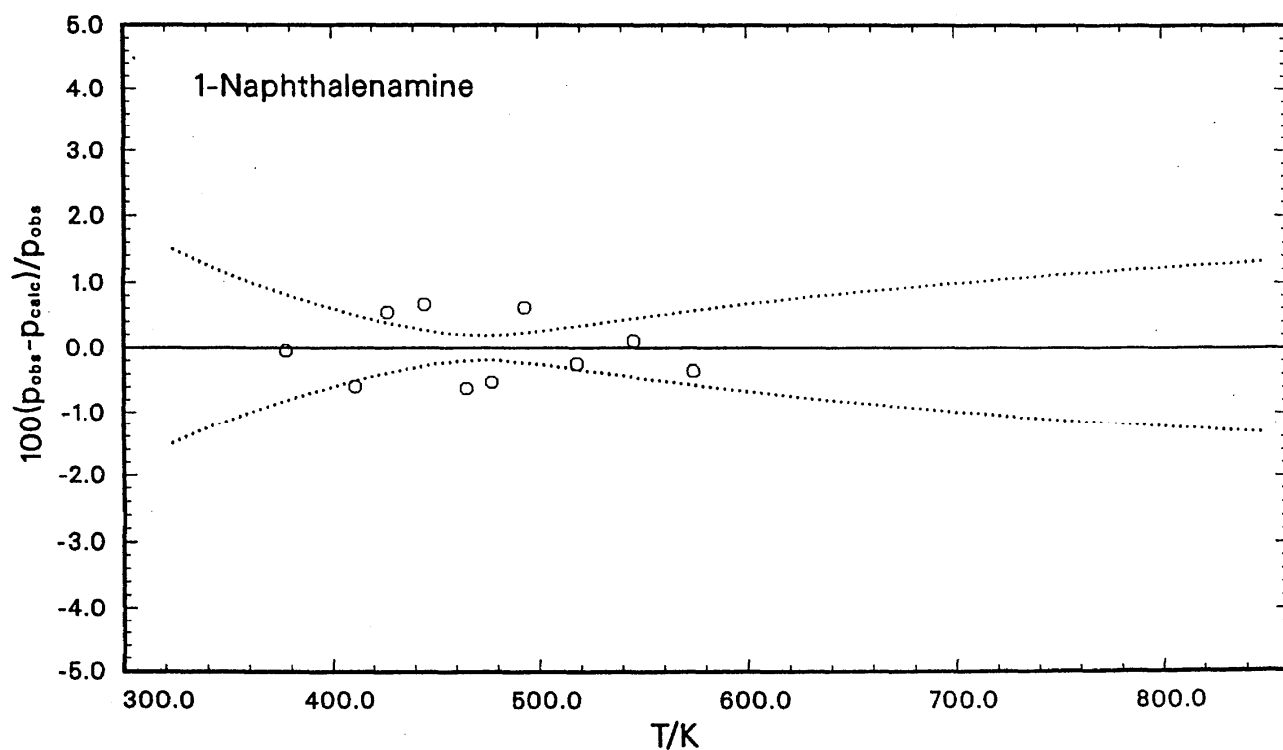


FIG. 22. Percent deviation of experimental vapor pressures for 1-naphthalenamine (liquid) from the Cox equation. $\circ$ (1947-83)*; * data from this reference used in the evaluation.

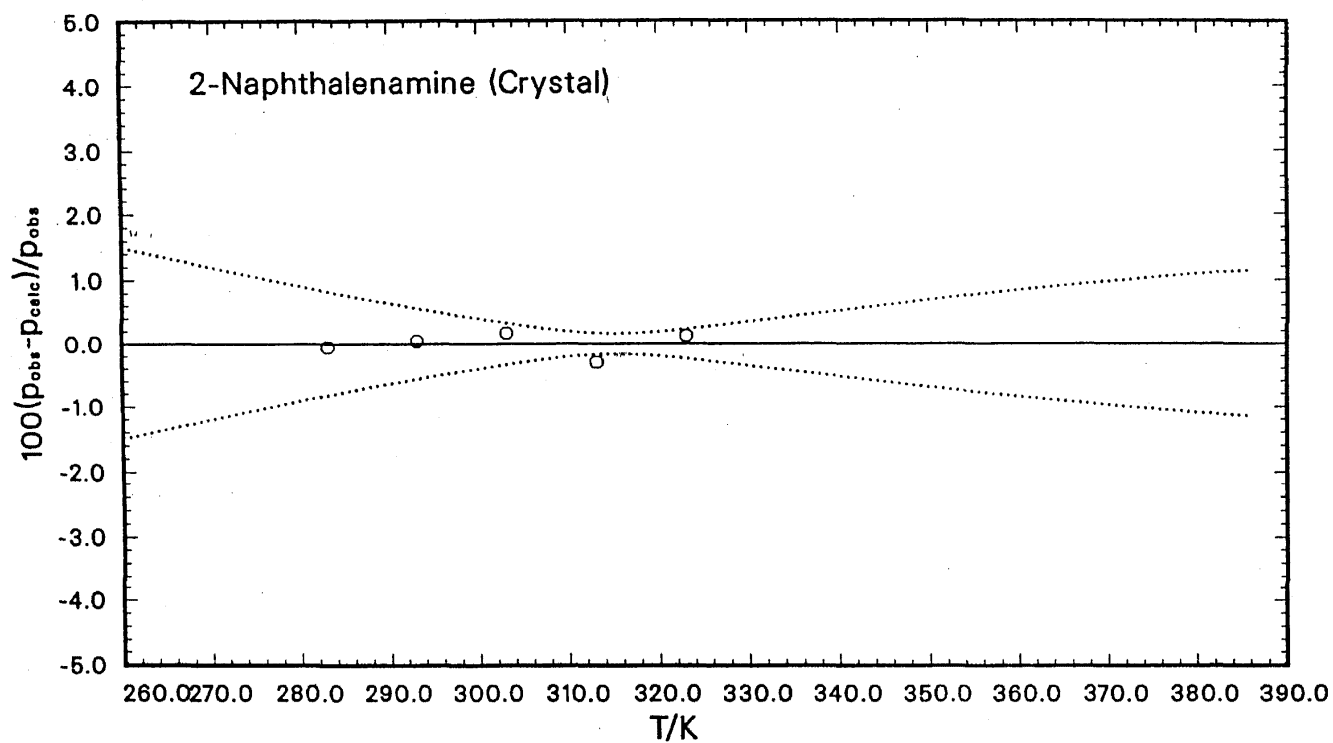


FIG. 23. Percent deviation of experimental vapor pressures for 2-naphthalenamine (crystal) from the Antoine equation. $\circ$ (1968-3)*; * data from this reference used in the evaluation.

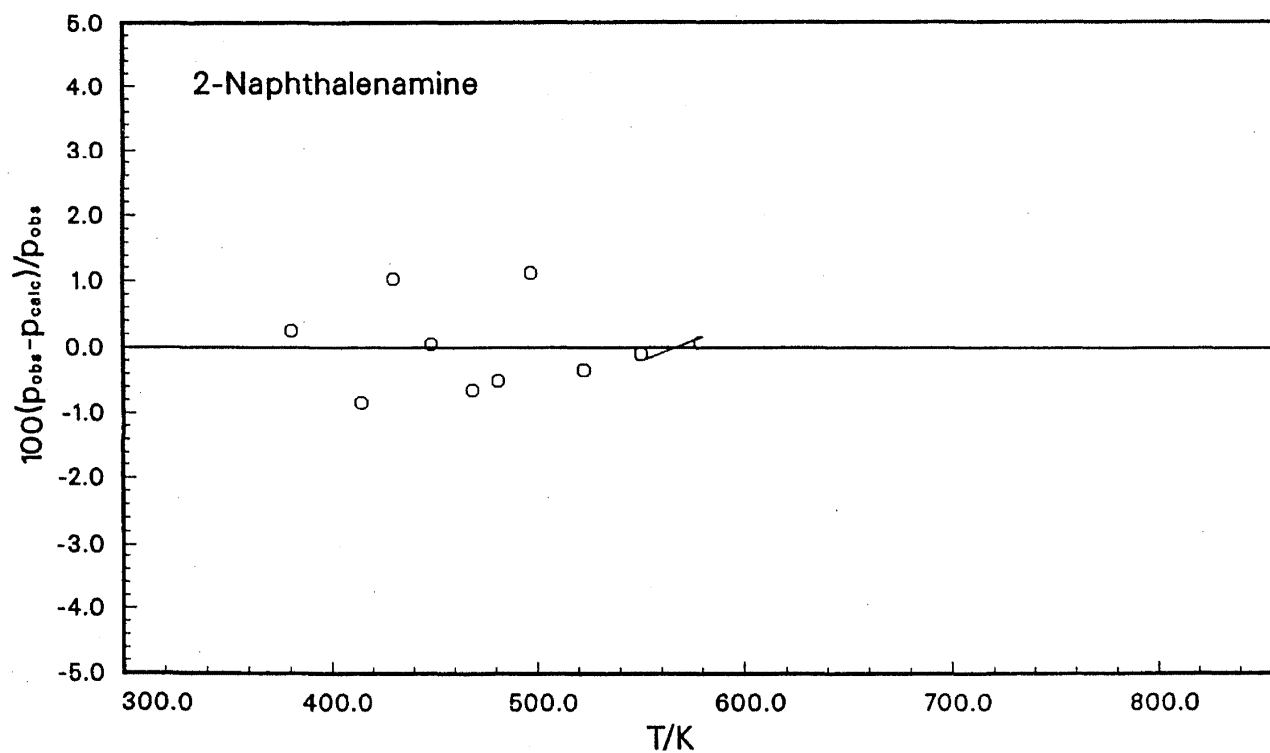


FIG. 24. Percent deviation of experimental vapor pressures for 2-naphthalenamine (liquid) from the Cox equation. $\circ$ (1947-83)*; * data from this reference used in the evaluation.

