Thermodynamic and Thermophysical Properties of Organic Nitrogen Compounds. Part I. Methanamine, Ethanamine, 1- and 2-Propanamine, Benzenamine, 2-, 3-, and 4-Methylbenzenamine

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The thermodynamic and thermophysical properties of eight primary amines, methanamine, ethanamine, 1- and 2-propanamine, benzenamine, and 2-, 3-, and 4-methylbenzenamine 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: critically evaluated data; methanamine; ethanamine; 1-propanamine; 2-propanamine; benzenamine; 2-methylbenzenamine; 3-methylbenzenamine; 4-methylbenzenamine; boiling temperature; freezing temperature; critical point; heat capacity; vapor pressure; enthalpy of vaporization; density; second virial coefficient; enthalpy of combustion; ideal gas thermodynamic properties; condensed phase thermodynamic properties; thermodynamics; thermochemistry; thermophysics.

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1. Introduction

1.1. Scope and Objectives

This report provides a compilation of a consistent set of evaluated physical and thermodynamic properties of a selected group of amines. 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 (formerly National Bureau of Standards).

Part 1 (this report) contains thermodynamic data of the following organic nitrogen compounds: methanamine, ethanamine, 1- and 2-propanamine, benzenamine, and 2-, 3-, and 4-methylbenzenamine. Literature data were evaluated for the following properties: normal boiling, freezing and triple-point temperatures, critical constants, vapor pressure, enthalpy of vaporization, density, second virial coefficients, 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 data, and temperature dependent selected data 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 sub-sections of Sec. 2. Merits of the available experimental and spectroscopic data 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 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 data 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 1985 (1986-333) were used for all calculations. Some of the results are in dimensionless forms derived with the gas constant of 8.31451 J mol^{-1} 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, the data were converted to the International Practical Temperature Scale of 1968 (IPTS-68) (1976-175); otherwise, values other than those for vapor pressures were used without conversion. There was a slight statistical advantage to making temperature scale corrections to vapor pressure data.

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:

methanamine, 74-89-5, CH_5N, aminomethane, methylamine;

ethanamine, 75-04-7, C_2H_7N, aminoethane, ethylamine;

1-propanamine, 107-10-8, C_3H_9N, 1-aminopropane, *n*-propylamine, propylamine;

2-propanamine, 75-31-0, C_3H_9N, 2-aminopropane, 2-propylamine, isopropylamine;

benzenamine, 62-53-3, C_6H_7N, aniline, phenylamine, aminobenzene;

2-methylbenzenamine, 95-53-4, C_7H_9N, 2-aminotoluene, *o*-aminotoluene, 2-methylaniline, *o*-methylaniline, *o*-toluidine, 1-amino-2-methylbenzene;

3-methylbenzenamine, 108-44-1, C_7H_9N, 3-aminotoluene, *m*-aminotoluene, 3-methylaniline, *m*-methylaniline, *m*-toluidine, 1-amino-3-methylbenzene;

4-methylbenzenamine, 106-49-0, C_7H_9N, 4-aminotoluene, *p*-aminotoluene, 4-methylaniline, *p*-methylaniline, *p*-toluidine, 1-amino-4-methylbenzene.

1.5. Procedures for Evaluation, Processing, and Selection of Data

The following steps were used in this compilation:

(i) Search the scientific literature, identify the sources of data and record the pertinent numerical values in the TRC Database.

(ii) Rate and evaluate the available data on the basis of accuracy and reliability and sort out the "best" numerical values.

(iii) 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.

(iv) Make preliminary choice of "reliable" values and, where appropriate, fit them to standard functions of temperature, pressure or other variables for further testing.

(v) Test the preliminary choices for internal thermodynamic consistency and make necessary adjustments to achieve consistency to within the experimental uncertainty.

(vi) Calculate the values of the derived properties from the final choices of the basic input data.

(vii) 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 data 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 this range. To obtain a smoothed set of selected values over the extended temperature range it was necessary to fit both sets of data to the same function of temperature. It was more common to have several sets of data of varying reliability for various temperature ranges which partially or completely overlapped. In fitting all of these data 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 data as well as desired, so the less reliable data 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 data to within the imprecisions of the original data, 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

$$\sigma(x) = \sigma_c(x) + x\sigma_f(x), \tag{1}$$

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

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, $Y(A_1, A_2, \ldots)$ of the parameters $A_1, A_2, \ldots$, was calculated from

$$\sigma(Y) = \Big[\sum_i \sum_j (\partial Y/\partial A_i)\sigma(A_i) \times C(A_i,A_j)(\partial Y/\partial A_j)\sigma(A_j)\Big]^{1/2}. \tag{2}$$

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 experimental data 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 data.

2.2. Vapor Pressure

The vapor pressure ($p_{\rm sat}$) measurements were smoothed with the Cox equation (1936-431):

$$\ln(p_{\rm sat}/p_{\rm ref}) = A_x[1 - 1/(T/T_{\rm ref})], \tag{3a}$$

where

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

$T_{\rm ref}$ and $p_{\rm ref}$ 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 $T_{\rm ref}$. 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 (1988-191). 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) 100 kPa to the critical pressure p_c. For the first two pressure ranges, the three parameter Antoine equation was used:

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

Compound	$\frac{T_m}{K}$	$\frac{T_b}{K}$	$\frac{T_c}{K}$	$\frac{p_c}{MPa}$	$\frac{V_c}{cm^3 \cdot mol^{-1}}$
Methanamine	179.708 ± 0.01[a]	266.80 ± 0.02	430.7 ± 0.2	7.614 ± 0.015	120 ± 6
Ethanamine	192.62 ± 0.05	289.74 ± 0.06	456.2 ± 1.0	5.63 ± 0.11	181 ± 5
1-Propanamine	188.389 ± 0.01[a]	320.370 ± 0.002	497 ± 1	4.72 ± 0.08	228 ± 11
2-Propanamine	178.011 ± 0.01[a]	304.905 ± 0.002	471.9 ± 0.5	4.54 ± 0.06	221 ± 11
Benzenamine	267.133 ± 0.01[a]	457.32 ± 0.08	699 ± 2	4.89 ± 0.12	280 ± 14
2-Methylbenzenamine	256.8 ± 0.1	473.49 ± 0.04	707 ± 2	4.37 ± 0.12	333 ± 17
3-Methylbenzenamine	241.9 ± 0.1	476.52 ± 0.04	707 ± 2	4.28 ± 0.12	333 ± 17
4-Methylbenzenamine	316.9 ± 0.1	473.57 ± 0.08	706 ± 2	4.58 ± 0.14	340 ± 17

[a] triple point temperature

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

Compound	A_0	$\sigma(A_0)^a$	A_1	$\sigma(A_1)^a$	A_2	$\sigma(A_2)^a$	T_b/K	$\sigma(T_b)$/K[a]	rmswd[b]
Methanamine	2.84924	0.00670	−0.51838	0.01353	0.15900	0.00614	266.797	0.016	0.60
Ethanamine	2.90190	0.02633	−0.64109	0.04701	0.20419	0.01976	289.738	0.055	0.65
1-Propanamine	2.91580	0.00554	−0.68989	0.00944	0.22235	0.00392	320.369	0.002	0.18
2-Propanamine	2.93670	0.00296	−0.74722	0.00564	0.24909	0.00256	304.905	0.002	0.31
Benzenamine	2.88571	0.01401	−0.58271	0.03131	0.18054	0.01617	457.318	0.079	1.08
2-Methylbenzenamine	3.18501	0.02530	−1.18083	0.04953	0.45370	0.02282	473.490	0.037	0.62
3-Methylbenzenamine	3.09998	0.02487	−0.98036	0.04841	0.36137	0.02209	476.522	0.039	0.61
4-Methylbenzenamine	3.07126	0.03643	−0.94617	0.07333	0.35468	0.03490	473.573	0.082	0.43

[a] see section 1.6

[b] rmswd = root-mean-squared-weighted deviation

TABLE 2a. Correlation matrix[a] for the Cox equation coefficients.

Compound	$C(A_0,A_1)$	$C(A_0,A_2)$	$C(A_0,T_b)$	$C(A_1,A_2)$	$C(A_1,T_b)$	$C(A_2,T_b)$
Methanamine	−0.99581	0.98380	0.50320	−0.99524	−0.55310	0.56901
Ethanamine	−0.99291	0.97980	−0.40649	−0.99637	0.38245	−0.35579
1-Propanamine	−0.99740	0.98844	−0.37025	−0.99663	0.36209	−0.34843
2-Propanamine	−0.99419	0.97603	−0.15302	−0.99310	0.12990	−0.10631
Benzenamine	−0.99484	0.98158	0.52424	−0.99529	−0.58443	0.61114
2-Methylbenzenamine	−0.99773	0.99206	−0.00176	−0.99809	−0.03142	0.05625
3-Methylbenzenamine	−0.99706	0.99069	−0.16781	−0.99801	0.14007	−0.11718
4-Methylbenzenamine	−0.99817	0.99356	−0.37395	−0.99851	0.33522	−0.29986

[a] see section 1.6

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

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
Methanamine											
179.708	0.178	230	13.85	280	177.9	320	704	370	2455	420	6311
190	0.541	240	25.59	290	261.8	330	935	380	3022	430	7447
200	1.406	250	44.57	298.15	350.6	340	1218	390	3681	430.7	7532
210	3.286	260	73.80	300	373.6	350	1561	400	4441		
220	7.01	270	116.86	310	519.1	360	1971	410	5314		
Ethanamine											
192.62	0.143	240	7.89	290	102.4	330	408	380	1435	430	3695
200	0.311	250	14.59	298.15	140.9	340	543	390	1768	440	4358
210	0.804	260	25.4	300	151.0	350	709	400	2154	450	5111
220	1.87	270	42.2	310	216.0	360	910	410	2600	456.2	5627
230	3.99	280	67.0	320	300.8	370	1151	420	3111		
1-Propanamine											
188.389	0.00927	250	3.148	300	45.601	360	350.06	420	1361.9	480	3700
200	0.03877	260	5.955	310	68.596	370	455.04	430	1639.6	490	4278
210	0.1144	270	10.633	320	99.980	380	581.9	440	1956.8	497	4723
220	0.3008	280	18.040	330	141.67	390	733.2	450	2317.2		
230	0.7150	290	29.259	340	195.75	400	911.8	460	2724		
240	1.5581	298.15	42.125	350	264.43	410	1120.3	470	3184		
2-Propanamine											
178.011	0.00790	240	3.721	298.15	78.045	350	423.6	410	1626.8	470	4453
190	0.03815	250	7.138	300	83.951	360	549.0	420	1957	471.9	4582
200	0.1194	260	12.865	310	122.22	370	700.2	430	2336		
210	0.3284	270	21.964	320	172.85	380	880.1	440	2769		
220	0.8080	280	35.752	330	238.24	390	1092.1	450	3261		
230	1.807	290	55.808	340	320.94	400	1339.7	460	3820		
Benzenamine											
267.133	0.00651	350	2.032	430	46.82	510	339	590	1318	670	3591
280	0.0206	360	3.30	440	62.9	520	413	600	1517	680	4004
290	0.0467	370	5.19	450	83.3	530	498	610	1738	690	4452
298.15	0.0867	380	7.95	460	108.6	540	596	620	1981	699	4887
300	0.0992	390	11.85	470	139.7	550	708	630	2248		
310	0.199	400	17.24	480	177.4	560	835	640	2541		
320	0.379	410	24.54	490	222.6	570	978	650	2862		
330	0.691	420	34.22	500	276.4	580	1139	660	3211		
340	1.208										

TABLE 3. Continued.

$\frac{T}{\mathrm{K}}$	$\frac{p_{sat}}{\mathrm{kPa}}$	$\frac{T}{\mathrm{K}}$	$\frac{p_{sat}}{\mathrm{kPa}}$	$\frac{T}{\mathrm{K}}$	$\frac{p_{sat}}{\mathrm{kPa}}$	$\frac{T}{\mathrm{K}}$	$\frac{p_{sat}}{\mathrm{kPa}}$	$\frac{T}{\mathrm{K}}$	$\frac{p_{sat}}{\mathrm{kPa}}$	$\frac{T}{\mathrm{K}}$	$\frac{p_{sat}}{\mathrm{kPa}}$
					2-Methylbenzenamine						
256.8	0.000469	330	0.321	410	15.28	490	149.6	570	681	650	2141
270	0.00213	340	0.596	420	21.65	500	186.6	580	798	660	2436
280	0.00599	350	1.055	430	30.03	510	230.2	590	929	670	2765
290	0.0153	360	1.79	440	40.85	520	281.4	600	1078	680	3135
298.15	0.0311	370	2.92	450	54.57	530	340.8	610	1244	690	3549
300	0.0362	380	4.62	460	71.73	540	409	620	1432	700	4012
310	0.0798	390	7.07	470	92.89	550	488	630	1642	707	4370
320	0.164	400	10.53	480	118.6	560	578	640	1877		
					3-Methylbenzenamine						
241.9	0.000058	320	0.135	410	13.37	500	176.4	590	920	680	3104
250	0.000172	330	0.265	420	19.13	510	219.2	600	1070	690	3502
260	0.00058	340	0.494	430	26.77	520	269.7	610	1238	700	3943
270	0.00179	350	0.879	440	36.75	530	328.7	620	1426	707	4280
280	0.00497	360	1.50	450	49.54	540	397	630	1637		
290	0.0126	370	2.47	460	65.69	550	476	640	1871		
298.15	0.0255	380	3.94	470	85.78	560	567	650	2133		
300	0.0298	390	6.08	480	110.4	570	670	660	2423		
310	0.0655	400	9.14	490	140.4	580	787	670	2746		
					4-Methylbenzenamine						
316.9	0.132	390	6.82	460	71.0	530	350	600	1141	670	2953
330	0.317	400	10.18	470	92.5	540	423	610	1321	680	3344
340	0.583	410	14.80	480	118.8	550	507	620	1524	690	3779
350	1.02	420	21.05	490	150.7	560	604	630	1750	700	4263
360	1.73	430	29.3	500	188.9	570	714	640	2003	706	4580
370	2.82	440	40.0	510	234.4	580	839	650	2286		
380	4.45	450	53.7	520	288.1	590	981.	660	2601		

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

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

$$\log_{10}(p_{\mathrm{sat}}/\mathrm{kPa}) = A_a - B_a/(T/\mathrm{K} + C_a) + D_a X_a^{''} + E_a X_a^{8} + F_a X_a^{12}, \tag{5}$$

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 data. The coefficients are listed in Table 4.

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

Compound	Range	A_a	B_a	C_a	$\frac{T_a^o}{K}$	n	E_a	F_a	T_c
Methanamine	a	6.1302	918.423	−46.47					
	b	6.4613	1010.93	−39.94					
	c	6.4613	1010.93	−39.94	273.15	4.2347	−197.27	10989.	430.7
Ethanamine	b	6.1203	964.494	−55.34					
	c	6.1203	964.494	−55.34	296.15	2.3232	−101.37	5974.	456.2
1-Propanamine	b	6.0574	1047.18	−61.91					
	c	6.0574	1047.18	−61.91	328.15	3.4191	145.88	−5001.	497.
2-Propanamine	b	6.0462	1000.85	−57.26					
	c	6.0462	1000.85	−57.26	328.15	2.4996	−99.29	21689.	471.9
Benzenamine	a	7.8189	2526.56	−13.50					
	b	6.2533	1590.91	−82.81					
	c	6.2533	1590.91	−82.81	470.15	4.6070	2871.	−545673.	699.
2-Methylbenzenamine	a	4.9997	1004.63	−148.36					
	b	6.0032	1488.77	−101.07					
	c	6.0032	1488.77	−101.07	485.15	1.9968	2684.9	−284086.	707.
3-Methylbenzenamine	a	6.0845	1491.71	−107.97					
	b	5.9726	1462.13	−107.96					
	c	5.9726	1462.13	−107.96	490.15	1.4196	792.9	−84601.	707.
4-Methylbenzenamine	a	5.2555	1109.60	−138.97					
	b	6.2867	1669.16	−83.84					
	c	6.2867	1669.16	−83.84	485.15	2.5203	2632.3	−787906.	706.

[a] In Eq. 5, $D_a = \log_{10} e = 0.43429$

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:

$$\rho_l = \rho_c\left[1 + A_1 x^{\epsilon} + x\sum_i A_i x^{(i-2)/m}\right], \tag{6}$$

where $i = 2$ to 4, $m = 2$, $\epsilon = 0.35$, $x = (1 - T/T_c)$, 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 $m > 1$. 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.

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:

$$(\rho_l + \rho_g)/2 = \rho_c + \alpha_m(1 - T/T_c), \tag{7}$$

TABLE 5. Coefficients[a] and their standard errors[b] for Eq. 6 representing densities of the liquids.

Compound	$A1$	$\sigma(A_1)$	A_2	$\sigma(A_2)$	A_3	$\sigma(A_3)$	A_4	$\sigma(A_4)$	rmswd[c]
Methanamine	2.72756	0.05765	−3.70256	0.46822	7.26323	0.93600	−3.71045	0.56658	4.21
Ethanamine	2.02707	0.00832	0.68726	0.04276	0.09905	0.04446			5.89
1-Propanamine	2.28708	0.01384	−0.40213	0.06078	0.97521	0.05656			6.37
2-Propanamine	1.93035	0.01071	0.27646	0.04759	0.41244	0.04388			1.13
Benzenamine	2.73925	0.09103	−3.12474	0.58812	5.30157	0.99722	−2.14627	0.51938	2.50
2-Methylbenzenamine	1.98053	0.00303	0.82364	0.00440					2.78
3-Methylbenzenamine	1.91047	0.00496	0.78919	0.00724					1.39
4-Methylbenzenamine	2.00055	0.00582	0.82247	0.00898					2.66

[a] see table 7 for values of ρ_c and Table 1 for T_c

[b] see section 1.6

[c] rmswd = root-mean-squared-weighted deviation

TABLE 5a. Correlation matrix[a] for coefficients in Eq. 6 representing densities of the liquids.

Compound	$C(A_1, A_2)$	$C(A_1, A_3)$	$C(A_1, A_4)$	$C(A_2, A_3)$	$C(A_2, A_4)$	$C(A_3, A_4)$
Methanamine	−0.98128	0.95547	−0.92847	−0.99432	0.98217	−0.99656
Ethanamine	−0.95509	0.89910		−0.98774		
1-Propanamine	−0.98951	0.97018		−0.99489		
2-Propanamine	−0.99510	0.98668		−0.99782		
Benzenamine	−0.99695	0.99117	−0.98320	−0.99849	0.99439	−0.99870
2-Methylbenzenamine	−0.99799					
3-Methylbenzenamine	−0.99822					
4-Methylbenzenamine	−0.99844					

[a] see section 1.6

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 ($p_{sat}/RT\rho_g$) was > 0.8. For the benzenamines, second virial coefficients were not available, so the range was limited to where the vapor pressure was > 1 bar. This procedure was tested with data where critical densities were available, see Table 15, and was shown to give reasonable agreement with experimental values of the critical density.

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

$\frac{T}{\mathrm{K}}$	$\frac{\rho_l}{\mathrm{kg\cdot m^{-3}}}$	$\frac{T}{\mathrm{K}}$	$\frac{\rho_l}{\mathrm{kg\cdot m^{-3}}}$	$\frac{T}{\mathrm{K}}$	$\frac{\rho_l}{\mathrm{kg\cdot m^{-3}}}$	$\frac{T}{\mathrm{K}}$	$\frac{\rho_l}{\mathrm{kg\cdot m^{-3}}}$	$\frac{T}{\mathrm{K}}$	$\frac{\rho_l}{\mathrm{kg\cdot m^{-3}}}$	$\frac{T}{\mathrm{K}}$	$\frac{\rho_l}{\mathrm{kg\cdot m^{-3}}}$
Methanamine											
179.708	788.3	230	736.0	280	678.2	320	627.6	370	555.1	415	453.
190	778.1	240	724.9	290	665.9	330	614.2	380	538.0	420	432.
200	767.9	250	713.5	298.15	655.8	340	600.3	390	519.	425	401.
210	757.5	260	702.0	300	653.4	350	586.0	400	497.	430	330.
220	746.9	270	690.2	310	640.7	360	570.9	410	470.	430.7	258.
Ethanamine											
192.62	793.1	250	732.4	300	674.5	360	593.6	420	481.7	450	369.
200	785.5	260	721.3	310	662.0	370	578.2	425	468.8	452	353.
210	775.2	270	709.9	320	649.3	380	561.8	430	454.6	454	332.
220	764.7	280	698.4	330	636.1	390	544.4	435	438.	455	316.
230	754.1	290	686.6	340	622.5	400	525.6	440	420.	456	284.
240	743.4	298.15	676.7	350	608.4	410	504.9	445	398.	456.2	248.
1-Propanamine											
188.389	820.2	250	760.3	300	710.03	360	644.9	420	567.3	480	439.
200	809.0	260	750.4	310	699.64	370	633.1	430	551.8	485	418.
210	799.3	270	740.5	320	689.09	380	621.0	440	535.0	490	391.
220	789.7	280	730.45	330	678.3	390	608.5	450	516.	495	345.
230	779.9	290	720.30	340	667.4	400	595.5	460	495.	496	326.
240	770.2	298.15	711.94	350	656.3	410	581.8	470	470.	497	259.
2-Propanamine											
178.011	805.2	240	744.53	298.15	683.36	350	622.61	410	536.0	460	412.
190	793.7	250	734.37	300	681.32	360	609.8	420	518.1	465	386.
200	784.1	260	724.07	310	670.14	370	596.5	430	498.	468	364.
210	774.3	270	713.64	320	658.71	380	582.6	440	475.	470	343.
220	764.5	280	703.05	330	647.01	390	568.1	450	448.	471	325.
230	754.58	290	692.28	340	634.99	400	552.6	455	432.	471.9	268.
Benzenamine											
267.133	1044.0	350	972.28	440	890.8	530	803.5	620	697.	680	569.
280	1033.12	360	963.42	450	881.5	540	793.1	630	682.	685	548.
290	1024.55	370	954.52	460	872.1	550	782.5	640	666.	690	520.
298.15	1017.54	380	945.58	470	862.6	560	771.7	650	648.	695	476.
300	1015.94	390	936.58	480	853.0	570	760.	655	638.	696	463.
310	1007.29	400	927.54	490	843.4	580	749.	660	627.	697	447.
320	998.60	410	918.45	500	833.6	590	737.	665	615.	698	423.
330	989.87	420	909.31	510	823.7	600	724.	670	602.	699	332.
340	981.10	430	900.1	520	813.7	610	711.	675	587.		

TABLE 6. Continued.

T/K	ρ_l/kg·m^{-3}	T/K	ρ_l/kg·m^{-3}	T/K	ρ_l/kg·m^{-3}	T/K	ρ_l/kg·m^{-3}	T/K	ρ_l/kg·m^{-3}	T/K	ρ_l/kg·m^{-3}
2-Methylbenzenamine											
256.8	1028.0	340	959.7	430	879.0	520	786.9	610	672.	690	498.
270	1017.5	350	951.1	440	869.4	530	775.	620	656.	695	477.
280	1009.47	360	942.4	450	859.7	540	764.	630	640.	698	461.
290	1001.35	370	933.7	460	849.9	550	752.	640	622.	700	449.
298.15	994.69	380	924.8	470	839.9	560	740.	650	603.	702	434.
300	993.18	390	915.9	480	829.7	570	727.	660	582.	704	415.
310	984.92	400	906.8	490	819.3	580	714.	670	559.	705	402.
320	976.60	410	897.7	500	808.7	590	700.	680	532.	706	385.
330	968.20	420	888.4	510	797.9	600	686.	685	516.	707	321.
3-Methylbenzenamine											
241.9	1029.0	330	959.13	430	871.9	530	770.	630	637.	685	515.
250	1022.7	340	950.8	440	862.6	540	759.	640	620.	690	497.
260	1015.0	350	942.4	450	853.1	550	747.	645	611.	695	476.
270	1007.2	360	934.0	460	843.4	560	735.	650	601.	698	460.
280	999.4	370	925.4	470	833.6	570	723.	655	591.	700	448.
290	991.51	380	916.8	480	823.6	580	710.	660	580.	702	434.
298.15	985.00	390	908.0	490	813.5	590	697.	665	569.	704	415.
300	983.52	400	899.2	500	803.1	600	683.	670	557.	705	402.
310	975.47	410	890.2	510	792.5	610	668.	675	545.	706	385.
320	967.34	420	881.1	520	781.	620	653.	680	531.	707	321.
4-Methylbenzenamime											
316.9	966.8	400	895.3	480	818.8	560	729.	640	612.	690	487.
330	956.01	410	886.2	490	808.5	570	717.	650	593.	695	465.
340	947.61	420	877.0	500	798.0	580	704.	660	573.	698	448.
350	939.13	430	867.7	510	787.3	590	690.	665	561.	700	435.
360	930.56	440	858.2	520	776.4	600	676.	670	549.	702	419.
370	921.9	450	848.6	530	765.2	610	662.	675	536.	704	396.
380	913.1	460	838.8	540	753.	620	646.	680	522.	705	378.
390	904.2	470	828.9	550	741.	630	630.	685	506.	706	315.

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

Compound	$\frac{\rho_c}{\mathrm{kg/m^3}}$	$\frac{\sigma(\rho_c)}{\mathrm{kg/m^3}}$	$\frac{\alpha_m}{\mathrm{kg/m^3}}$	$\frac{\sigma(\alpha_m)}{\mathrm{kg/m^3}}$	$C(\rho_c,\alpha_m)$	$\frac{\alpha_m}{\rho_c}$
Methanamine	258.14	0.36	235.34	0.86	−0.9837	0.9117
Ethanamine[b]	253.79	0.31	248.43	0.77	−0.9855	0.9789
1-Propanamine	259.58	0.24	242.25	0.62	−0.9801	0.9332
2-Propanamine[b]	253.90	0.24	240.80	0.61	−0.9619	0.9484
Benzenamine	332.51	0.17	307.43	0.33	−0.9900	0.9246
2-Methylbenzenamine	321.31	0.81	304.28	1.43	−0.9951	0.9470
3-Methylbenzenamine	321.67	1.08	295.34	1.93	−0.9955	0.9181
4-Methylbenzenamine	315.17	0.75	305.76	1.47	−0.9961	0.9702

[a] see section 1.6

[b] data not used for adopted ρ_c; experimental data available.

2.4. Second Virial Coefficients

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

$$p/\rho RT = 1 + B\rho \tag{8}$$

were evaluated. The selected values of the second virial coefficient were smoothed using

$$B = A_b + C_b e^{(D_b/T)}. \tag{9}$$

For correlation of data of limited range, this equation was cast into reduced form,

$$B = A_r\rho_c + C_b e^{D_r(T_c/T)}, \tag{10}$$

where the values of A_r and D_r were determined from the data for methylamine with the critical constants from Table 1. The coefficients to Eq. (9) are listed in Table 8 where, if the imprecision is not listed for a coefficient, the value was estimated with the aid of Eq. (10). Values of the second virial coefficient at selected temperatures are listed in Table 9.

TABLE 8. Coefficients of Eq. 9 with their correlation coefficients[a] for the second virial coefficients.

Compound	$\frac{A_b}{\mathrm{cm^3/mol}}$	$\frac{\sigma(A_b)}{\mathrm{cm^3/mol}}$	$\frac{C_b}{\mathrm{cm^3/mol}}$	$\frac{\sigma(C_b)}{\mathrm{cm^3/mol}}$	$\frac{D_b}{\mathrm{K}}$	$\frac{\sigma(D_b)}{\mathrm{K}}$	rmswd[b]	$C(A_b,C_b)$	$C(A_b,D_b)$	$C(C_b,D_b)$
Methanamine	15.50	5.02	-30.28	1.87	822	16	1.1	−0.9927	−0.9872	0.9990
Ethanamine	23.50		-46.74	2.27	852	16	16.9			0.9947
1-Propanamine	29.45		-47.51	0.44	928		0.9			
2-Propanamine	28.50		-44.43	0.73	881		1.5			

[a] see section 1.6 [b] rmswd = root-mean-squared-weighted deviation

TABLE 9. Second virial coefficients calculated from Eqs. 9 and 10 at selected temperatures.