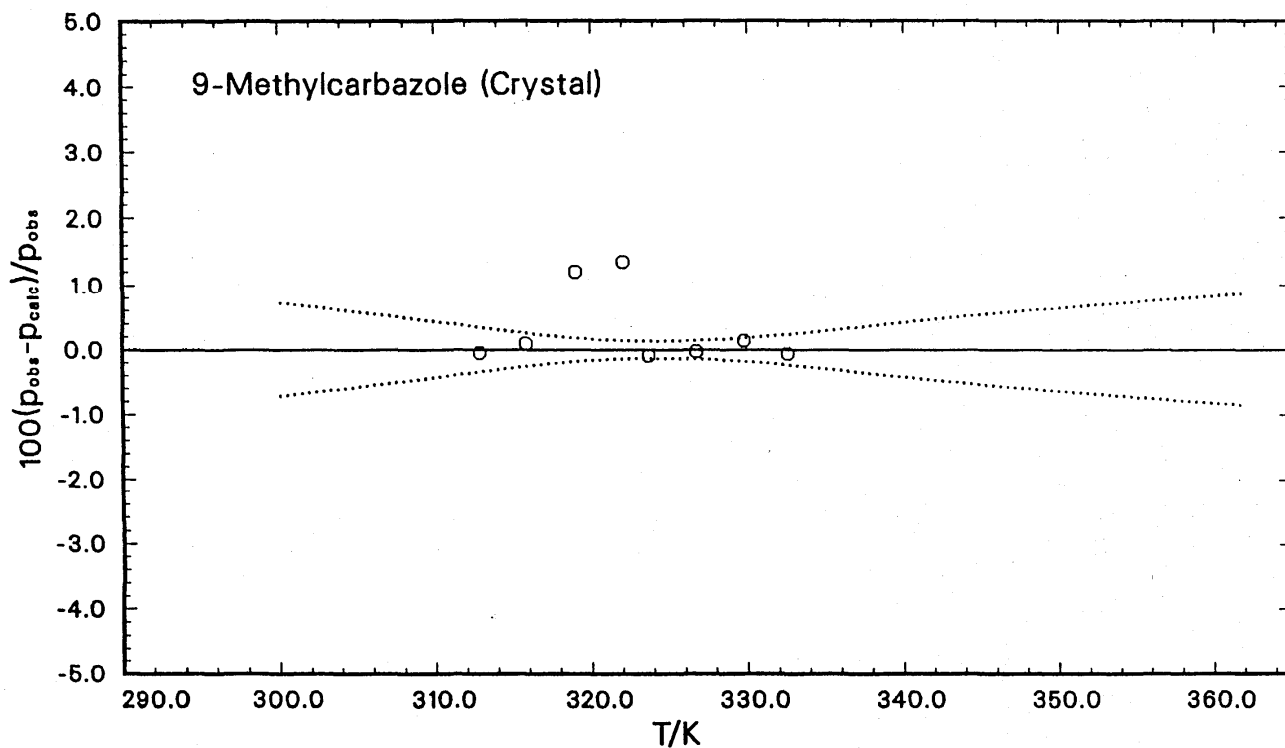


FIG. 25. Percent deviation of experimental vapor pressures for 9-methylcarbazole (crystal) from the Antoine equation. $\circ$ (1990-65)*; * data from this reference used in the evaluation.

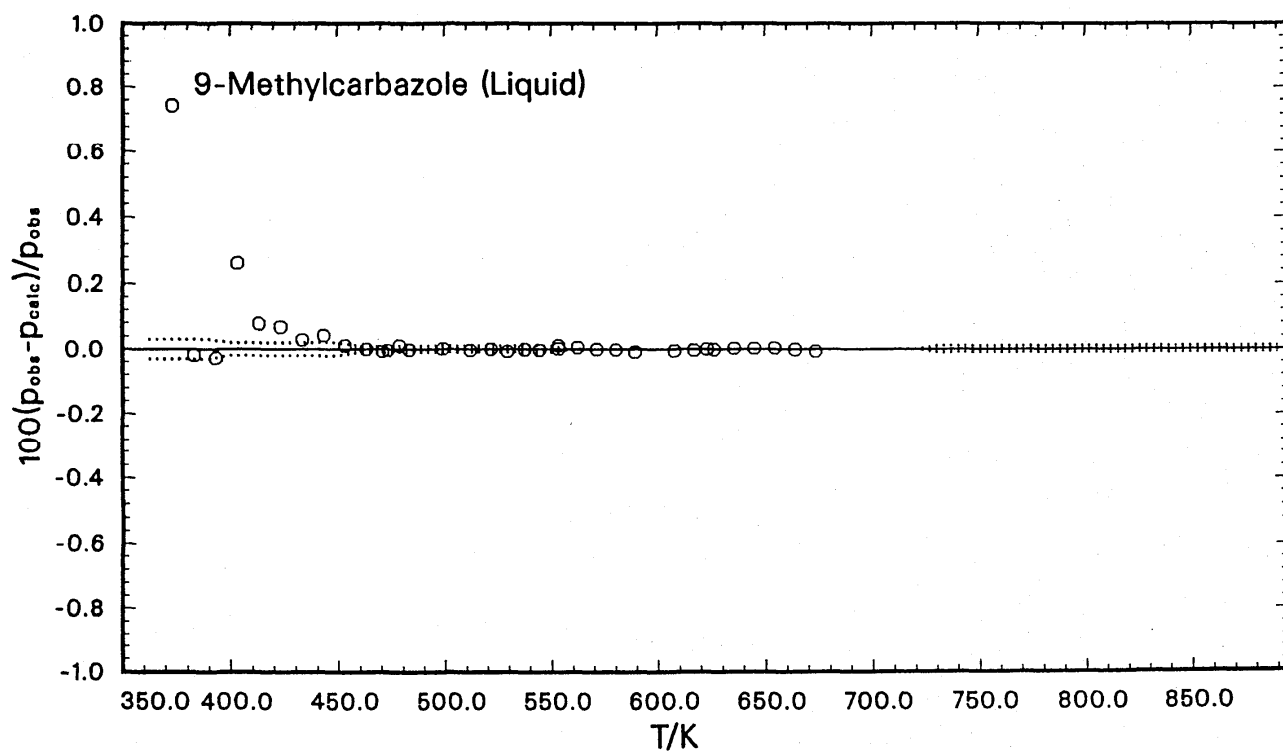


FIG. 26. Percent deviation of experimental vapor pressures for 9-methylcarbazole (liquid) from the Cox equation. $\circ$ (1992-100)*; * data from this reference used in the evaluation.

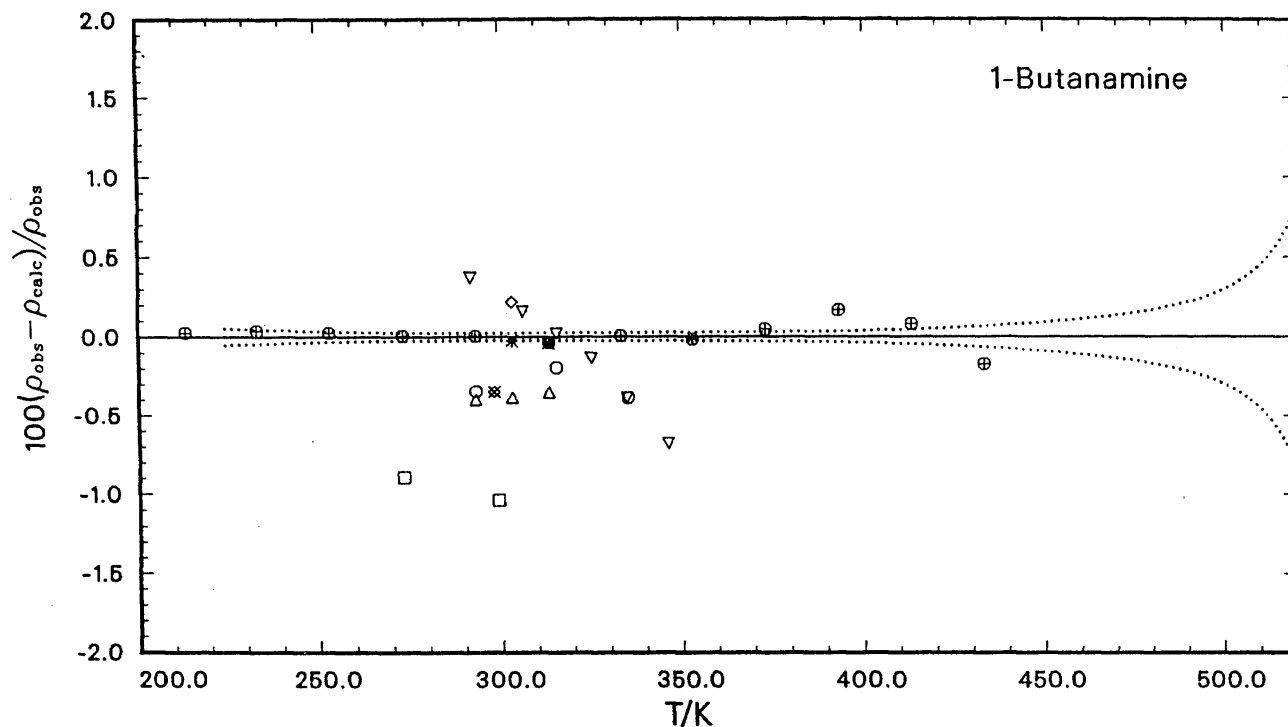


FIG. 27. Percent deviation of experimental saturated liquid densities for 1-butanamine from [Eq. (6)]. $\square$ (1871–21); ∇ (1944–125); $\circ$ (1948–262); $\oplus$ (1959–218)*; $\triangle$ (1972–237); $+$ (1978–77)*; $\times$ (1979–96); $\diamond$ (1979–209); * data from this reference used in the evaluation.