$\frac{T}{K}$	$\frac{B}{cm^3 \cdot mol^{-1}}$	$\frac{T}{K}$	$\frac{B}{cm^3 \cdot mol^{-1}}$	$\frac{T}{K}$	$\frac{B}{cm^3 \cdot mol^{-1}}$	$\frac{T}{K}$	$\frac{B}{cm^3 \cdot mol^{-1}}$	$\frac{T}{K}$	$\frac{B}{cm^3 \cdot mol^{-1}}$	$\frac{T}{K}$	$\frac{B}{cm^3 \cdot mol^{-1}}$
Methanamine											
170	−3790	260	−699	340	−324	430	−189	520	−131	610	−101
180	−2890	270	−620	350	−301	440	−180	530	−127	620	−98
190	−2270	280	−554	360	−281	450	−172	540	−123	630	−96
200	−1820	290	−499	370	−263	460	−165	550	−119	640	−93
210	−1500	298.15	−461	380	−247	470	−158	560	−115	650	−91
220	−1250	300	−453	390	−233	480	−152	570	−112	660	−89
230	−1060	310	−413	400	−220	490	−146	580	−109	670	−87
240	−910	320	−379	410	−209	500	−141	590	−106	680	−85
250	−795	330	−350	420	−198	510	−136	600	−103		
Ethanamine											
240	−1600	280	−956	310	−706	350	−509	390	−391	430	−315
250	−1380	290	−858	320	−646	360	−474	400	−369	440	−300
260	−1210	298.15	−790	330	−594	370	−443	410	−349	450	−286
270	−1070	300	−776	340	−549	380	−416	420	−331	460	−274
1-Propanamine											
250	−1910	270	−1440	290	−1136	300	−1018	320	−834	340	−698
260	−1650	280	−1277	298.15	−1038	310	−918	330	−761	350	−643
2-Propanamine											
250	−1470	270	−1132	290	−898	300	−809	320	−668	340	−564
260	−1287	280	−1004	298.15	−824	310	−733	330	−612	350	−522

2.5. Enthalpy of Vaporization or Sublimation

Enthalpies of vaporization from the literature were tested for consistency through the Claperyon equation with our selections of vapor pressure, liquid density, and second virial coefficient data. Values listed are the molar enthalpy of vaporization from the condensed phase x to the ideal gas $\Delta_x^{g,id}H$ rather than to the saturated vapor $\Delta_x^g H$. The selection of values was made from the combined data. Recommended values are listed in Table 10.

2.6. Enthalpy of Combustion and Formation

The enthalpies of combustion were usually available for the substances in the condensed phase (either liquid or crystal). Accepted values for the enthalpies of formation of the combustion products at 298.15 K, listed in Table 21 (1978-115), were used to derive enthalpies of formation. Enthalpies of vaporization and the second virial coefficients given in this report were used to derive enthalpies of formation for the ideal gas. The results were tested against values estimated from enthalpies of formation of related compounds. If the inconsistencies appeared to be too large and the experimental values were of suspected merit, the estimated values of the enthalpies of formation were adopted. Recommended values of enthalpies of formation in the condensed and ideal gas state at 298.15 K are listed in Table 11.

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

Compound	phase x	$\Delta_x^{g,id}H^a/\mathrm{kJ\cdot mol^{-1}}$
Methanamine	l	24.74±0.10
Ethanamine	l	26.66±0.20
1-Propanamine	l	31.37±0.10
2-Propanamine	l	28.57±0.10
Benzenamine	l	55.83±0.10
2-Methylbenzenamine	l	62.7±0.5
3-Methylbenzenamine	l	62.7±0.5
4-Methylbenzenamine	s	78.8±0.5

[a] Uncertainties 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.

	Ideal gas		liquid or crystal	
Temperature	0 K	298.15 K	298.15 K	
Compound	$\Delta_f H^\circ/\mathrm{kJ\cdot mol^{-1}}$			phase[c]
Methanamine	−7.82 ± 0.41	−22.53±0.41	−47.27±0.40	l
Ethanamine	−26.65 ± 0.51	−47.47±0.51	−74.13±0.50	l
1-Propanamine	−42.36 ± 0.39	−70.10±0.39	−101.47±0.38	l
2-Propanamine	−56.90 ± 0.68	−83.70±0.68	−112.27±0.67	l
Benzenamine	−65.58 ± 0.81	87.46±0.81	31.63±0.80	l
2-Methylbenzenamine	84.28 ± 2.1	56.4 ±2.0	−6.3 ±2.1	l
3-Methylbenzenamine	83.37 ± 2.1	54.6 ±2.0	−8.1 ±2.1	l
4-Methylbenzenamine	83.96 ± 2.1	55.3 ±2.0	−23.5 ±2.1	s

[a] for formation reactions $n\mathrm{C}(graphite) + (m/2)\mathrm{H_2}(g) + (1/2)\mathrm{N_2}(g) \rightarrow \mathrm{C}_n\mathrm{H}_m\mathrm{N}(s, l, \text{ or } g)^c$

[b] uncertainties are two standard error estimates.

[c] s for crystal, l for liquid, and g for gas.

2.7. Condensed Phase Heat Capacities and Related Thermal Properties

Where calorimetric data for the condensed phases were available to near 10 K, the dimensionless thermodynamic functions C_{sat}/R, $\Delta_0^l S/R$, $\Delta_0^l G/RT$ and $\Delta_0^T H/RT$ along the vapor saturation lines were derived from numerical integrations of the heat-capacity data and from the enthalpies of transition. The results are listed in Table 12.

TABLE 12. Thermodynamic properties for the condensed phases at vapor saturation.[a]

$\frac{T}{K}$	$\frac{C_{sat}}{R}$	$\frac{\Delta_0^T S}{R}$	$\frac{-\Delta_0^T G}{RT}$	$\frac{\Delta_0^T H}{RT}$
		Methanamine (cII)		
0	0.000	0.000	0.000	0.000
10	0.068	0.023	0.006	0.017
15	0.224	0.076	0.019	0.057
20	0.497	0.174	0.044	0.129
25	0.813	0.319	0.084	0.235
30	1.168	0.498	0.138	0.360
35	1.546	0.705	0.204	0.502
40	1.935	0.937	0.281	0.657
45	2.322	1.188	0.367	0.820
50	2.659	1.450	0.462	0.988
60	3.279	1.989	0.672	1.317
70	3.841	2.539	0.899	1.640
80	4.272	3.080	1.138	1.942
90	4.729	3.609	1.383	2.226
100	5.181	4.132	1.632	2.500
101.469	5.209	4.207	1.669	2.539
		Methanamine (cI)		
101.469	5.185	4.367	1.669	2.698
110	5.447	4.796	1.895	2.901
120	5.716	5.282	2.157	3.125
130	5.973	5.749	2.416	3.334
140	6.162	6.200	2.670	3.530
150	6.431	6.633	2.920	3.713
160	6.664	7.055	3.165	3.890
170	6.914	7.467	3.406	4.061
179.708	7.170	7.858	3.636	4.222
		Methanamine (*l*)		
179.708	11.960	11.963	3.636	8.327
180	11.957	11.982	3.650	8.332
190	11.905	12.627	4.105	8.521
200	11.952	13.239	4.547	8.692
210	12.045	13.824	4.975	8.850
220	12.077	14.385	5.390	8.995
230	12.258	14.926	5.793	9.134
240	12.212	15.447	6.184	9.263
250	12.174	15.944	6.565	9.379
260	12.170	16.426	6.935	9.491
270	12.111	16.880	7.295	9.585
280	12.247	17.323	7.645	9.678
290	12.264	17.753	7.986	9.767
298.15	12.279	18.093	8.258	9.836
300	12.282	18.169	8.319	9.851

[a] The percentage imprecision in the listed properties is 2 for 10 to 50 K and 0.2 above 50 K.

TABLE 12. Continued.[a]

$\frac{T}{K}$	$\frac{C_{sat}}{R}$	$\frac{\Delta_0^T S}{R}$	$\frac{-\Delta_0^T G}{RT}$	$\frac{\Delta_0^T H}{RT}$
1-Propanamine (c)				
0	0.000	0.000	0.000	0.000
10	0.138	0.046	0.012	0.035
15	0.440	0.154	0.040	0.116
20	0.874	0.337	0.089	0.248
25	1.381	0.585	0.162	0.423
30	1.899	0.883	0.257	0.626
35	2.410	1.214	0.369	0.844
40	2.900	1.569	0.497	1.071
45	3.355	1.936	0.637	1.300
50	3.786	2.312	0.785	1.527
60	4.580	3.075	1.103	1.971
70	5.266	3.832	1.439	2.394
80	5.879	4.577	1.785	2.792
90	6.434	5.301	2.136	3.166
100	6.947	6.007	2.487	3.519
110	7.429	6.691	2.839	3.852
120	7.894	7.358	3.188	4.170
130	8.338	8.008	3.534	4.474
140	8.786	8.642	3.876	4.766
150	9.251	9.264	4.215	5.049
160	9.751	9.876	4.550	5.327
170	10.303	10.484	4.881	5.603
180	10.951	11.091	5.208	5.882
188.389	11.516	11.601	5.480	6.119
1-Propanamine (*l*)				
188.389	18.482	18.606	5.480	13.126
190	18.512	18.766	5.595	13.171
200	18.683	19.717	6.274	13.443
210	18.814	20.633	6.938	13.694
220	18.923	21.514	7.582	13.930
230	19.021	22.354	8.206	14.149
240	19.103	23.165	8.810	14.355
250	19.174	23.951	9.404	14.546
260	19.245	24.701	9.977	14.726
270	19.314	25.431	10.536	14.895
280	19.387	26.131	11.079	15.054
290	19.470	26.815	11.613	15.205
298.15	19.549	27.354	12.035	15.322
300	19.569	27.475	12.126	15.349
310	19.677	28.119	12.634	15.487
320	19.807	28.748	13.127	15.619
330	19.961	29.357	13.611	15.748
340	20.146	29.956	14.084	15.876

[a] The percentage imprecision in the listed properties is 2 for 10 to 50 K, and 0.2 above 50 K.

TABLE 12. Continued.[a]

$\frac{T}{\mathrm{K}}$	$\frac{C_{\mathrm{sat}}}{R}$	$\frac{\Delta_0^T S}{R}$	$\frac{-\Delta_0^T G}{RT}$	$\frac{\Delta_0^T H}{RT}$
		2-Propanamine (c)		
0	0.000	0.000	0.000	0.000
10	0.270	0.092	0.023	0.068
15	0.746	0.290	0.076	0.212
20	1.299	0.577	0.163	0.414
25	1.859	0.926	0.280	0.647
30	2.381	1.312	0.419	0.893
35	2.858	1.716	0.576	1.140
40	3.287	2.126	0.744	1.382
45	3.669	2.536	0.920	1.615
50	4.022	2.941	1.102	1.839
60	4.661	3.732	1.475	2.257
70	5.221	4.493	1.852	2.640
80	5.749	5.225	2.228	2.997
90	6.254	5.931	2.601	3.330
100	6.756	6.617	2.968	3.648
110	7.257	7.284	3.330	3.953
120	7.751	7.936	3.687	4.249
130	8.266	8.577	4.038	4.538
140	8.809	9.209	4.385	4.824
150	9.399	9.836	4.728	5.109
160	10.070	10.464	5.067	5.397
170	10.878	11.098	5.403	5.695
178.011	11.551	11.613	5.670	5.942
		2-Propanamine (l)		
178.011	17.576	16.558	5.670	10.892
180	17.646	16.759	5.796	66.878
190	17.978	17.719	6.395	11.325
200	18.265	18.650	6.983	11.664
210	18.511	19.546	7.562	11.986
220	18.721	20.411	8.125	12.287
230	18.895	21.247	8.679	12.572
240	19.033	22.058	9.222	12.837
250	19.154	22.838	9.750	13.089
260	19.265	23.588	10.264	13.323
270	19.374	24.319	10.772	13.546
280	19.483	25.024	11.270	13.756
290	19.601	25.713	11.758	13.955
298.15	19.710	26.256	12.146	14.111
300	19.735	26.378	12.231	14.146
310	19.879	27.027	12.699	14.328
320	20.038	27.661	13.157	14.504

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[a] The percentage imprecision in the listed properties is 2 for 10 to 50 K, and 0.2 above 50 K.

TABLE 12. Continued.[a]

$\frac{T}{K}$	$\frac{C_{sat}}{R}$	$\frac{\Delta_0^T S}{R}$	$\frac{-\Delta_0^T G}{RT}$	$\frac{\Delta_0^T H}{RT}$
		Benzenamine (c)		
0	0.000	0.000	0.000	0.000
10	0.159	0.053	0.013	0.040
15	0.508	0.176	0.045	0.132
20	1.037	0.393	0.103	0.290
25	1.586	0.683	0.189	0.494
30	2.137	1.023	0.299	0.724
35	2.628	1.391	0.429	0.963
40	3.030	1.772	0.573	1.200
45	3.490	2.156	0.727	1.429
50	3.831	2.543	0.889	1.653
60	4.443	3.298	1.228	2.070
70	4.952	4.022	1.576	2.446
80	5.423	4.713	1.925	2.788
90	5.883	5.379	2.272	3.107
100	6.279	6.020	2.615	3.405
110	6.724	6.639	2.953	3.686
120	7.181	7.243	3.286	3.958
130	7.615	7.834	3.613	4.222
140	8.106	8.417	3.935	4.482
150	8.623	8.994	4.253	4.741
160	9.130	9.567	4.567	4.999
170	9.701	10.138	4.878	5.259
180	10.259	10.708	5.186	5.521
190	10.843	11.278	5.492	5.786
200	11.429	11.849	5.796	6.054
210	12.035	12.421	6.097	6.324
220	12.680	12.996	6.398	6.598
230	13.321	13.573	6.697	6.876
240	13.969	14.154	6.996	7.158
250	14.582	14.737	7.294	7.443
260	15.177	15.320	7.591	7.729
267.133	15.570	15.736	7.803	7.933

[a] The percentage imprecision in the listed properties is 2 for 10 to 50 K, and 0.2 above 50 K.

TABLE 12. Continued.[a]

$\frac{T}{K}$	$\frac{C_{sat}}{R}$	$\frac{\Delta_0^T S}{R}$	$\frac{-\Delta_0^T G}{RT}$	$\frac{\Delta_0^T H}{RT}$
		Benzenamine (*l*)		
267.133	22.511	20.482	7.803	12.679
270	22.525	20.722	7.939	12.783
280	22.699	21.544	8.410	13.133
290	22.818	22.343	8.877	13.466
298.15	23.082	22.979	9.254	13.725
300	23.109	23.122	9.339	13.783
310	23.328	23.882	9.796	14.086
320	23.657	24.628	10.248	14.380
330	23.892	25.360	10.695	14.665
340	24.071	26.076	11.137	14.939
350	24.291	26.777	11.574	15.203
360	24.495	27.464	12.005	15.459
370	24.678	28.138	12.432	15.705
380	24.865	28.798	12.854	15.944
390	25.053	29.447	13.272	16.175
400	25.241	30.083	13.684	16.399
410	25.427	30.709	14.092	16.617
420	25.738	31.327	14.495	16.833
430	25.831	31.934	14.893	17.041
440	25.925	32.529	15.287	17.242
450	26.019	33.112	15.677	17.436
460	26.113	33.685	16.062	17.623

[a] The percentage imprecision in the listed properties is 2 for 10 to 50 K, and 0.2 above 50 K.

2.8. Ideal Gas Thermal Functions

The thermodynamic properties of the ideal gas were calculated from spectroscopically derived data with standard statistical mechanical methods for a rigid-rotor, harmonic-oscillator molecular model with modifications for internal rotations and inversion about the nitrogen atom. The ideal gas thermodynamic properties in dimensionless units (i.e., divided by R) include heat capacity (C_p°/R), entropy $\Delta_0^T S^\circ/R$, Gibbs energy function $\Delta_0^T G^\circ/RT$, enthalpy function $\Delta_0^T H^\circ/RT$, enthalpy of formation $\Delta_f H^\circ/RT$, and Gibbs energy of formation $\Delta_f G^\circ/RT$. 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.

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

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

$\frac{T}{\mathrm{K}}$	$\frac{-\Delta_0^T G^\circ}{RT}$	$\frac{\Delta_0^T H^\circ}{RT}$	$\frac{\Delta_0^T S^\circ}{R}$	$\frac{C_p^\circ}{R}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f G^\circ}{RT}$
			Methanamine			
0	0.000	0.000	0.000	0.000	infinite	infinite
50	16.872	4.014	20.885	4.029	−24.776	−13.891
100	19.672	4.096	23.767	4.364	−16.150	0.094
150	21.360	4.248	25.609	4.733	−12.628	5.889
200	22.605	4.413	27.018	5.091	−10.830	9.250
273.16	24.019	4.679	28.698	5.751	−9.418	12.397
298.15	24.433	4.780	29.212	6.020	−9.088	13.205
300	24.462	4.787	29.250	6.041	−9.066	13.261
400	25.901	5.248	31.149	7.237	−8.072	15.724
500	27.127	5.766	32.893	8.426	−7.320	17.442
600	28.226	6.300	34.526	9.493	−6.688	18.719
700	29.236	6.825	36.061	10.429	−6.136	19.708
800	30.181	7.328	37.509	11.251	−5.645	20.494
900	31.072	7.805	38.877	11.976	−5.205	21.133
1000	31.918	8.255	40.172	12.615	−4.807	21.661
1100	32.724	8.677	41.402	13.179	−4.448	22.067
1200	33.497	9.074	42.570	13.676	−4.123	22.475
1300	34.238	9.445	43.682	14.113	−3.828	22.793
1400	34.950	9.792	44.743	14.498	−3.561	23.067
1500	35.637	10.117	45.755	14.836	−3.318	23.304
			Ethanamine			
0	0.000	0.000	0.000	0.000	infinite	infinite
50	19.102	4.297	23.399	4.826	−73.077	−55.338
100	22.214	4.699	26.913	5.396	−41.865	−16.538
150	24.185	5.047	29.232	6.094	−30.552	−1.998
200	25.685	5.400	31.085	6.837	−24.820	5.927
273.16	27.448	5.951	33.399	8.117	−20.221	12.914
298.15	27.978	6.152	34.130	8.604	−19.149	14.634
300	28.016	6.168	34.183	8.640	−19.076	14.752
400	29.908	7.039	36.946	10.663	−16.006	19.785
500	31.576	7.955	39.531	12.529	−13.933	23.121
600	33.107	8.853	41.960	14.121	−12.373	25.518
700	34.536	9.705	44.241	15.470	−11.127	27.328
800	35.885	10.500	46.384	16.633	−10.093	28.744
900	37.164	11.239	48.404	17.653	−9.213	29.881
1000	38.385	11.927	50.311	18.557	−8.450	30.811
1100	39.552	12.567	52.118	19.362	−7.781	31.514
1200	40.671	13.163	53.834	20.079	−7.187	32.236
1300	41.747	13.720	55.467	20.717	−6.658	32.790
1400	42.783	14.241	57.024	21.285	−6.182	33.265
1500	43.782	14.728	58.510	21.791	−5.754	33.677

TABLE 13. Continued.

$\frac{T}{\mathrm{K}}$	$\frac{-\Delta_0^T G^\circ}{RT}$	$\frac{\Delta_0^T H^\circ}{RT}$	$\frac{\Delta_0^T S^\circ}{R}$	$\frac{C_p^\circ}{R}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f G^\circ}{RT}$
			1-Propanamine			
0	0.000	0.000	0.000	0.000	infinite	infinite
50	22.591	4.173	26.763	4.618	−114.285	−90.542
100	25.647	4.743	30.390	6.022	−64.391	−30.311
150	27.692	5.384	33.076	7.273	−46.437	−8.067
200	29.325	5.998	35.324	8.413	−37.322	3.918
273.16	31.326	6.886	38.212	10.267	−29.986	14.356
298.15	31.942	7.199	39.141	10.965	−28.278	16.902
300	31.987	7.222	39.209	11.018	−28.162	17.076
400	34.242	8.533	42.775	13.910	−23.298	24.455
500	36.291	9.883	46.174	16.600	−20.056	29.286
600	38.210	11.201	49.412	18.929	−17.638	32.719
700	40.032	12.452	52.483	20.924	−15.715	35.289
800	41.772	13.621	55.393	22.646	−14.122	37.280
900	43.440	14.709	58.148	24.141	−12.769	38.864
1000	45.042	15.718	60.761	25.442	−11.598	40.147
1100	46.585	16.655	63.240	26.576	−10.573	41.097
1200	48.072	17.524	65.596	27.563	−9.668	42.083
1300	49.507	18.330	67.837	28.424	−8.865	42.825
1400	50.893	19.078	69.971	29.175	−8.147	43.455
1500	52.233	19.774	72.007	29.832	−7.505	43.995
			2-Propanamine			
0	0.000	0.000	0.000	0.000	infinite	infinite
50	20.409	4.137	24.546	4.615	−149.316	−123.356
100	23.465	4.795	28.260	6.261	−81.836	−45.626
150	25.548	5.525	31.073	7.676	−57.961	−17.588
200	27.234	6.228	33.462	8.992	−45.842	−2.739
273.16	29.324	7.235	36.559	11.011	−36.043	9.952
298.15	29.972	7.581	37.554	11.732	−33.764	13.003
300	30.019	7.607	37.627	11.786	−33.609	13.211
400	32.400	9.012	41.412	14.643	−27.193	21.923
500	34.561	10.401	44.962	17.202	−23.038	27.517
600	36.575	11.721	48.296	19.379	−20.035	31.438
700	38.476	12.951	51.426	21.233	−17.715	34.346
800	40.280	14.088	54.368	22.831	−15.842	36.584
900	42.001	15.139	57.140	24.222	−14.283	38.358
1000	43.647	16.109	59.756	25.438	−12.957	39.792
1100	45.225	17.007	62.232	26.501	−11.812	40.867
1200	46.741	17.837	64.578	27.430	−10.813	41.956
1300	48.199	18.607	66.807	28.243	−9.933	42.787
1400	49.605	19.321	68.926	28.954	−9.154	43.493
1500	50.961	19.985	70.946	29.577	−8.460	44.101

TABLE 13. Continued.

$\frac{T}{\mathrm{K}}$	$\frac{-\Delta_0^T G^\circ}{RT}$	$\frac{\Delta_0^T H^\circ}{RT}$	$\frac{\Delta_0^T S^\circ}{R}$	$\frac{C_p^\circ}{R}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f G^\circ}{RT}$
			Benzenamine			
0	0.000	0.000	0.000	0.000	infinite	infinite
50	21.881	4.288	26.169	4.323	−166.485	−151.393
100	24.887	4.461	29.349	5.160	−89.048	−65.698
150	26.781	4.955	31.735	6.796	−62.329	−35.359
200	28.298	5.655	33.953	8.756	−48.823	−19.462
273.16	30.240	6.902	37.143	11.896	−37.845	−6.033
298.15	30.864	7.367	38.231	12.982	−35.280	−2.836
300	30.910	7.401	38.311	13.062	−35.106	−2.618
400	33.303	9.337	42.639	17.127	−27.886	6.404
500	35.593	11.245	46.838	20.505	−23.262	12.097
600	37.803	13.021	50.823	23.195	−19.987	16.033
700	39.933	14.633	54.566	25.344	−17.515	18.920
800	41.983	16.085	58.069	27.096	−15.564	21.126
900	43.955	17.392	61.346	28.550	−13.976	22.865
1000	45.849	18.571	64.420	29.776	−12.652	24.267
1100	47.670	19.638	67.308	30.820	−11.529	25.208
1200	49.421	20.608	70.029	31.716	−10.563	26.380
1300	51.106	21.493	72.599	32.489	−9.724	27.191
1400	52.729	22.303	75.032	33.158	−8.989	27.884
1500	54.293	23.046	77.340	33.740	−8.341	28.482
			2-Methylbenzenamine			
0	0.000	0.000	0.000	0.000	infinite	infinite
50	22.945	4.464	27.409	4.872	189.934	213.153
100	26.186	4.999	31.185	6.398	87.584	121.326
150	28.362	5.826	34.188	8.600	54.762	92.940
200	30.170	6.809	36.979	10.930	38.562	79.630
273.16	32.522	8.382	40.904	14.450	25.661	69.732
298.15	33.280	8.941	42.221	15.661	22.751	67.612
300	33.335	8.983	42.318	15.750	22.557	67.472
400	36.231	11.262	47.494	20.366	14.920	62.146
500	38.986	13.492	52.478	24.326	10.666	59.315
600	41.633	15.576	57.209	27.564	8.066	57.618
700	44.179	17.484	61.663	30.207	6.382	56.511
800	46.629	19.215	65.844	32.392	5.248	55.737
900	48.984	20.784	69.768	34.224	4.464	55.167
1000	51.249	22.208	73.457	35.778	3.912	54.727
1100	53.427	23.503	76.930	37.105	3.516	54.127
1200	55.524	24.685	80.209	38.245	3.228	54.081
1300	57.543	25.767	83.310	39.228	3.015	53.831
1400	59.489	26.760	86.249	40.080	2.856	53.614
1500	61.367	27.673	89.040	40.820	2.733	53.421

TABLE 13. Continued.

$\frac{T}{\mathrm{K}}$	$\frac{-\Delta_0^T G^\circ}{RT}$	$\frac{\Delta_0^T H^\circ}{RT}$	$\frac{\Delta_0^T S^\circ}{R}$	$\frac{C_p^\circ}{R}$	$\frac{\Delta_f H^\circ}{RT}$	$\frac{\Delta_f G^\circ}{RT}$
3-Methylbenzenamine						
0	0.000	0.000	0.000	0.000	infinite	infinite
50	23.784	4.784	28.568	4.805	188.679	210.739
100	27.135	4.975	32.110	5.815	86.772	119.590
150	29.255	5.582	34.838	7.860	53.994	91.521
200	30.974	6.441	37.415	10.203	37.800	78.431
273.16	33.197	7.932	41.130	13.837	24.923	68.769
298.15	33.915	8.480	42.395	15.090	22.026	66.713
300	33.968	8.521	42.489	15.183	21.832	66.577
400	36.729	10.793	47.521	19.941	14.253	61.452
500	39.380	13.041	52.421	23.999	10.058	58.764
600	41.947	15.153	57.100	27.309	7.512	57.172
700	44.431	17.088	61.519	30.002	5.873	56.147
800	46.829	18.846	65.675	32.225	4.780	55.438
900	49.142	20.439	69.581	34.087	4.031	54.921
1000	51.372	21.884	73.256	35.662	3.510	54.525
1100	53.520	23.200	76.720	37.007	3.141	53.962
1200	55.591	24.400	79.991	38.161	2.877	53.947
1300	57.588	25.497	83.086	39.156	2.685	53.725
1400	59.515	26.504	86.020	40.016	2.544	53.532
1500	61.376	27.431	88.806	40.764	2.438	53.359
4-Methylbenzenamine						
0	0.000	0.000	0.000	0.000	infinite	infinite
50	23.079	4.767	27.846	4.730	190.079	212.861
100	26.413	4.959	31.373	5.855	87.465	121.020
150	28.533	5.593	34.126	7.937	54.477	92.716
200	30.258	6.469	36.726	10.279	38.182	79.502
273.16	32.492	7.973	40.465	13.918	25.223	69.734
298.15	33.213	8.524	41.737	15.173	22.308	67.652
300	33.266	8.565	41.831	15.266	22.113	67.515
400	36.041	10.848	46.889	20.029	14.485	62.316
500	38.706	13.102	51.808	24.081	10.261	59.580
600	41.284	15.217	56.501	27.380	7.693	57.953
700	43.778	17.152	60.930	30.062	6.038	56.901
800	46.184	18.909	65.093	32.275	4.931	56.171
900	48.505	20.500	69.005	34.128	4.171	55.637
1000	50.741	21.943	72.684	35.697	3.639	55.227
1100	52.895	23.256	76.151	37.036	3.262	54.652
1200	54.970	24.453	79.424	38.186	2.990	54.627
1300	56.972	25.549	82.520	39.176	2.791	54.397
1400	58.902	26.553	85.456	40.034	2.644	54.195
1500	60.766	27.478	88.244	40.779	2.532	54.016

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 nonreacting 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.

Methanamine. Our selected value for the boiling temperature agrees with the results of Holmberg (1962-353), Aston *et al.* (1937-248), Hsia (1931-328), Plank and Vahl (1931-336), and Gibbs (1905-45) within our estimated uncertainties of those measurements. The value of Berthoud (1917-30) is about 1 K low, primarily due to inaccurate low pressure measurements. The majority of his measurements were at pressures much higher than atmospheric pressure.

The selected value of the freezing temperature was based primarily on the careful triple-point temperature determination of Aston *et al.* (1937-248) who used a well-characterized sample having an impurity of 0.025 mole %. The result of Timmermans and Mattaar (1921-17), although high, agrees with our recommendation to within the estimated uncertainty. The estimated uncertainty of 0.1 K given by Emeleus and Briscoe (1937-434) appears optimistic. Other measurements of the atmospheric boiling temperature, generally of lower accuracy, are listed in (1889-19), (1905-45), (1931-269), (1950-248), (1952-41), (1952-42).

Ethanamine. Our selected value for the boiling temperature agrees with the results of Timmermans (1912-127 and 1914-135), Lecat (1946-272), Holmberg (1962-353), Lempe *et al.* (1966-195) and Anderson and Shimanskaya (1969-163) within the respective estimated uncertainties. The selected freezing temperature was based primarily on the results of Timmermans (1914-135). The boiling temperature of Landenburg and Krugel (1900-32) is about 2 K higher than the selected value and their freezing temperature is about 2 K lower, both of which indicates an appreciable amount of low volatility impurity. Other measurements of the atmospheric boiling temperature, generally of lower accuracy, are listed in (1850-2), (1872-18), (1896-26), (1899-19), (1912-10), (1950-248).