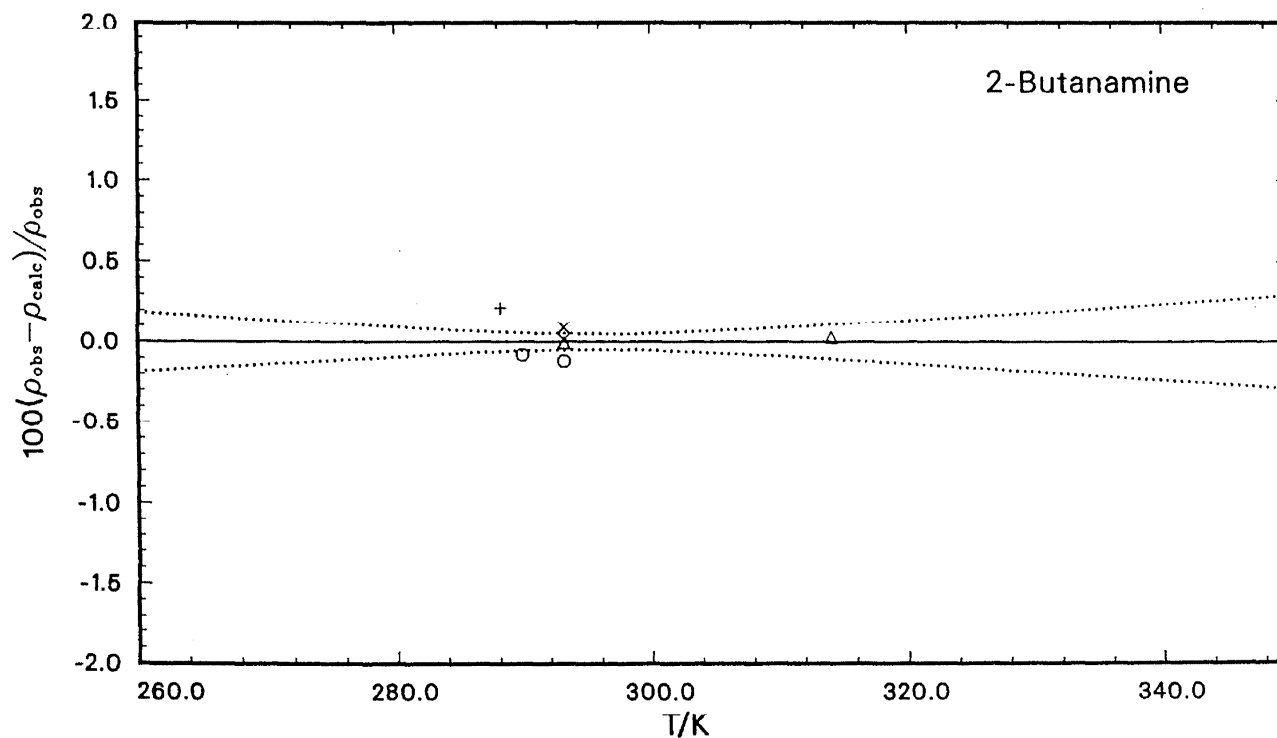


FIG. 28. Percent deviation of experimental saturated liquid densities for 2-butanamine from [Eq. (6)]. $\circ$ (1895–49)*; $\diamond$ (1903–28)*; $+$ (1930–63)*; $\triangle$ (1948–262)*; $\times$ (1978–78)*; * data from this reference used in the evaluation.

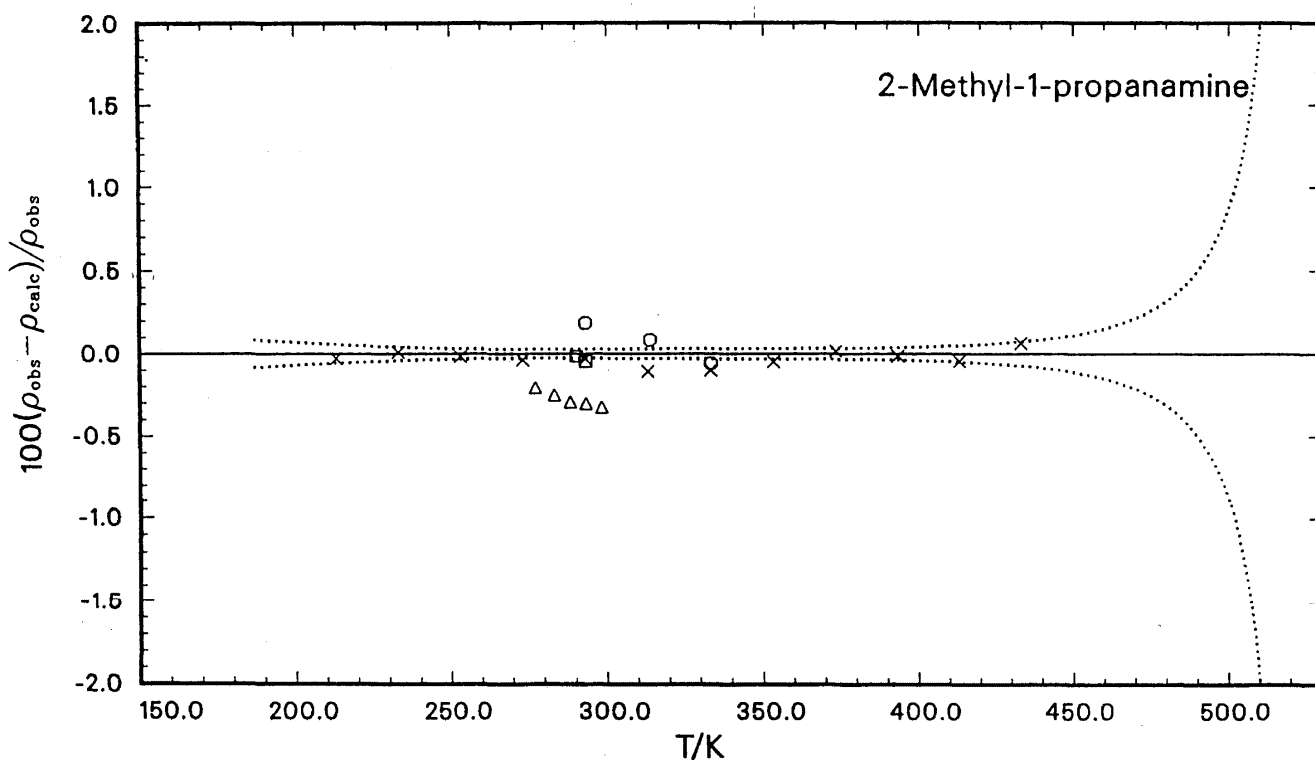


FIG. 29. Percent deviation of experimental saturated liquid densities for 2-methyl-1-propanamine from [Eq. (6)]. Δ (1889-26); $\square$ (1895-49); $\circ$ (1948-262)*; $\times$ (1959-218)*; * data from this reference used in the evaluation.

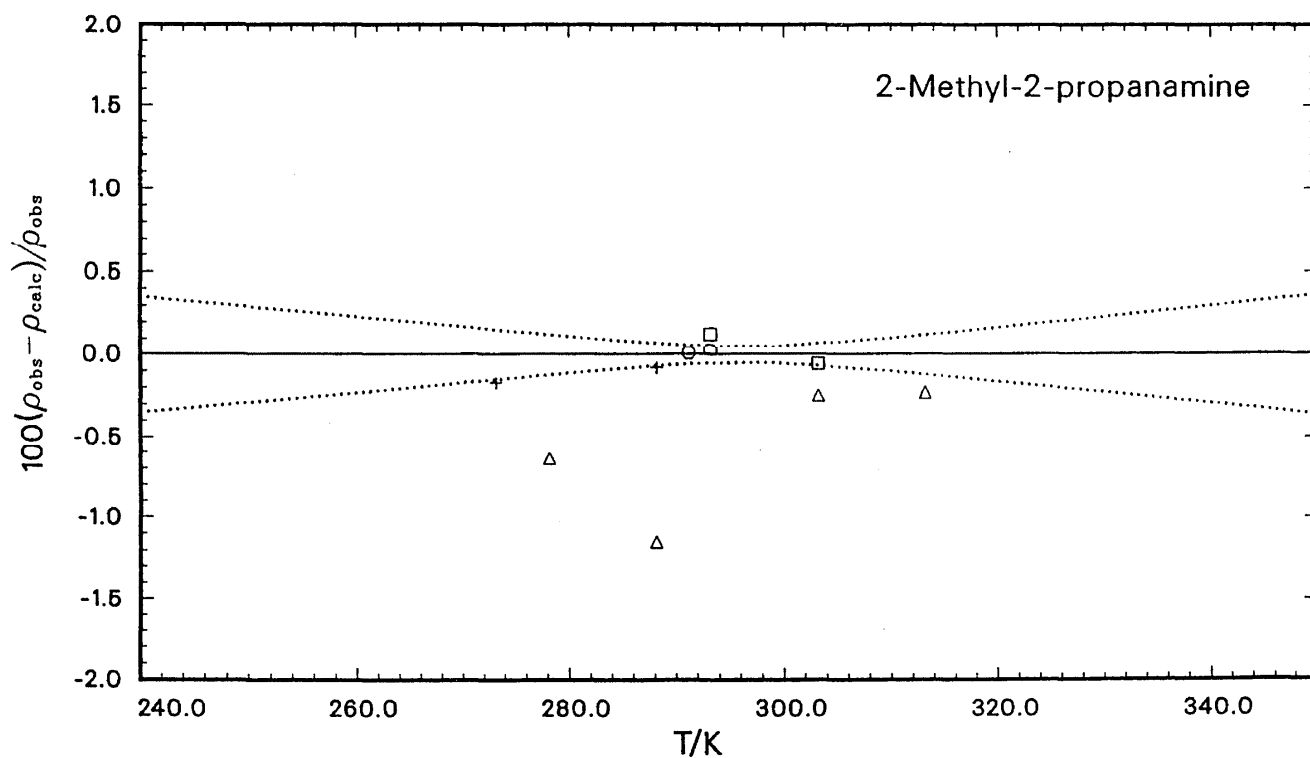


FIG. 30. Percent deviation of experimental saturated liquid densities for 2-methyl-2-propanamine from [Eq. (6)]. $\circ$ (1897-43)*; Δ (1965-387)*; $\square$ (1973-148)*; $+$ (1978-36)*; * data from this reference used in the evaluation.

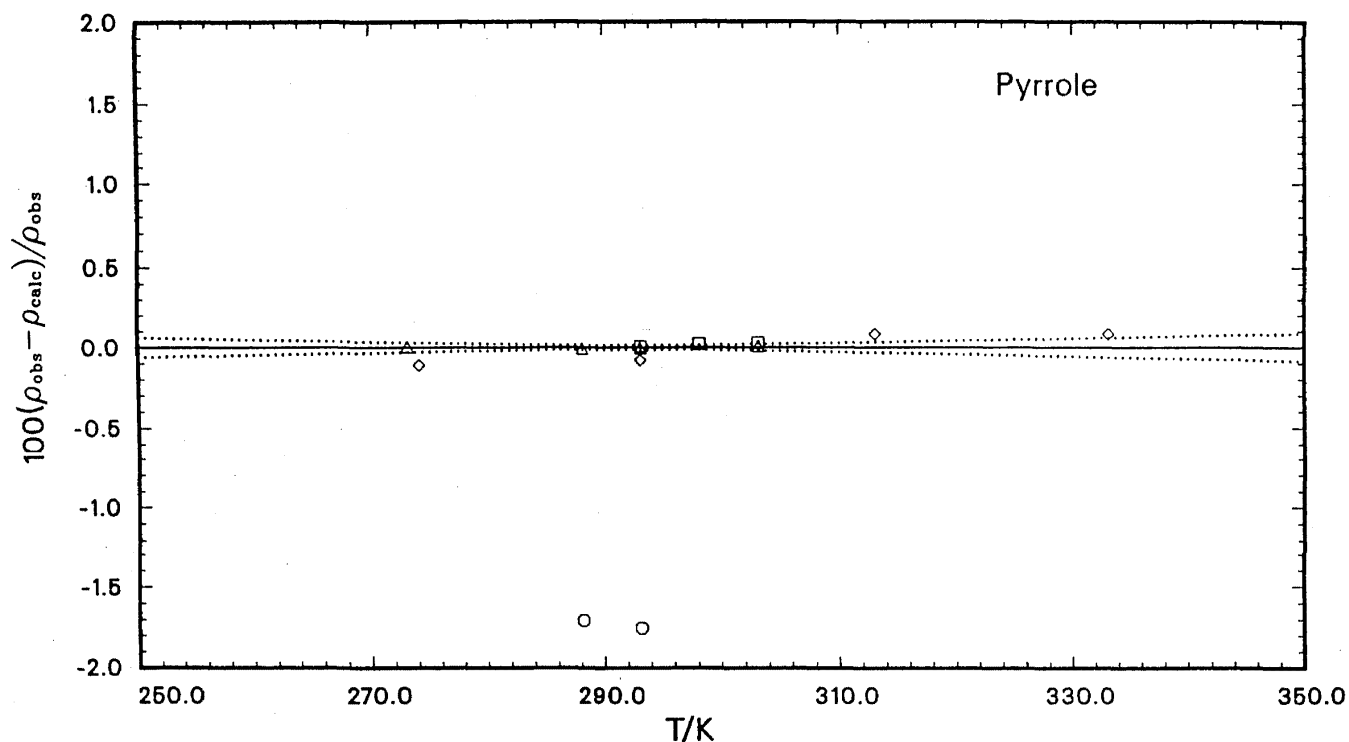


FIG. 31. Percent deviation of experimental saturated liquid densities for pyrrole from values calculated from [Eq. (6)]. + (1895-49); ○ (1937-487); ◇ (1955-11); △ (1955-485)*; □ (1958-216)*; * data from this reference used in the evaluation.

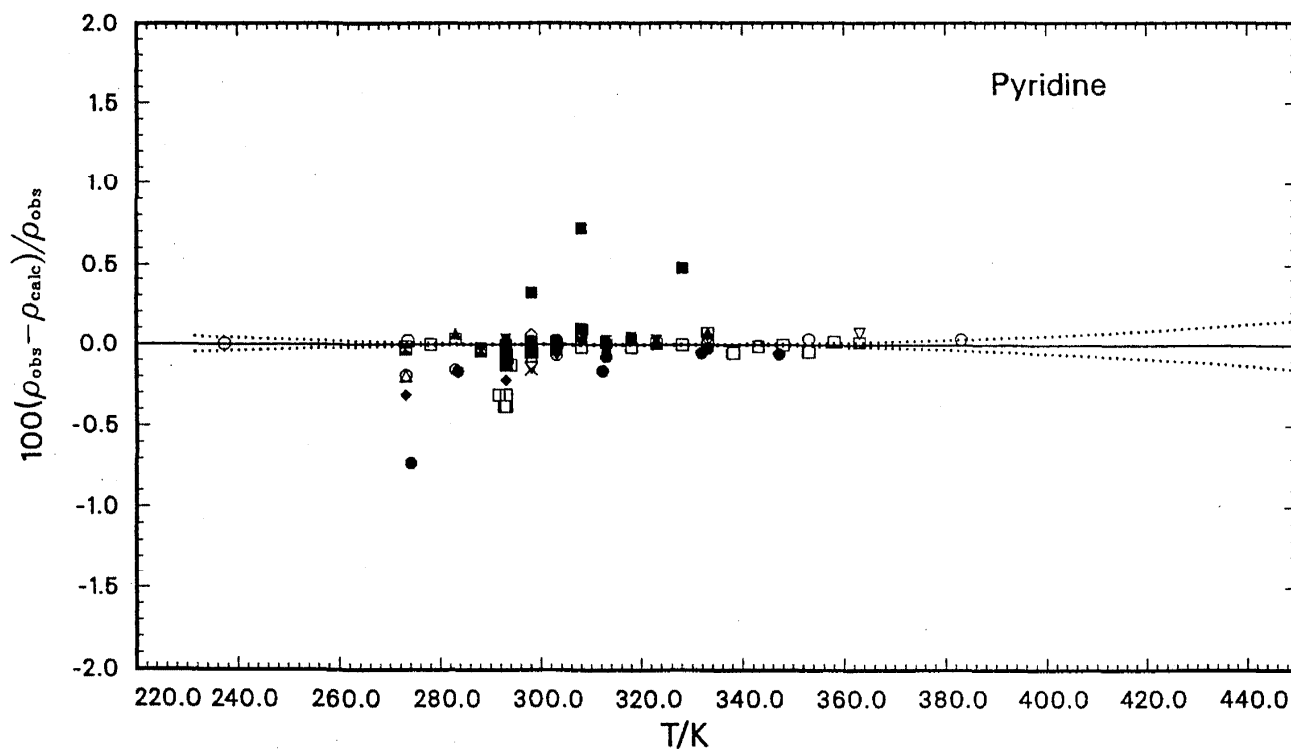


FIG. 32. Percent deviation of experimental saturated liquid densities for pyridine from values calculated from [Eq. (6)]. □ (1895-49); ○ (1907-128); ● (1908-112); △ (1908-126); + (1910-58); ○ (1916-37); × (1926-210); □ (1932-322)*; ▽ (1935-418); ▢ (1937-146); ◇ (1945-205); ■ (1949-43); ▲ (1949-264)*; ◆ (1953-615); * (1954-31); ● (1955-11); ♦ (1956-639)*; ⊕ (1958-216)*; ⌘ (1967-321)*; ⊞ (1971-130)*; ▼ (1971-213)*; ⊗ (1973-222)*; ⌘ (1979-207); ▢ (1980-121)*; ■ (1986-2); * data from this reference used in the evaluation.