1-Propanamine. Our selected value for the boiling temperature was based on the ebulliometric measurements of Osborn and Douslin (1968-206). It also agrees with that of Krichevtsov and Komarov (1970-165) within the limits of their uncertainty. The other published data 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 triple point temperature of Finke *et al* (1972-140). It agrees with the freezing temperature value of Vasil'ev *et al.* (1971-154) within the estimated uncertainties; however, the value of Timmermans and Mattaar (1921 17) is almost 2 K higher. Other measurements of the atmospheric boiling temperature, generally of lower accuracy, are listed in (1862-2), (1869-15), (1872-26), (1882-30), (1886-28), (1889-26), (1895-49), (1896-5), (1900-73), (1919-64), (1924-82), (1948-262), (1949-167), (1950 248), (1951-569), (1952-42), (1952-385), (1968-195).

2-Propanamine. Our selected value for the boiling temperature agrees with the results of 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) and is 6 K higher than the value published by Timmermans (1921-19), confirming a considerable impurity in the Timmermans sample. Other measurements of the atmospheric boiling temperature, generally of lower accuracy, are listed in (1895-49), (1909-1), (1949-166), (1949-167), (1968-195), (1970-5).

Benzenamine. The selected value of the boiling temperature agrees within the estimated uncertainties with the published results. The selected value of the freezing temperature was based upon the adiabatic calorimetric result for the triple-point temperature by Hatton *et al.* (1962-3) whose sample was 99.98 mole % pure. The agreement with other results listed are commensurate with the purities and accuracies of the temperature measurements. Other measurements of the atmospheric boiling temperature, generally of lower accuracy, are listed in (1850-10), (1884-15), (1888-39), (1896-28), (1902-64), (1912-127), (1914-135), (1914-136), (1916-232), (1920-95), (1923-73), (1924-167), (1926-91), (1930-279), (1935-68), (1937-254), (1941-332), (1944-125), (1946-272), (1950-531), (1954-670), (1954-674), (1960-289), (1962-363), (1965-333), (1966-203), (1979-93).

2-Methylbenzenamine. Our selected value for the boiling temperature agrees with the published results within the estimated uncertainties. The freezing temperatures are grouped about two distinct values, one around 249 K and the other around 257 K. The low values were ascribed to a metastable phase which melts at around 249 K. The selected value was based on the results of Timmermans (1921-19), (1952-50). Other measurements of the atmospheric boiling temperature, generally of lower accuracy, are listed in (1896-28), (1920-95), (1921-19), (1932-79), (1944-125), (1946-272), (1960-288), and (1951-569).

3-Methylbenzenamine. Our selected value for the boiling temperature agrees with the published results within the estimated uncertainties. The selected value of the freezing temperature was based on the results of Timmermans and Hennaut-Roland (1935-68). It is 0.8 K higher than that of Dreisbach and Martin (1949-120), but it agrees with the other published values within the estimated uncertainties. Other measurements of the atmospheric boiling temperature, generally of lower accuracy, are listed in (1896-28),

TABLE 14. Available freezing and normal boiling temperatures

$\frac{T_b}{K}$	$\frac{\sigma(T_b)^a}{K}$	$\frac{T_m}{K}$	$\frac{\sigma(T_m)^a}{K}$	Author(s)	Ref.
Methanamine					
266.45	0.5	–	–	Gibbs	1905-45
265.60	0.09	–	–	Berthoud	1917-30
–	–	180.65	1.0	Timmermans and Mattaar	1921-17
266.56	0.1	–	–	Plank and Vahl	1931-336
266.70	0.05	–	–	Hsia	1931-328
–	–	179.70	0.07	McNeight and Smyth	1936-137
266.87	0.09	179.71^b	0.05	Aston *et al.*	1937-248
–	–	180.05	0.3	Emeleus and Briscoe	1937-434
267.05	0.2	180.05	0.4	Roberts *et al.*	1939-387
266.65	0.2	–	–	Holmberg	1962-353
Ethanamine					
–	–	187.95	0.5	Landenburg and Krugel	1899-19
292.65	2.0	189.4	1.0	Landenburg and Krugel	1900-32
289.70	0.2	–	–	Timmermans	1910-58
289.70	0.2	–	–	Timmermans	1912-127
289.75	0.2	192.60	0.2	Timmermans	1914-135
–	–	189.99	0.2	Timmermans	1921-19
–	–	192.15	0.5	Pohland and Mehl	1933-369
289.75	0.2	192.15	0.3	Roberts *et al.*	1939-387
289.75	0.05	–	–	Lecat	1946-272
289.75	1.0	–	–	James	1952-42
289.75	0.5	–	–	Holmberg	1962-353
289.80	0.05	–	–	Lempe *et al.*	1966-195
290.15	1.0	–	–	Anderson and Shimanskaya	1969-163
1-Propanamine					
320.95	0.3	190.15	0.1	Timmermans and Mattaar	1921-17
322.4	0.2	–	–	Butler *et al.*	1935-366
322.85	0.5	–	–	Lecat	1946-272
322.15	1.0	–	–	Glaser and Rüland	1957-76
321.6	1.0	–	–	Costello and Bowden	1959-218
321.8	1.0	–	–	Holmberg	1962-353
321.65	0.5	–	–	Sudaricov *et al.*	1963-316
320.379	0.005	–	–	Osborn and Douslin	1968-206
321.0	1.0	–	–	Krichevtsov and Komarov	1970-165
–	–	188.36	0.07	Vasil'ev *et al.*	1971-154
–	–	188.389^b	0.005	Finke *et al.*	1972-140

[a] See section 1.6. [b] triple point temperature corrected to IPTS-68

TABLE 14. Continued.

$\frac{T_b}{K}$	$\frac{\sigma(T_b)^a}{K}$	$\frac{T_m}{K}$	$\frac{\sigma(T_m)^a}{K}$	Ref.	
				2-Propanamine	
306.15	0.3	171.95	0.6	Timmermans	1921-19
304.8	0.5	–	–	Koob *et al.*	1951-626
306.0	1.0	–	–	Costello and Bowden	1959-218
307.15	1.5	–	–	Holmberg	1962-353
304.926	0.001	–	–	Osborn and Douslin	1968-206
305.01	0.2	–	–	Komarov and Krichevtsov	1969-165
–	–	178.019[b]	0.005	Finke *et al.*	1972-140
				Benzenamine	
–	–	267.05	0.1	Timmermans	1909-118
457.55	0.5	–	–	Timmermans	1910-58
–	–	266.95	0.05	Timmermans	1912-127
457.50	0.2	–	–	Knowles	1920-94
–	–	267.1	0.05	Lang	1928-196
457.45	0.5	–	–	Buehler *et al.*	1932-79
–	–	266.86	0.05	Parks *et al.*	1933-94
457.35	0.1	–	–	Green and Spinks	1945-173
457.05	0.1	266.85	0.05	Dreisbach and Martin	1949-120
–	–	267.01	0.1	Timmermans	1952-50
–	–	267.12	0.15	Witschonke	1954-24
–	–	266.61	0.1	Rock and Sieg	1955-605
–	–	267.13	0.07	McDonald *et al.*	1959-109
457.85	0.3	–	–	Costello and Bowden	1959-218
457.25	0.3	–	–	Ellis and Razavipour	1959-304
457.5	0.5	–	–	Sheveleva *et al.*	1959-305
457.09	0.5	–	–	Kurtyka	1961-263
457.03	0.15	–	–	Stadnicki	1962-32
–	–	267.133[b]	0.005	Hatton *et al.*	1962-3
457.65	0.4	–	–	Katti and Chaudhri	1964-292
457.25	0.3	–	–	Campbell *et al.*	1968-211
–	–	267.10	0.05	Brunet and Gubbins	1969-164
457.65	0.5	267.65	0.4	Pawlowski and Wieckowska	1980-66

[a] See section 1.6. [b] triple point temperature corrected to IPTS-68

TABLE 14. Continued.

$\frac{T_\mathrm{b}}{\mathrm{K}}$	$\frac{\sigma(T_\mathrm{b})^a}{\mathrm{K}}$	$\frac{T_\mathrm{m}}{\mathrm{K}}$	$\frac{\sigma(T_\mathrm{m})^a}{\mathrm{K}}$	Ref.	
				2-Methylbenzenamine	
–	–	257.7	0.7	Knoevenagel	1907-127
473.85	0.2	(248.8)	0.2	Timmermans	1914-135
–	–	256.75	0.3	Timmermans	1921-19
–	–	(248.75)	0.3	Timmermans	1921-19
472.85	0.5	–	–	Grimm and Patrick	1923-73
472.99	0.2	–	–	Berliner and May	1927-2
473.45	0.3	–	–	Lecat	1930-279
473.55	0.05	–	–	Timmermans and Hennaut-Roland	1935-68
473.45	0.07	(249.47)	0.05	Dreisbach and Martin	1949-120
–	–	256.75	0.5	Timmermans	1952-50
473.35	0.3	–	–	Kurtyka	1961-263
473.35	0.5	–	–	Kurtyka and Kurtyka	1979-93
				3-Methylbenzenamine	
–	–	242.15	0.4	O'Connor	1924-186
476.30	0.2	241.65	0.4	Dessart	1926-22
476.01	0.2	–	–	Berliner and May	1927-2
476.3	0.05	–	–	Timmermans	1927-21
476.35	0.3	–	–	Lecat	1930-279
476.15	0.5	–	–	Buehler *et al.*	1932-79
476.55	0.05	241.92	0.05	Timmermans and Hennaut-Roland	1935-68
476.2	0.1	–	–	Lecat	1943-221
476.49	0.07	242.75	0.05	Dreisbach and Martin	1949-120
–	–	241.9	0.3	Timmermans	1952-50
476.35	0.2	–	–	Glaser and Rüland	1957-76
				4-Methylbenzenamine	
–	–	316.85	0.3	Cauwood and Turner	1915-45
473.5	0.2	–	–	Berliner and May	1927-2
473.65	0.3	–	–	Lecat	1930-279
–	–	316.55	0.4	Buehler *et al.*	1932-79
–	–	316.15	0.5	Bernouli and Veillon	1932-307
473.70	0.3	316.9	0.1	Timmermans and Hennaut-Roland	1937-146
–	–	317.15	0.5	Barcelo *et al.*	1951-569
473.55	0.2	–	–	Glaser and Rüland	1957-76
–	–	316.85	0.4	Rastogi *et al.*	1963-367

[a] See section 1.6. () indicates the melting point of metastable form

(1946-272), and (1951-569).

4-Methylbenzenamine. Our selected value for the boiling temperature agrees with the published results within the estimated uncertainties. The selected value of the freezing temperature was based on the results of Timmermans and Hennaut-Roland (1937-146). Other measurements of the atmospheric boiling temperature, generally of lower accuracy, are listed in (1896-28), (1946-272), and (1944-125).

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.

Methanamine. Vincent and Chappius (1886-11) determined the critical temperature and critical pressure of methanamine for a sample that was reported to be pure. Berthoud (1917-30) also determined the critical temperature and critical pressure using samples prepared by Kahlbaum by alkylation of ammonia and subsequently purified by fractional crystallization followed by a number of fractional distillations over barium oxide. Kay and Young (1974-179) reported Weaver's value of the critical temperature and critical pressure of methanamine. The selected values are those determined by Weaver. The critical volume was estimated by a procedure (1989-1) based on those of Lydersen (1955-593) and Ambrose (1979-58) and calculated from the rectilinear diameter. The rectilinear diameter value was selected because the method gave good agreement with literature critical volumes for ethanamine and 2-propanamine, where the liquid and vapor densities were measured close to the critical temperature.

Ethanamine. The critical temperature and critical pressure were determined by Vincent and Chappius (1886-11), and Berthoud (1917-30). Pohland and Mehl (1933-369) reported the critical temperature and density. The purity of the sample used by Vincent and Chappius is unknown. The samples used by Berthoud and by Pohland and Mehl were reported to be "pure." The selected critical pressure was that obtained by extrapolation of the Cox equation to the selected critical temperature. The selected value of the critical volume was based on the measurements of Pohland and Mehl (1933-369); they used their vapor density measurements to 451 K and their liquid density measurements to 410 K with unpublished data from I. G. Faben. The critical volume was calculated from the equation for the rectilinear line given by Pohland and Mehl, $\frac{1}{2}(\rho_l+\rho_g)/(\mathrm{kg\,m^{-3}}) = 248.5 + 261.7(1 - T/T_c)$ (from 300 to 456.2 K), with our selected critical temperature.

1-Propanamine. The critical temperature and critical pressure of 1-propanamine were determined by Vincent and Chappius (1886-11) and by Berthoud (1917-30). The critical temperature determined by Berthoud was selected. The samples used by Berthoud were prepared by Kahlbaum with methods discussed above for methylamine. The selected critical pressure was that obtained by extrapolation of the Cox equation to the selected critical temperature. The estimated critical volume (1989-1) differed by 9 $\mathrm{cm^3\,mol^{-1}}$ from the value calculated from the rectilinear diameter. The latter value was selected.

2-Propanamine. The only values available for this compound are those determined by Kobe and Mathews (1970-5). The samples used by these authors were purified by distillation. The critical constants determined by them are selected.

Benzenamine. The critical temperature and pressure were determined by Guye and Mallet (1902-63). Kudchadker *et al.* (1968-31) noted that these values have a considerable uncertainty. The experimental values agree with the estimated values (1989-1). The selected critical pressure was that obtained by extrapolation of the Cox equation to the experimental critical temperature. The selected critical volume was calculated from the rectilinear diameter, and this value disagrees considerably with the estimated value (1989-1).

2-Methylbenzenamine. The critical temperature and critical pressure of this compound were determined by Glaser and Rüland (1957-76). Their pressure seems inordinately low, but it roughly corresponds to the vapor pressure at their reported critical temperature, which is 13 K below our selected value. We deemed these values unreliable as they differ considerably from predicted values. The selected critical temperature was estimated by Somayajulu (1989-1). The selected critical pressure was that obtained by extrapolation of the Cox equation to the selected critical temperature. The selected critical volume was calculated from the rectilinear diameter.

3-Methylbenzenamine. The critical temperature and critical pressure determined by Glaser and Rüland (1957-76) were considered unreliable. The selected value of the critical temperature was estimated by Somayajulu (1989-1). The agreement between the experimental and the estimated values of p_c and T_c is somewhat better than that for 2-methylbenzenamine. The selected critical pressure was that obtained by extrapolation of the Cox equation to the selected critical temperature. The selected critical volume was calculated from the rectilinear diameter.

4-Methylbenzenamine. Both the critical temperature and critical pressure determined by Glaser and Rüland (1957-76) disagree with estimated values (1979-58), (1989-1). The calculated value of the pressure from the Cox equation at the experimental critical temperature is significantly higher than the experimental value of the critical pressure. The estimated critical temperature (1989-1) was selected. The selected critical pressure was obtained from the Cox equation, and the selected critical volume was calculated from the rectilinear diameter.