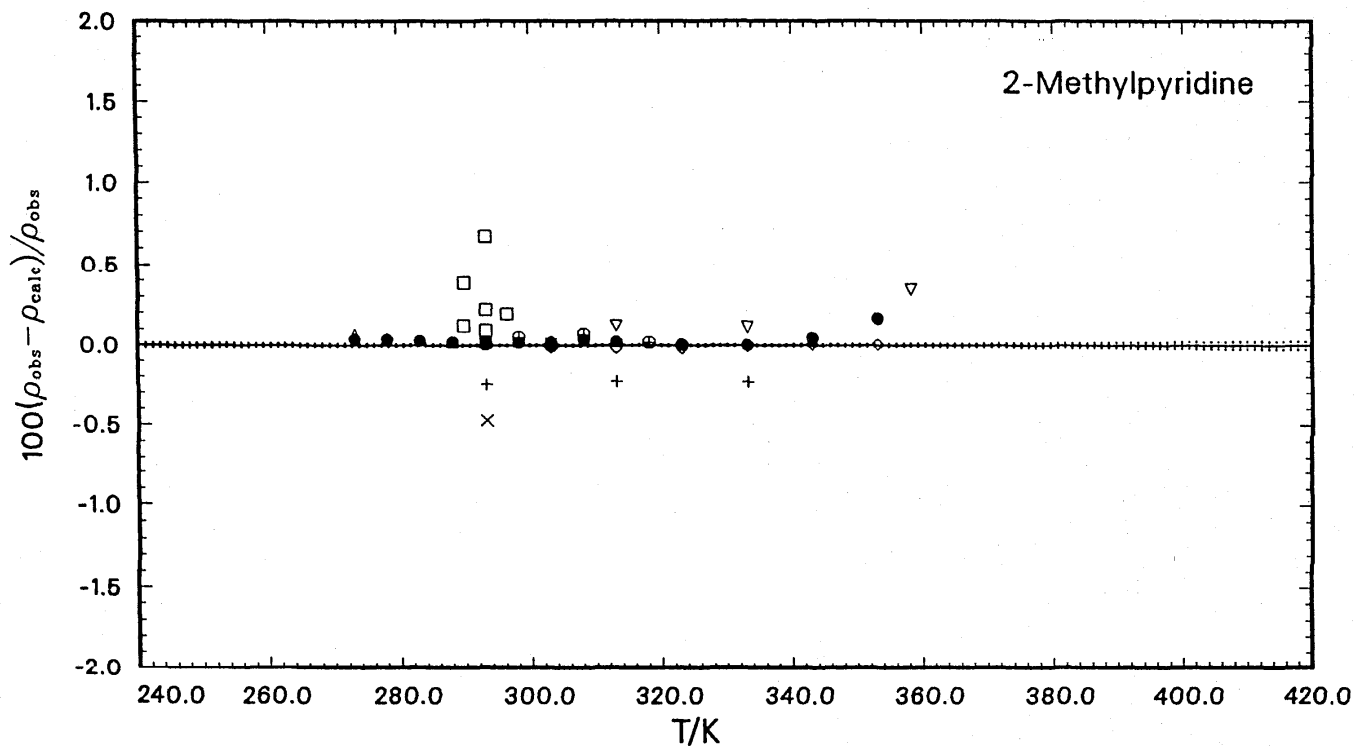


FIG. 33. Percent deviation of experimental saturated liquid densities for 2-methylpyridine from values calculated from [Eq. (6)]. $\square$ (1895–49); $\diamond$ (1948–442)*; $\circ$ (1954–31); $\triangle$ (1955–485); $+$ (1956–639); $\times$ (1958–216); ∇ (1960–119); $\oplus$ (1971–213)*; $\bullet$ (1984–95)*; * data from this reference used in the evaluation.

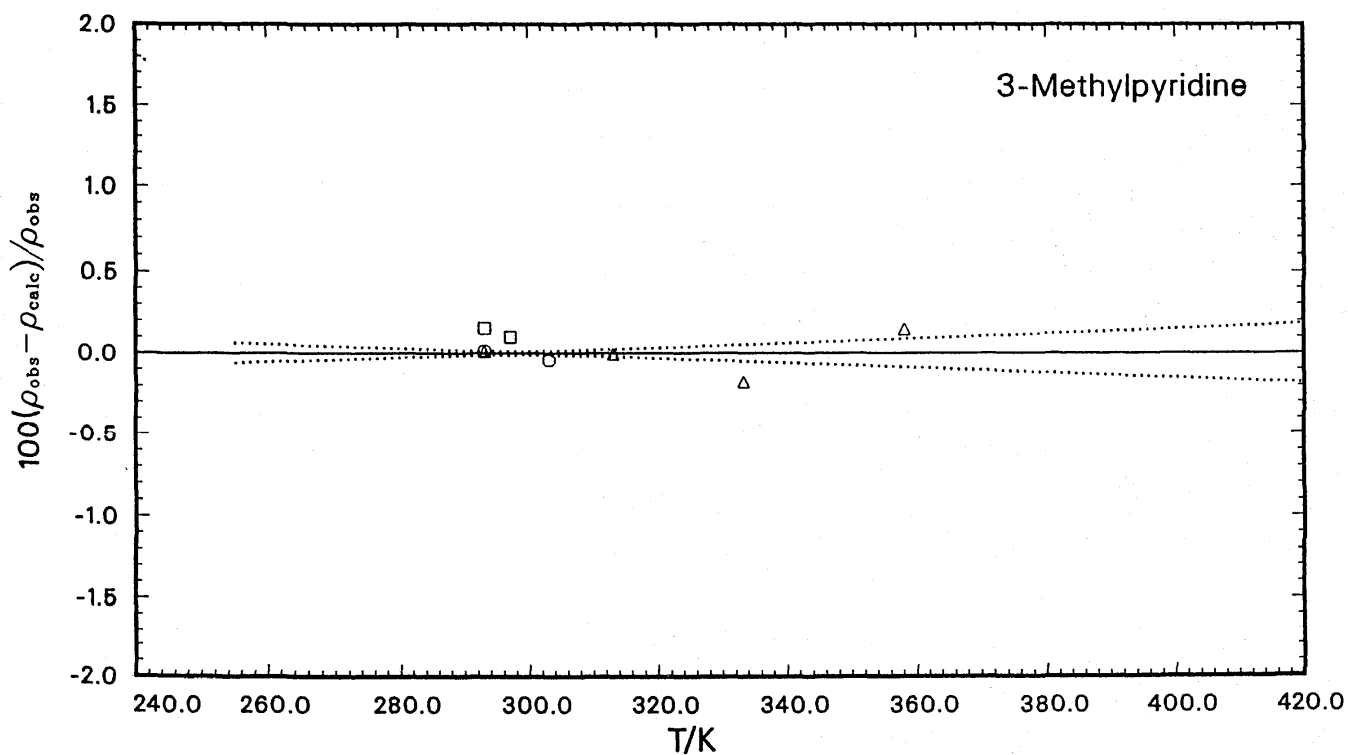


FIG. 34. Percent deviation of experimental saturated liquid densities for 3-methylpyridine from values calculated from [Eq. (6)]. $\square$ (1895–49); $\circ$ (1954–31)*; $\triangle$ (1960–119)*; * data from this reference used in the evaluation.

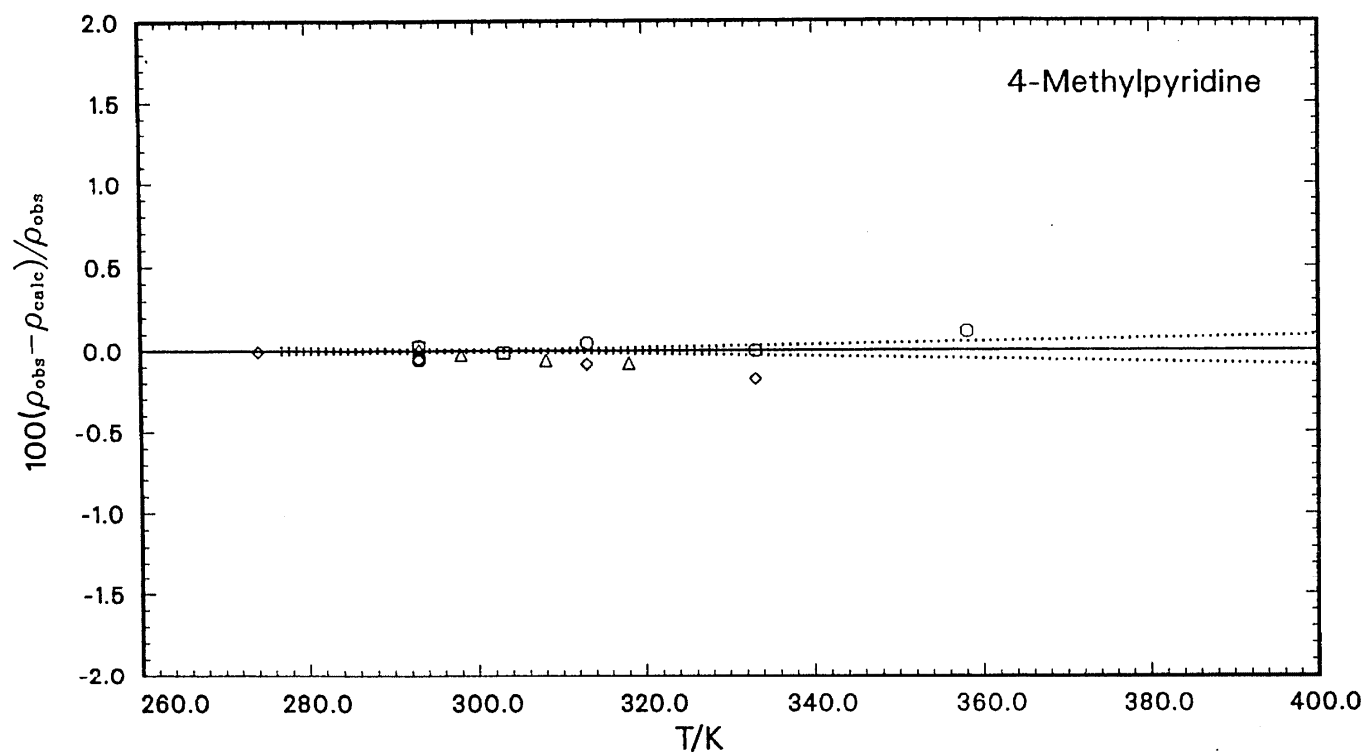


FIG. 35. Percent deviation of experimental saturated liquid densities for 4-methylpyridine from values calculated from [Eq. (6)]. $\square$ (1954-31)*; $\diamond$ (1955-11); $\circ$ (1960-119)*; $\triangle$ (1971-213)*; * data from this reference used in the evaluation.

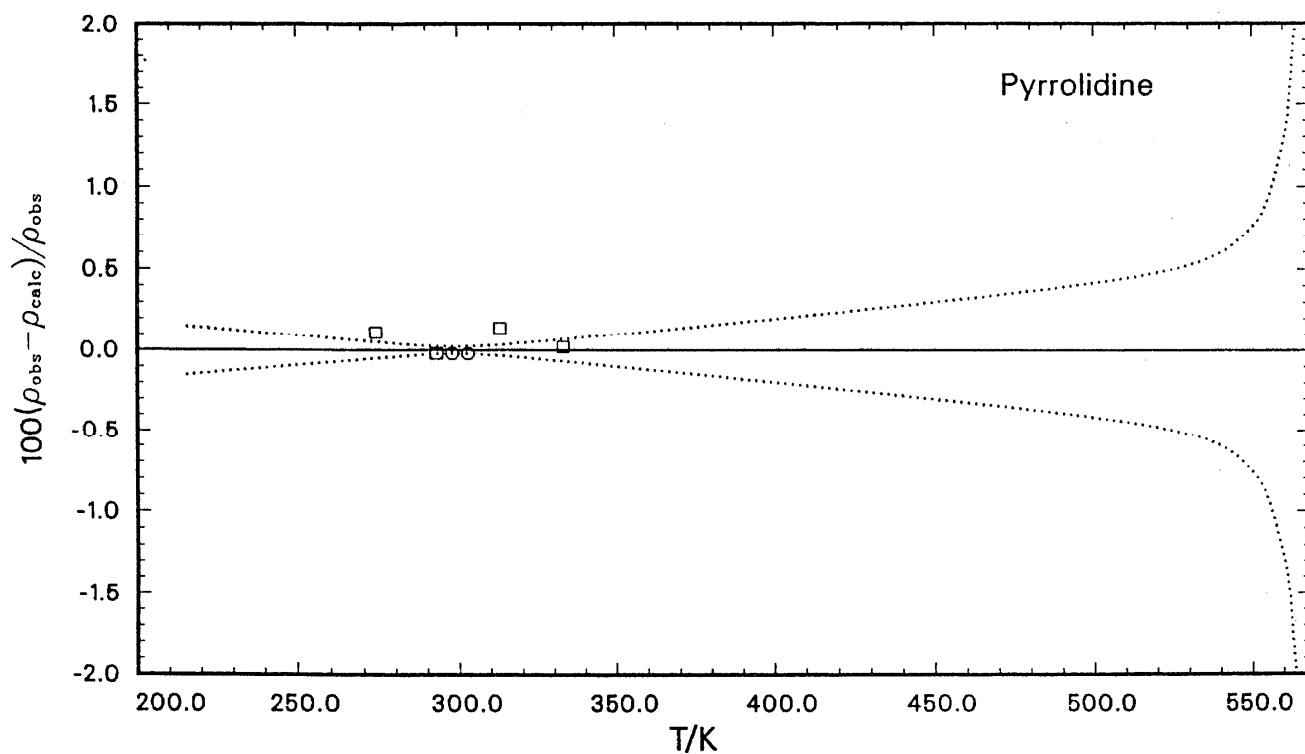


FIG. 36. Percent deviation of experimental saturated liquid densities for pyrrolidine from values calculated from [Eq. (6)]. $\square$ (1955-11); $\circ$ (1958-216)*; * data from this reference used in the evaluation.

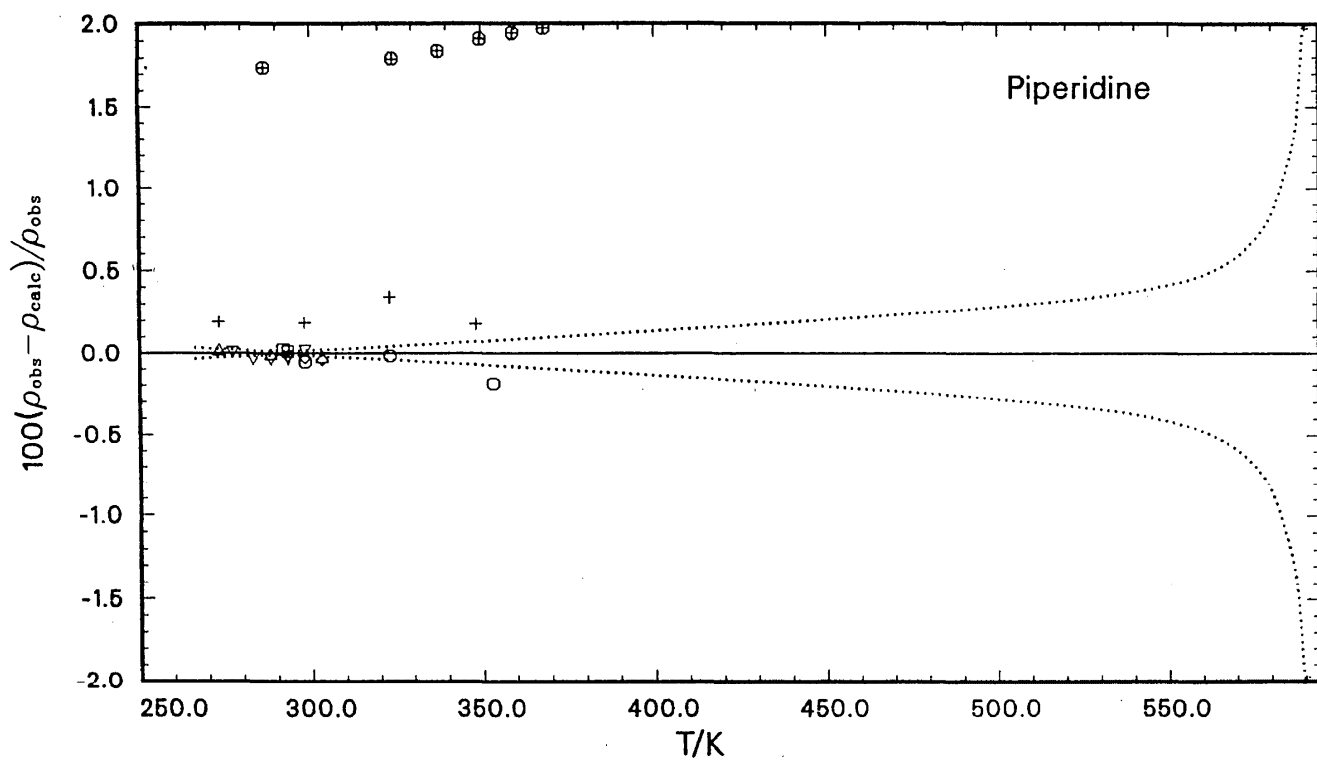


FIG. 37. Percent deviation of experimental saturated liquid densities for piperidine from values calculated from [Eq. (6)]. ∇ (1889-26)*; $\square$ (1895-49); $\circ$ (1913-179); $\triangle$ (1937-146)*; $\oplus$ (1944-126); $+$ (1947-402)*; $\diamond$ (1960-369)*; * data from this reference used in the evaluation.