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.
				Methanamine			
428	2	7.30	0.3	–	–	Vincent and Chappius	1886-11
430	1	7.56	0.1	–	–	Berthoud	1917-30
430.7	0.2	7.614	0.015	–	–	Kay and Young	1974-181
430.8	0.5	7.65	0.05	138	10	Li and Kiran	1988-83
432.1^{b}	1.0^{b}	7.13^{b}	0.2^{b}	127^{b}	5^{b}	Somayajulu	1989-1
–	–	$7.532^{b,c}$	$0.03^{b,c}$	$120^{b,d}$	$6^{b,d}$	TRC – this work	
				Ethanamine			
450	10	6.69	1.0	–	–	Vincent and Chappius	1886-11
456.4	1	5.63	0.5	–	–	Berthoud	1917-30
456.2	1	–	–	181.4	5	Pohland and Mehl	1933-369
455^{b}	1.0^{b}	5.74^{b}	0.2^{b}	181.9^{b}	2^{b}	Somayajulu	1989-1
–	–	$5.63^{b,c}$	$0.11^{b,c}$	$177.6^{b,d}$	$5^{b,d}$	TRC – this work	
				1-Propanamine			
491	10	5.07	1.0	–	–	Vincent and Chappius	1886-11
497	1	4.74	0.5	–	–	Berthoud	1917-30
497	1.5	4.73	0.2	–	–	Glaser and Rüland	1957-76
492^{b}	2^{b}	4.78^{b}	0.2^{b}	237^{b}	5^{b}	Somayajulu	1989-1
–	–	$4.72^{b,c}$	$0.08^{b,c}$	$228^{b,d}$	$11^{b,d}$	TRC – this work	
				2-Propanamine			
471.9	0.5	4.54	0.05	221	5	Kobe and Mathews	1970-5
469^{b}	2^{b}	4.63^{b}	0.2^{b}	235^{b}	5^{b}	Somayajulu	1989-1
–	–	$4.54^{b,c}$	$0.06^{b,c}$	$233^{b,d}$	$11^{b,d}$	TRC – this work	
				Benzenamine			
699	2	5.31	0.5	–	–	Guye and Mallet	1902-64
699	6	–	–	–	–	Livingston *et al.*	1980-5
699^{b}	2^{b}	5.3^{b}	0.2^{b}	293^{b}	5^{b}	Somayajulu	1989-1
	–	$4.89^{b,c}$	$0.12^{b,c}$	$280^{b,d}$	$14^{b,d}$	TRC – this work	
				2-Methylbenzenamine			
694	2	3.75	0.3	–	–	Glaser and Rüland	1957-76
706^{b}	2^{b}	4.44^{b}	0.5^{b}	–	–	Ambrose	1979-58
707^{b}	2^{b}	4.58^{b}	0.1^{b}	348^{b}	5^{b}	Somayajulu	1989-1
–	–	$4.37^{b,c}$	$0.12^{b,c}$	$333^{b,d}$	$17^{b,d}$	TRC – this work	

TABLE 15. Continued.

$\frac{T_c}{K}$	$\frac{\sigma(T_c)^a}{K}$	$\frac{p_c}{MPa}$	$\frac{\sigma(p_c)^a}{MPa}$	$\frac{V_c}{cm^3 \cdot mol^{-1}}$	$\frac{\sigma(V_c)^a}{cm^3 \cdot mol^{-1}}$	Author(s)	Ref.
				3-Methylbenzenamine			
709	2	4.15	0.3	–	–	Glaser and Rüland	1957-76
706^b	2^b	4.17^b	0.5^b	–	–	Ambrose	1979-58
707^b	2^b	4.32^b	0.1^b	348^b	5^b	Somayajulu	1989-1
–	–	$4.28^{b,c}$	$0.12^{b,c}$	$333^{b,d}$	$17^{b,d}$	TRC – this work	
				4-Methylbenzenamine			
667	5	2.38	0.7	–	–	Glaser and Rüland	1957-76
702^b	2^b	4.17^b	0.5^b	–	–	Ambrose	1979-58
706^b	2^b	4.45^b	0.1^b	348^b	5^b	Somayajulu	1989-1
–	–	$4.58^{b,c}$	$0.14^{b,c}$	$340^{b,d}$	$17^{b,d}$	TRC – this work	

[a] See section 1.6; [b] estimated values; [c] from Cox vapor pressure equation with selected T_c in Table 1; [d] from fit to rectilinear diameter line with selected T_c in Table 1.

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 data 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. (3)]. 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 the eight compounds involved in this study.

Methanamine. Felsing and Thomas (1929-227), Hsia (1931-328), Emeleus and Briscoe (1937-434) and Wolff *et al.* (1964-344 and 1968-205) used static methods to measure the vapor pressure of methanamine; owing to questions of the degree of outgassing, their data were excluded. Aston *et al.* (1937-248) used a highly purified sample (99.975 mole %) and a static method for measuring the vapor pressure. They showed their vapor pressure values were the same after 50 mole % of the sample was removed by distillation. Their data were given the highest weight. To cover temperatures up to the critical temperature, the data of Wolff *et al.* (1962-354) and of Berthoud (1917-30) were used but were given less weight than that of Aston *et al.* Percent deviations of the experimental values from the vapor pressures calculated from the Cox equation are shown in Fig. 1.

Ethanamine. Bittrich *et al.* (1962-170) used an ebulliometric method to measure the vapor pressure at temperatures up to 288 K and a static method at higher temperatures. They used a static method in their later work (1963-320), and it was excluded from the fit.

Berthoud (1917-30) measured the vapor pressure between the boiling and the critical temperatures, and Wolff *et al.* (1964-344) measured the vapor pressure up to the boiling temperature using a static method. All these data were used in fitting the vapor pressure equations. The data by Pohland and Mehl (1933-369) and by Roberts *et al.* (1939-387) were excluded.

Percent deviations of the experimental values from the vapor pressures calculated from the Cox equation are plotted in Fig. 2.

1-Propanamine. For 1-propanamine the data by Glaser and Rüland (1957-76), by Srivastava *et al.* (1986-5), and isolated points from references (1941-101 and 1968-195) were excluded. All other available data were used but the data of Osborn and Douslin (1968-206) were given the highest weight while Berthoud's (1917-30) were given the lowest. Figure 3 shows that percent deviations from the vapor pressures calculated from the Cox equation are less than ± 1% except for the data of Glaser and Rüland which showed deviations as much as − 11% at 360 K. Their values were excluded from Fig. 3 to permit more resolution on the plot.

2-Propanamine. The low-temperature data (lower than 273 K) of Osborn and Douslin (1968-206) were measured by a static method using an inclined-piston apparatus. These

TABLE 16. Available vapor pressure data.

Range K	$\sigma(T)^a$ K	Range kPa	$\sigma_c(p_{sat})^a$ kPa	$10^3 \cdot \sigma_f(p_{sat})^a$	sl[b]	Meth.[c]	Author(s)	Ref.
				Methanamine				
266-370	0.05	96-2400	0.1	1.5	1	S	Berthoud	1917-30
380-427	0.05	2500-7460	0.04	2.0	1	S	Berthoud	1917-30
193-263	0.01	0.9-87	0.01	1.5	0	S	Felsing and Thomas	1929-227
196-282	0.05	86-198	0.01	1.5	0	U	Hsia	1931-328
190-267	0.005	0.5-103	0.001	0.3	1	S	Aston *et al.*	1937-248
216-263	0.01	5-86	0.01	1.5	0	S	Emeleus and Briscoe	1937-434
218-293	0.1	6-292	0.01	1.5	1	S	Wolff and Hopfner	1962-354
218-293	0.1	6-292	0.01	1.5	0	S	Wolff *et al.*	1964-344
253-293	0.1	53-292	0.01	1.5	0	S	Wolff and Wurtz	1968-205
				Ethanamine				
288-404	0.05	96-2400	0.1	1.5	1	S	Berthoud	1917-30
417-456.3	0.05	3000-5600	0.04	2.0	1	S	Berthoud	1917-30
211-297	0.1	1-140	0.05	1.0	0	S	Pohland and Mehl	1933-369
223-283	0.05	3-78	0.03	2.0	0	S	Roberts *et al.*	1939-387
275-288	0.05	50-93	0.1	2.0	1	E	Bittrich *et al.*	1962-170
297-323	0.05	130-326	0.1	2.0	1	S	Bittrich *et al.*	1962-170
273-323	0.05	50-327	0.05	1.5	0	S	Bittrich *et al.*	1963-320
218-293	0.1	1-116	0.01	1.5	1	S	Wolff *et al.*	1964-344
				1-Propanamine				
320-451	0.05	96-2400	0.1	1.5	1	S	Berthoud	1917-30
460-496	0.05	2700-4740	0.04	2.0	1	S	Berthoud	1917-30
322-485	0.5	101-4050	0.05	1.5	0	S	Glaser and Rüland	1957-76
243-293	0.1	4-34	0.01	1.5	1	S	Wolff *et al.*	1964-344
296-351	0.001	39-270	0.01	0.15	1	E	Osborn and Douslin	1968-206
297-348	0.005	42-250	0.01	1.0	0	S	Srivastava *et al.*	1986-5
				2-Propanamine				
277-305	0.55	29-100	0.1	2.5	0	U	Colpy *et al.*	1941-101
213-243	0.001	0.4-4.5	0.0005	0.15	1	S	Osborn and Douslin	1968-206
213-334	0.001	0.4-270	0.002	0.15	1	E	Osborn and Douslin	1968-206
305-471	0.025	100-4540	0	1.5	1	S	Kobe and Mathews	1970 -5
				Benzenamine				
350-458	0.05	2-100	0.01	1.5	0	S	Ramsay and Young	1885-25
403-457	0.05	19-101	0.01	1.5	0	S	Ramsay and Young	1886-62
404-456	0.05	20-103	0.01	1.5	0	S	Neubeck	1887-59
316-457	0.01	0.1-101	0.05	1.0	0	S	Kahlbaum	1898-2
404-457	0.2	20-101	0.05	2.0	0	E	Beckmann and Liesche	1915-88
365-424	0.05	4-39	0.01	1.0	1	E	Garrick	1927-156
473-643	0.1	149-2677	0.1	2.0	1	E	Lastovtsev	1937-438
273-323	0.02	0.01-0.4	0.005	2.0	0	G	Gurevich and Sigalovskaya	1937-437
330-388	0.05	0.7-11	0.05	1.5	0	S	Gould *et al.*	1947-337
386-457	0.01	10-101	0.05	1.5	0	S	Dreisbach and Shrader	1949-113
324-353	0.02	0.4-2.4	0.007	2.0	0	S	Holtzlander and Riggle	1955-604
267-353	0.05	0.007-2.4	0.001	1.5	1	S	Roeck and Sieg	1955-2
363-457	0.01	3.8-101	0.015	1.5	0	S	Crutzen *et al.*	1957-486
376-458	0.05	6.8-105	0.001	1.5	1	E	McDonald *et al.*	1959-109
438-457	0.01	53-101	0.07	1.5	0	E	Stadnicki	1962-32
434-457	0.01	53-101	0.07	1.5	0	E	Stadnicki	1962-33
434-457	0.01	53-101	0.07	1.5	0	E	Stadnicki	1962-34
434-457	0.01	53-101	0.07	1.5	1	E	Stadnicki	1963-321
313-453	0.5	0.3-88	0.1	2.0	0	S	Danov and Shinyaeva	1965-382
298-323	0.05	0.08-0.5	0.005	1.0	0	S	Pannetier *et al.*	1965-388
298-341	0.01	0.05-1.1	0.005	1.0	0	S	Campbell *et al.*	1968-211
308-371	0.5	0.13-5.3	0.05	2.0	0	S	Gopal and Rizvi	1968-210
313-387	0.03	0.25-10.5	0.003	0.35	0	S	Maher and Smith	1979-94
277-393	0.03	0.02-13	0.003	0.35	1	S	Maher and Smith	1980-20

TABLE 16. Continued.

Range K	$\sigma(T)^a$ K	Range kPa	$\sigma_c(p_{sat})^a$ kPa	$10^3 \cdot \sigma_f(p_{sat})^a$	sl^b	Meth.^{c}	Author(s)	Ref.
2-Methylbenzenamine								
415-472	0.1	20-101	0.1	5.0	0	S	Neubeck	1887-59
319-473	0.01	0.1-101	0.05	1.0	1	S	Kahlbaum	1898-2
392-473	0.01	7.6-101	0.05	1.5	1	E	Dreisbach and Shrader	1949-113
473-690	0.1	101-3500	0.05	2.0	1	S	Glaser and Rüland	1957-76
3-Methylbenzenamine								
422-476	0.1	19-101	0.1	5.0	0	S	Neubeck	1887-59
323-383	0.01	0.1-5	0.05	1.0	1	S	Kahlbaum	1898-2
394-476	0.01	7.6-101	0.05	1.5	1	E	Dreisbach and Shrader	1949-113
476-704	0.1	101-4050	0.05	2.0	1	S	Glaser and Rüland	1957-76
4-Methylbenzenamine								
416-474	0.1	18-101	0.1	5.0	0	S	Neubeck	1887-59
320-380	0.01	0.1-5	0.05	1.0	1	S	Kahlbaum	1898-2
473-641	0.1	101-2026	0.05	2.0	1	S	Glaser and Rüland	1957-76

[a] See section 1.6. [b] 1 for data selected and 0 for data not selected for least squares fit.

[c] Method of measurement: S, static; E, ebulliometric; G, gas saturation; and U, unspecified.

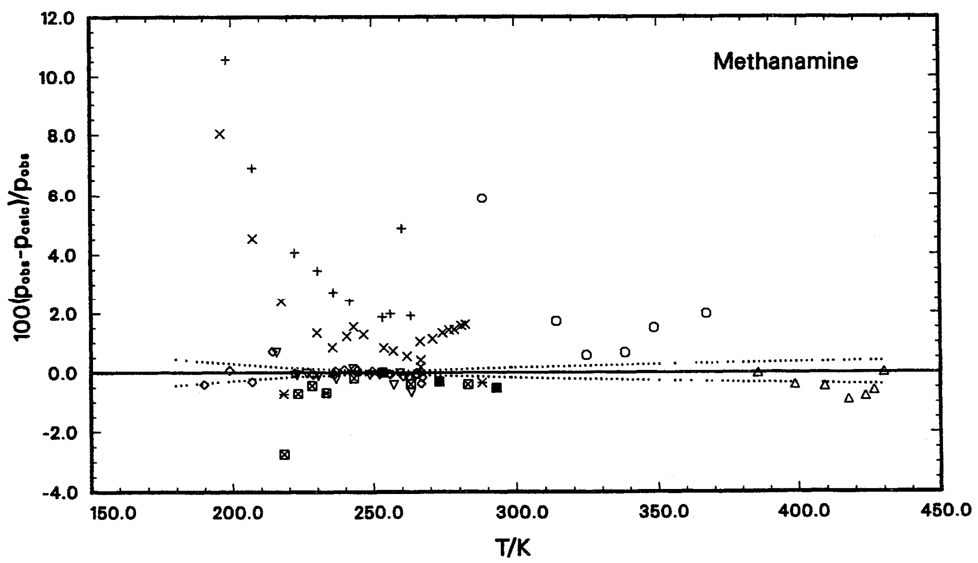

FIG. 1. Percent deviation of experimental vapor pressures for methanamine from the Cox equation. ○,△ Berthoud (1917-30)*; + Felsing and Thomas (1929-227); ×Hsia (1931-328); ◇ Aston *et al.* (1937-248)*; ▽ Emeleus and Briscoe (1937-434); ⊠ Wolff and Hopfner (1962-354)*; × Wolff *et al.* (1964-344); ◇ Wolff and Wurtz (1968-205); with * after reference number for data used in fitting.