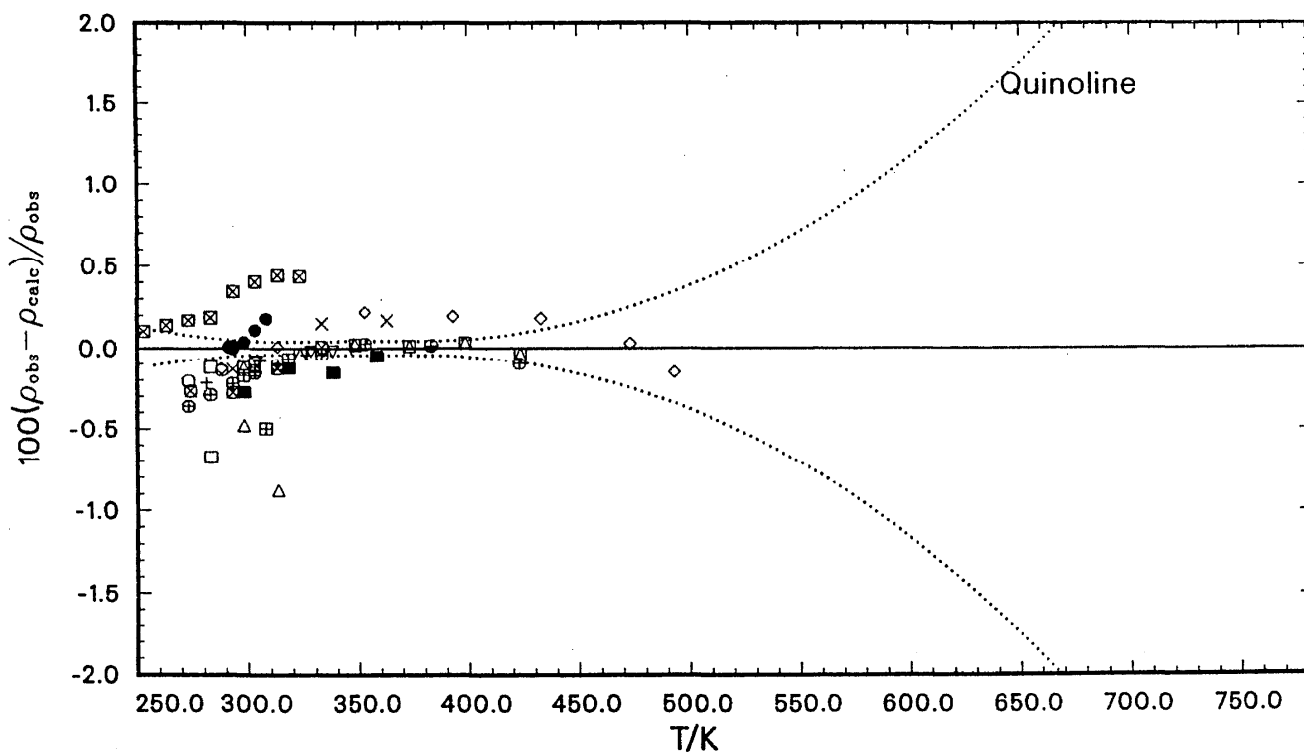


FIG. 38. Percent deviation of experimental saturated liquid densities for quinoline from values calculated from [Eq. (6)]. $\square$ (1884-28); $\diamond$ (1907-64); ∇ (1908-112); $+$ (1911-44); $\oplus$ (1916-37); $\circ$ (1937-146); $\bullet$ (1949-43); $\triangle$ (1951-444); $\times$ (1954-674); $\oplus$ (1955-11); $\boxtimes$ (1965-231)*; $\boxtimes$ (1984-246); $\blacksquare$ (1986-86); $\boxtimes$ (1988-551)*; * data from this reference used in the evaluation.

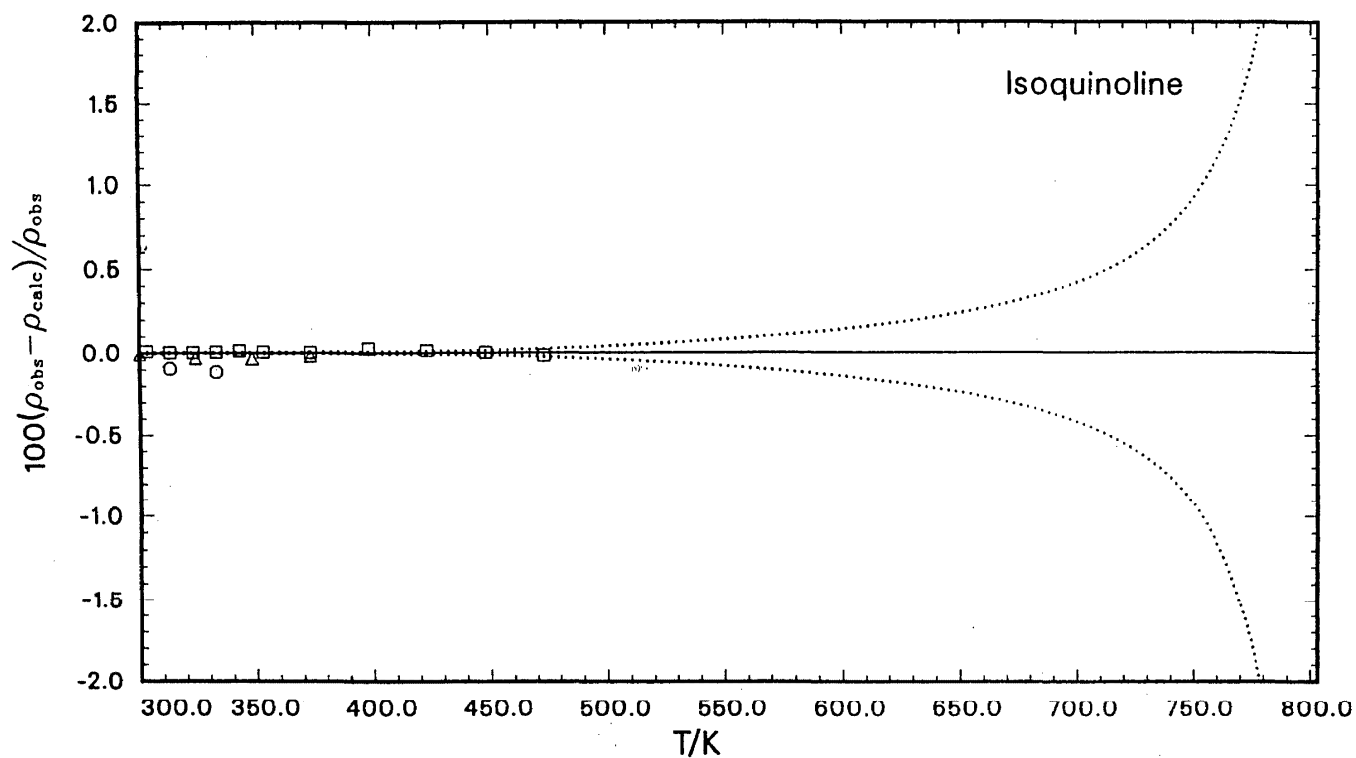


FIG. 39. Percent deviation of experimental saturated liquid densities for isoquinoline from values calculated from [Eq. (6)]. $\square$ (1949-545)*; $\circ$ (1955-11); $\triangle$ (1988-551)*; * data from this reference used in the evaluation.

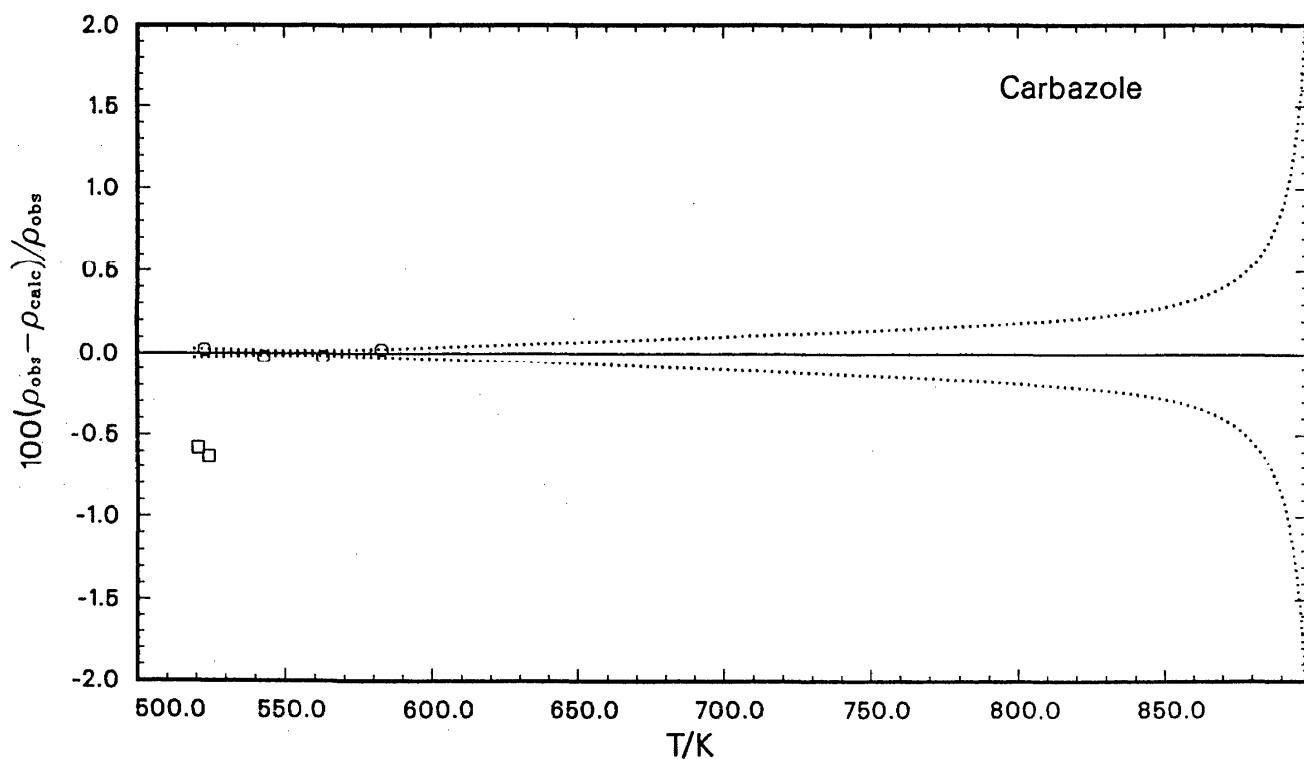


FIG. 40. Percent deviation of experimental saturated liquid densities for carbazole from values calculated from [Eq. (6)]. $\square$ (1931-8); $\circ$ (1972-326)*; * data from this reference used in the evaluation.