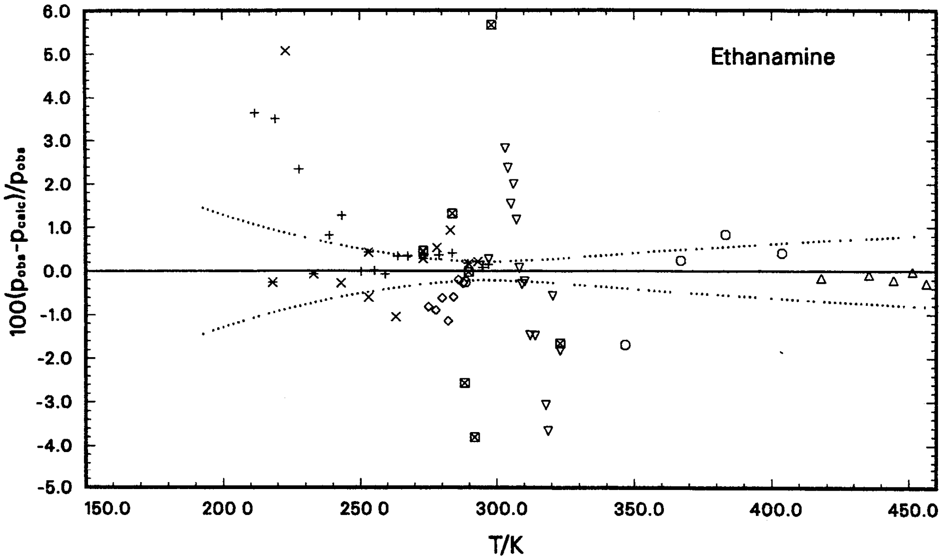

FIG. 2. Percent deviation of experimental vapor pressures for ethanamine from the Cox equation. O,Δ Berthoud (1917-30)*; + Pohland and Mehl (1933-369); ×Roberts *et al.* (1939-387); Bittrich *et al.* (1962-170)*, ◇ by dynamic method, ▽ static; ⊠ Bittrich *et al.* (1963-320); ×Wolff *et al.* (1964-344)*; with * after reference number for data used in fitting.

data were given lower weight than their higher temperature data which were obtained by an ebulliometric method. Kobe and Mathews (1970-5) only gave an equation for their measured values which were focused to determine the critical temperature; however, they did measure a near atmospheric pressure boiling temperature that is in good agreement (0.04 kPa) with our recommended value. The data of Osborn and Douslin (1968-206) along with 16 values calculated at temperatures from 345 K to T_c for the data of Kobe and Mathews (1970-5) were used to fit the Cox equation. The distri-

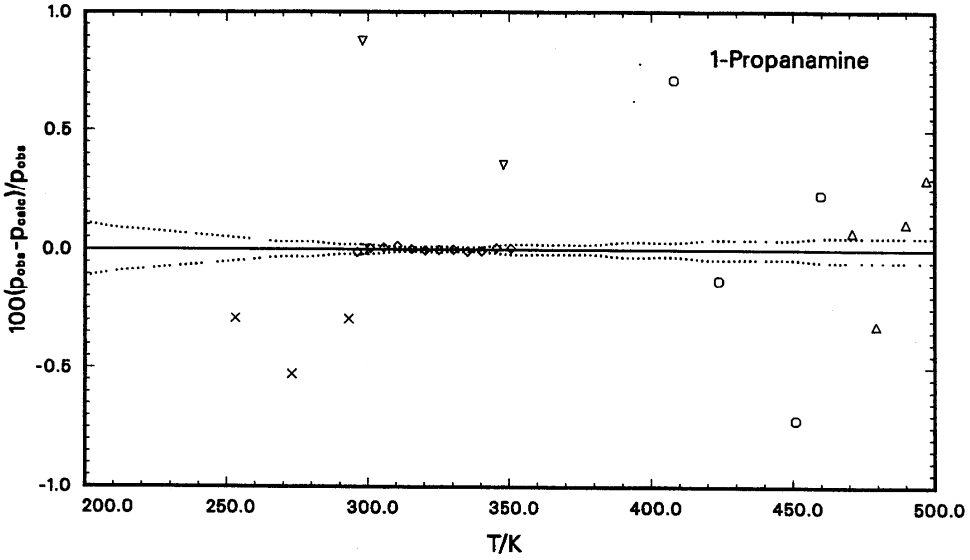

FIG. 3. Percent deviation of experimental vapor pressures for 1-propanamine from the Cox equation. O,Δ Berthoud (1917-30)*; ×Wolff *et al* (1964-344)*; Osborn and Doulsin (1968-206)*; ▽ Srivastava *et al.* (1986-5); with * after reference number for data used in fitting.

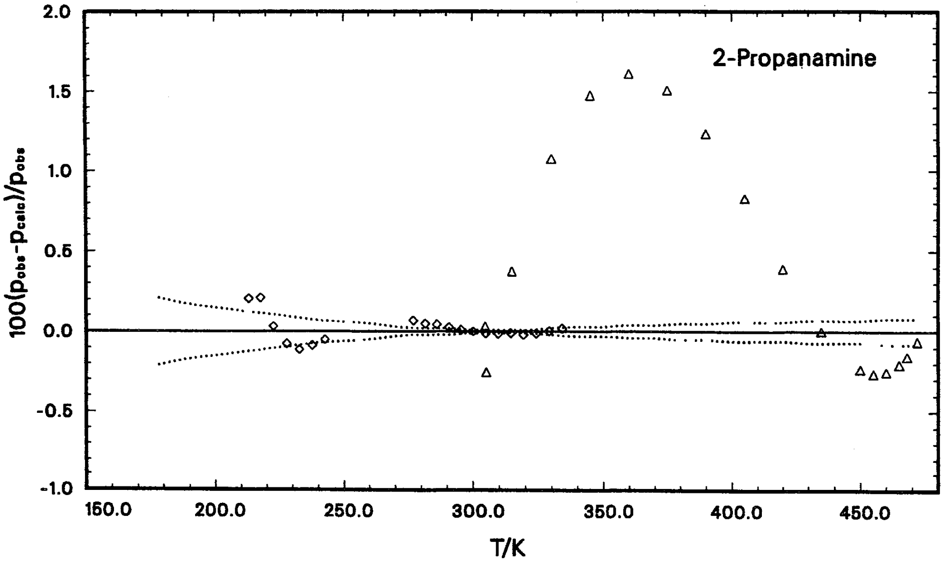

FIG. 4. Percent deviation of experimental vapor pressures for 2-propanamine from the Cox equation. ○ Colpy *et al.* (1941-101); △ Kobe and Mathews (1970-5)*; ◇ Osborn and Douslin (1968-206)*; with * after reference number for data used in fitting.

bution of the calculated values that were used is shown in Fig. 4.

Copley *et al.* (1941-101) reported vapor pressure data at 277.7 and 405.4 K. The purity and the method of measurement were not specified. Their vapor pressure values were 7.7 and 4% lower than those of Osborn and Douslin. The single point at 63.7 kPa reported in (1968-195) is in good agreement, 0.06%, with the selected values. The percent deviations of the experimental values from vapor pressures calculated from the Cox equation are shown in Fig. 4. Also shown are percent deviations from the Cox equation for 16 values calculated from the equation of Kobe and Mathews (1970-5).

Benzenamine. Many vapor pressure data have been reported for benzenamine in the last hundred years. In the nineteenth century, Ramsay and Young (1885-25, 1886-62 and 1887-58) and Kahlbaum (1898-2) measured the vapor pressure. Beckmann and Liesche (1915-88) used a sample of unspecified purity and their uncertainties were high. Holtzlander and Riggle (1955-604), and Crutzen *et al.* (1957-486) used static methods on samples of unspecified purities. Rock and Sieg (1955-2) and Gurevich and Sigalovskaya (1937-437) used gas saturation methods. Danov and Shinyaeva (1965-382), Gopal and Rizvi (1968-210), Gould *et al.* (1947-337), Campbell *et al.* (1968-211) and Dreisbach and Shrader (1949-113) used static methods, and their uncertainties were very high. The data of Maher and Smith (1979-94) were less precise than expected. The above mentioned data along with isolated points reported in references (1932-116, 1953-610, 1954-622, 1962-363, 1974-136) were not given weight in this evaluation.

Garrick (1927-156), Lastovtsev (1937-438), McDonald *et al.* (1959-109), and Stadnicki (1962-32, 1962-33, 1962-34, 1963-321) used ebulliometric methods in measuring the vapor pressure, and their data were used in this evaluation. However only one of the apparently repeated sets of data by Stadnicki was used. The data of Maher and Smith (1980-20) were also used; they used static methods on carefully purified and degassed samples. Percent deviations of the experimental values from those calculated from the Cox equation are shown in Fig. 5.

2-Methylbenzenamine. The data of Neubeck (1887-59) and the single point of reference (1921-19) were not used in the evaluation. The vapor pressures that Kahlbaum (1898-2) and Dreisbach and Shrader (1949-113) measured up to the boiling temperature and that Glaser and Rüland (1957-76) measured between the boiling and critical temperatures were selected for further evaluation. At low temperatures, the data of Dreisbach and Shrader were given higher weight than that of Kahlbaum, although the latter covered a wider range of temperature. The deviations of the experimental values from those calculated from the Cox equation are shown in Fig. 6. The data of Kahlbaum shows significant deviations at the lowest temperatures for this compound as well as for the other benzenamines considered in this work.

3-Methylbenzenamine. The data of Kahlbaum (1898-2) and Dreisbach and Shrader (1949-113) were used at low temperatures and the data of Glaser and Rüland (1957-76) were used at high temperatures. The data of Neubeck (1887-59) and the isolated point reported in reference (1921-19) were not used in the analysis. Percent deviations of the experimental vapor pressures from values calculated with the Cox equation are shown in Fig. 7.

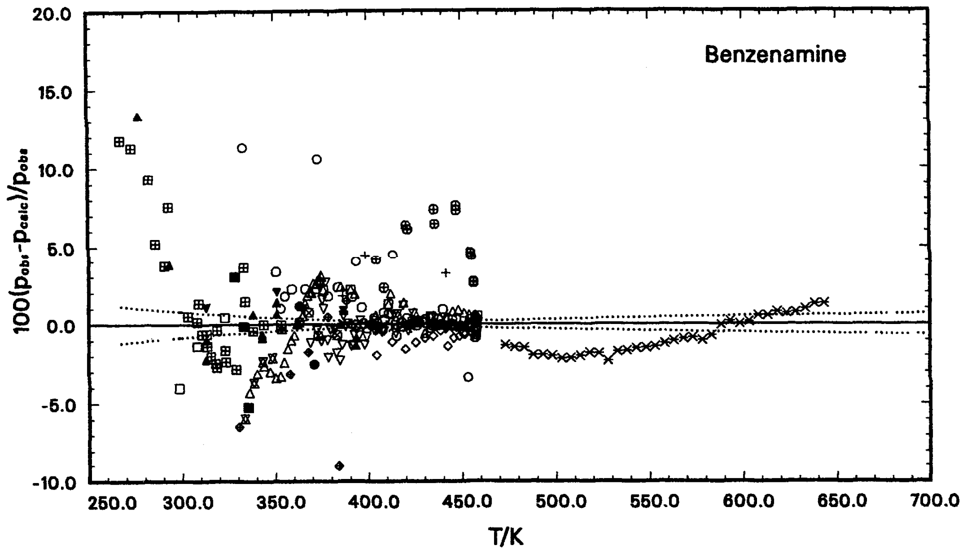

FIG. 5. Percent deviation of experimental vapor pressures for benzenamine from the Cox equation. ○ Ramsay and Young (1885-25); × Ramsay and Young (1886-62); ⊕ Ramsay and Young (1887-58); △ Kahlbaum (1898-2); ◇ Beckmann and Liesche (1915-88); ▽ Garrick (1927-156)*; × Lastovtsev (1937-438); ⊠ Gurevich and Sigalovskaya (1937-437); ◇ Gould *et al.* (1947-337); + Dreisbach and Shrader (1949-113)*; △ Holtzlander and Riggle (1955-604); □ Roeck and Sieg (1955-2)*; ⊗ Crutzen *et al* (1957-486); □ McDonald *et al.* (1959-109)*; ◆ Stadnicki (1962-32, 1962-33, 1962-34, 1963-321*); ○ Danov and Shinyaeva (1965-382); □ Pannetier *et al.* (1965-388); ■ Campbell *et al.* (1968-211); ● Gopal and Rizvi (1968-210); ▼ Maher and Smith (1979-94); ▲ Maher and Smith (1980-20)*; with * after reference number for data used in fitting.

4-Methylbenzenamine. The final evaluation was made with the measurements made by Kahlbaum (1898-2) up to the boiling temperature and by Glaser and Rüland (1957-76) between the boiling and critical temperatures. The results of Neubeck (1887-59) and the single point at 373 K (1895-49) were excluded. Percent deviations of experimental values from those calculated with the Cox equation are shown in Fig. 8.