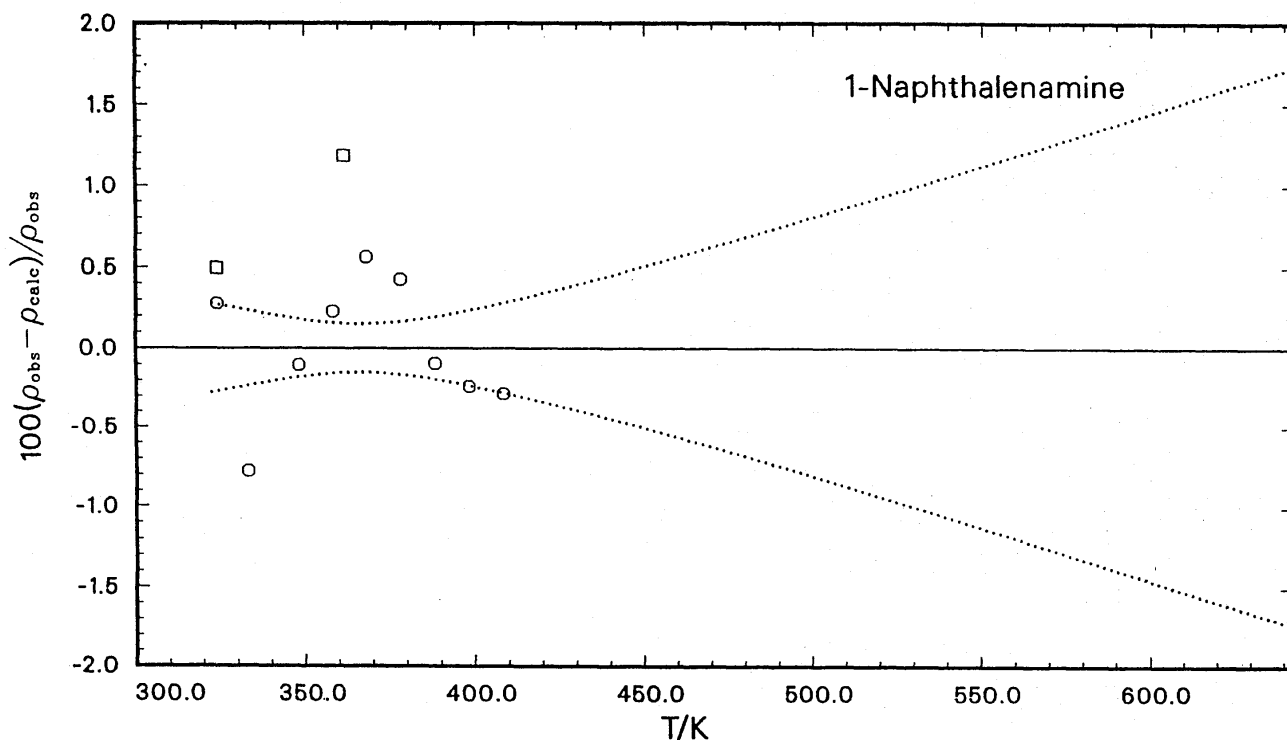


FIG. 41. Percent deviation of experimental saturated liquid densities for 1-naphthalenamine from values calculated from [Eq. (6)]. □ (1892-22); ○ (1907-112)*; * data from this reference used in the evaluation.

4. Discussion

The 23 Nitrogen compounds evaluated in the study are considered to be important compounds in the development of empirical correlations for the estimation of properties of their respective homologous series. The reliability of any estimation procedure depends on the accuracy and reliability of the basic values used in establishing the estimation parameters. Predictive methods were used to derive some of the recommended values, particularly the critical properties and enthalpies of formation. It is necessary to use predicted critical properties when there is no experimental results as these values are required for a proper extrapolation of vapor pressure, density, and virial coefficients. The evaluations in this work indicated the lack of quality measurements on thermophysical properties for many of the compounds studied. In particular these are few measurements of the critical density of the majority of compounds. Values of critical density are important in many prediction schemes and the use of the critical temperature and pressure measurements along with an assumed critical compressibility ratio can lead to values of the critical density in error by 15 per cent. For many of the higher molecular

weight compounds, it is not possible to make measurements at the critical point due to decomposition.

There are few reliable vapor pressure measurements over an adequate temperature range for 2- and 3-methylpyrrole, indole, and 1- and 2-naphthalenamine. For these compounds there is also a lack of reliable density measurements.

There is no experimental data on enthalpies of combustion for 2- and 3-methylpyrrole. Only low accuracy measurements have been made on the enthalpies of combustion of 1- and 2-naphthalenamine. Low-temperature heat capacity measurements are available for only 14 of the 23 compounds of interest. There is a lack of spectroscopic data for 9-methylcarbazole so that the ideal gas thermodynamic properties cannot be calculated using statistical mechanical technique.

The agreement achieved between ideal gas entropy values derived from evaluated experimental data using the third law of thermodynamics and statistical mechanical calculations were satisfactory except for acridine and phenanthridine, where the differences can be explained by the uncertainties in the enthalpies of vaporization and vapor pressure data. The majority of the reliable thermodynamic and physical property measurements have been made at NIPER, Bartlesville, OK.

5. Symbols and Notation

Subscripts and indexes, general

c	for value of T , p , V , or ρ at the critical point
f	for formation of the substance from its elements, each in their standard states
g	for vapor in equilibrium with liquid
i, j, m, n	integer index
l	for liquid in equilibrium with vapor
r	for coefficient to reduced variable in Eq. (10); for reduced variable in Eq. (12); for moment of inertia; for rotational potential function
ref	at reference pressure (101.325 kPa) in Cox vapor pressure equation [Eq. (3a or 3b)]
sat	for value of C_{sat} or p_{sat} determined with an infinitesimal amount of vapor(here) in equilibrium with the condensed phase (l , or c)
tr	for value at a transition temperature

Superscripts

see other variables and notations, and functional notation below

Other variables and designations

$A_a, B_a, \dots, F_a$	coefficients in extended Antoine equation [Eq. (5)]
A_d, A_d	coefficients in Eq. (13) for $-\text{NH}_2$ inversion
A_i	least squares adjusted parameter in Eqs. (2), (3a), and (6)
A_r	coefficient to ρ_c in Eq. (10) for second virial coefficient
A_x	exponential function in Eqs. (3a–3b)
A', A'', C_1, C_s	molecular symmetry species
B	second virial coefficient in Eqs. (8–10)
C	carbon symbol
C_b	coefficient to exponential term in Eqs. (9–10)
$C(A_i, A_j)$	element in correlation matrix in Eq. (2)
C_{end}	heat capacity determined at constant end (sat or p)
D_r	coefficient to (T_c/T) in exponential term of Eq. (10)
F	$= h/8\pi^2 c I_r$, function for internal rotation
F_i	coefficient in $\sum_i F_i \cos i\theta$ for angle dependent function for internal rotation
G	molar Gibbs energy
H	hydrogen symbol
H	molar enthalpy
I_a, I_b , and I_c	moments of inertia about the three principal orthogonal axes
I_r	reduced moment of inertia for relative rotation about a bond
L	number of degrees of freedom involved in rotation about C–N and C–C bonds
N	nitrogen symbol
N	number of atoms in each molecule
S	molar entropy
T	temperature

T_a°	nearest integer value of temperature in Kelvin at which the vapor pressure is 130 kPa in the extended Antoine equation [Eq. (5)]
T_b	boiling temperature at 101.325 kPa
T_m	freezing temperature at 101.325 kPa in air
V	molar volume; potential function
V_n	coefficients in potential function for relative rotation about a bond
V_r	potential function for relative rotation about a bond
$V_w(z \text{ or } r/r_o)$	potential function for inversion of $-\text{NH}_2$ where z and r/r_o are the relative motion displacements
X_a	$= (T - T_a^\circ)/T_c$ in the extended Antoine equation [Eq. (5)]
a, b	coefficients in potential function for $-\text{NH}_2$ inversion
cr	crystal
g	gas
l	liquid
n	exponent to X_a in extended Antoine equation [Eq. (5)]
p	pressure
p_{sat}	vapor pressure
p_{tp}	triple point pressure
rmswd	$\sqrt{\frac{\sum (Y_{\text{calc}} - Y_{\text{obs}})^2}{n}}$
x	$= \{1 - T/(T_c)\}$ in Eq. (6)
x	condensed phase
α_m	coefficient to $(1 - T/T_c)$ in Eq. (7)
Δ	see functional notation below
ϵ	$= 0.35$, exponent to x in Eq. (6)
θ	angle of rotation
ν_i	fundamental vibrational frequency
ν_{inv}	bending frequency between lowest two energy levels for inversion about a nitrogen atom
$\nu_{\text{tor}}(0 \rightarrow 1)$	torsional frequency for transition between lowest two energy levels
ρ	density
σ	molecular symmetry number
$\sigma(x)$	imprecision in the variable x with $\sigma_c(x)$ constant contribution and $\sigma_f(x)$ fractional contribution

Constants and units

$^\circ\text{C}$	degree celsius, temperature
J	joule, energy
K	kelvin, temperature
Pa	pascal = newton/(meter) ² , pressure
R	$= 8.314510 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$, gas constant
c	$= 2.99792458 \cdot 10^8 \text{ m}\cdot\text{s}^{-1}$, speed of light
cm^{-1}	$\approx 29979.2458 \text{ MHz}$, wavenumber
e	$= 2.71828\dots$, Napierian base
h	$= 6.6260755 \cdot 10^{-34} \text{ J}\cdot\text{Hz}$, Plank's constant
m	meter
mol	$= 6.0221367 \cdot 10^{23}$ molecules, mole
s	second

π	= 3.1415...
$\cos(\theta)$	cosine of angle θ
$\ln(Z)$	logarithm of Z for Napierian base, e
$\log_{10}(Z)$	logarithm of Z for base 10
$Y^\circ Z'$	angle of Y degrees and Z minutes
$Y(A_1, A_2, \dots)$	variable Y as a function of the parameters, $A_1, A_2, \dots$
Z°	value of Z (C, H, S, G) at 100 kPa, standard state
$Z(\text{ph}, T)$	value of Z ($C_p, \Delta_f H^\circ$, etc.) for phase ph at temperature T
$\Delta_q Z$	change in variable Z (G, H, S) for process q (f or tr)
$\Delta_{s1}^{s2} Z$	change in variable Z (G, H, S) in passing between states $s1$ to $s2$

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