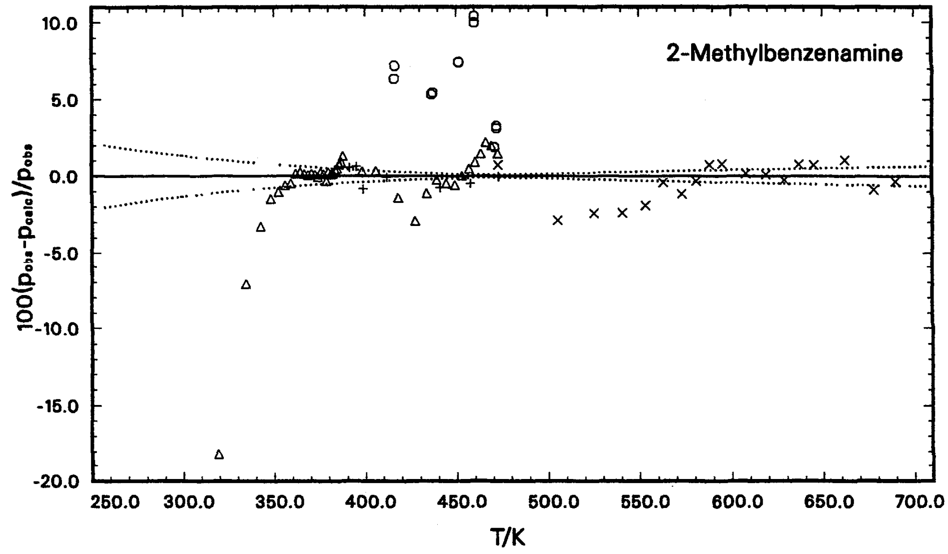

FIG. 6. Percent deviation of experimental vapor pressures for 2-methylbenzenamine from the Cox equation. ○ Neubeck (1887-59); △ Kahlbaum (1898-2)*; + Dreisbach and Shräder (1949-113)*; × Glaser and Rüland (1957-76)*; with * after reference number for data used in fitting.

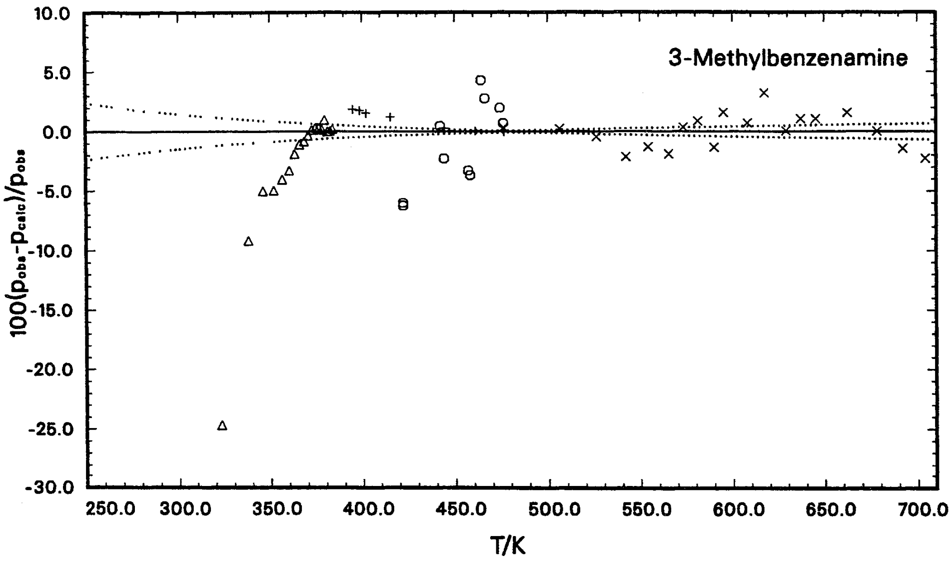

FIG. 7. Percent deviation of experimental vapor pressures for 3-methylbenzenamine from the Cox equation. O Neubeck (1887-59); △ Kahlbaum (1898-2)*; + Dreisbach (1949-113)*; × Glaser and Rüland (1957-76)*; with * after reference number for data used in fitting.

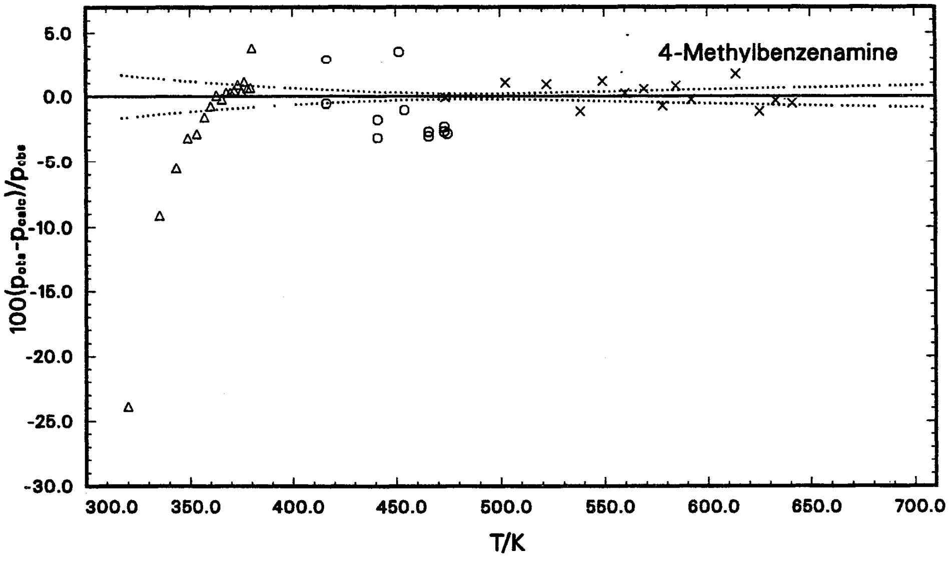

FIG. 8. Percent deviation of experimental vapor pressures for 4-methylbenzenamine from the Cox equation. O Neubeck (1887-59); △ Kahlbaum (1898-2)*; × Glaser and Rüland (1957-76)*; with * after reference number for data used in fitting.

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 pressure 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.

Methanamine. The values of Felsing and Thomas (1929-227) and of Isakova *et al.* (1966-198) were used to fit Eq. (6). The values of the latter were about 0.25% lower than the former in the region of overlap, 281 to 293 K. The values of Le Fevre and Russell (1947-335) were about 0.35% lower than the selected values while that of Hofmann (1889-19) was in good agreement with the selections. The root-mean-square-weighted-deviation for the fit to Eq. (6) with four adjustable constants was four times higher than expected for an optimum fit and a proper choice of experimental imprecisions. The cyclic sign changes in the deviations, Fig. 9, indicated that Eq. (6) was not entirely adequate; however, additional terms in Eq. (6) were not warranted by the data.

Ethanamine. The values of Swift (1942-92), Barcelo *et al.* (1950-529), and Pohland and Mehl (1933-369) were selected in determining the three coefficients in Eq. 6; the temperature range of the values was too limited to justify inclusion of a fourth term. The selected values and the remaining values (1850-2, 1889-26, 1910-58, and 1912-127) were consistent with the experimental values as shown by the deviations from Eq. (6), see Fig. 10. Measurements reported at single temperatures by (1850-7) and (1889-19) were not given any weight in the evaluation.

1-Propanamine. The values reported by Vogel (1948-262) and Costello and Bowden (1959-218) were selected, and were represented to within their experimental imprecisions by Eq. (6) with three adjustable parameters. The deviations are shown in Fig. 11. The remaining values at isolated temperatures (1952-385, 1968-195) and those prior to 1920 (1872-26, 1886-28, 1889-26, 1891-28, 1893-55, 1895-49, 1910-66, and 1919-64) were represented to within 0.3%. Larger deviations were found for the values from the remaining literature, (1869-15) 1.2%; (1970-165) 10%.

2-Propanamine. The values used in determining the three constants in the density equation were those of Vogel (1948-262) and of Costello and Bowden (1959-218). The values from the references, (1868-12, 1895-49, 1954-310, 1968-195, and 1969-165), that reported only one or two points were not included in the fit; however, they were within the expected accuracy of the data used in the fit. The excluded results of Shirai (1956-45) showed slightly more scatter, as much as 0.2%, than had been anticipated from the assigned imprecisions. The results of Hough *et al.* (1950-523) were as much as 1% higher than the accepted values.

Kobe and Mathews (1970-5) used isochoric measurements to determine liquid and vapor densities up to the critical temperature, but they only reported their value of the critical density and the constants for the rectilinear diameter $\frac{1}{2}(\rho_l+\rho_g)/(\text{kg m}^{-3}) = 268.2 - 218.8(1 - T/T_c)$ (from 453 to 471.9 K). Their values of the critical temperature and density were used as constraints on the density equation.

Benzenamine. Over 200 separate values of the density at varied temperatures have been reported in the literature as

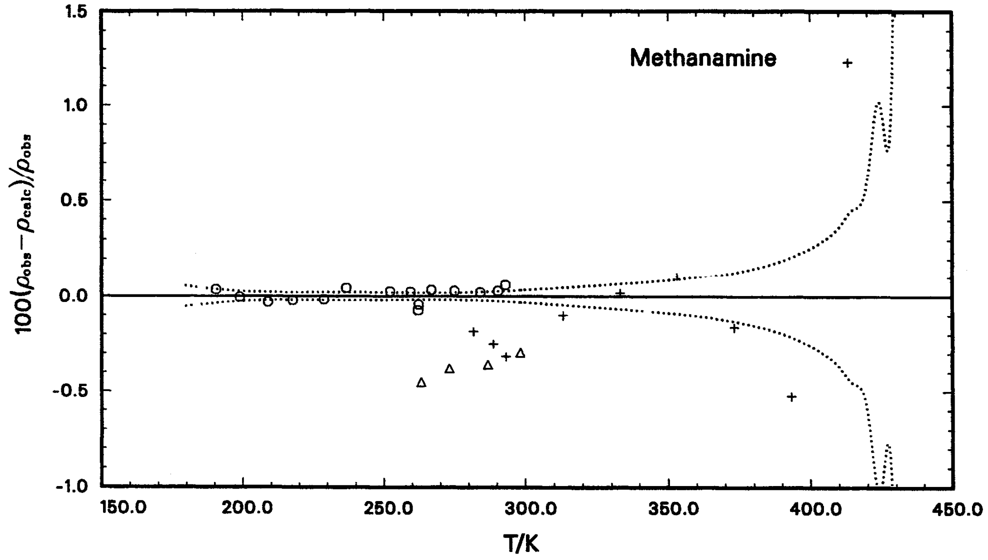

FIG. 9. Percent deviation of experimental saturated liquid densities for methanamine from Eq. (6). ○ Felsing and Thomas (1929-227)*; △ Le Fevre and Russell (1947-335); + Isakova *et al.* (1966-198)*; with * after reference number for data used in fitting.

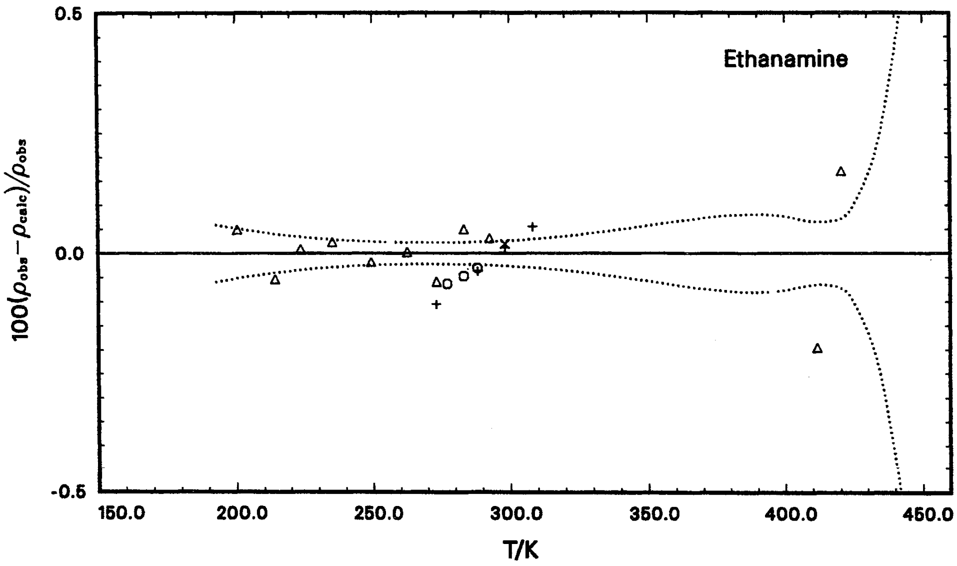

FIG. 10. Percent deviation of experimental saturated liquid densities for ethanamine from Eq. (6). ○ Perkin (1889-26); △ Pohland and Mehl (1933-369)*; + Swift (1942-92)*; × Barcelo *et al.* (1950-529); with * after reference number for data used in fitting.

summarized in Table 17. The four constants in the density equation were determined from the values for which a one is in the *sl* column of Table 17. Additional data not indicated in Table 17 are available at isolated points (1850-10, 1880-2, 1888-35, 1888-39, 1894-56, 1895-49, 1898-2, 1902-64, 1909-133, 1910-58, 1912-127, 1913-73, 1913-163, 1914-108, 1920-94, 1924-127, 1931-211, 1932-116, 1933-418, 1937-254, 1945-173, 1949-535, 1949-536, 1957-486, 1959-304, 1960-

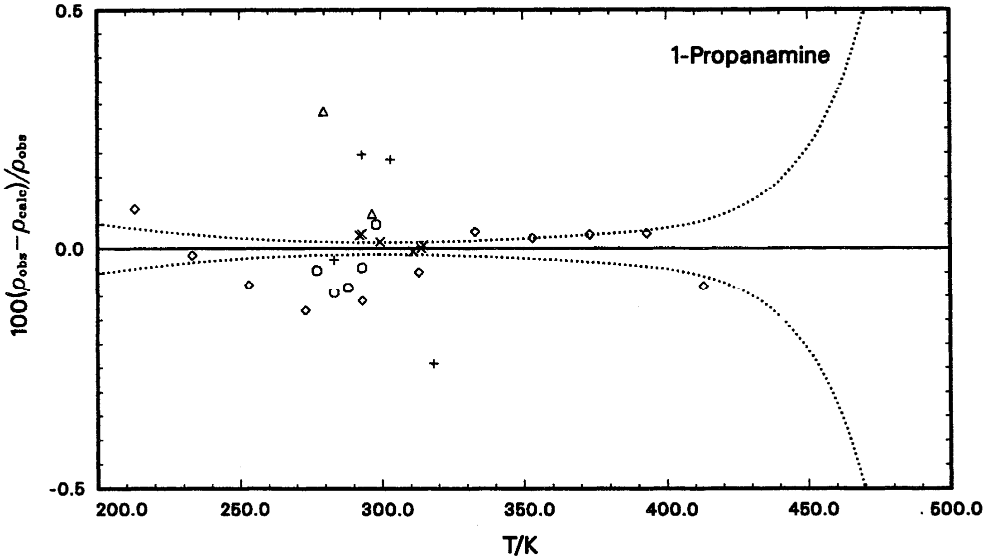

FIG. 11. Percent deviation of experimental saturated liquid densities for 1-propanamine from Eq. (6). ○ Perkin (1889-26); △ Gladstone (1891-28); + Turner and Merry (1910-66); × Vogel (1948-262)*; ◇ Costello and Bowden (1959-218)*; with * after reference number for data used in fitting.

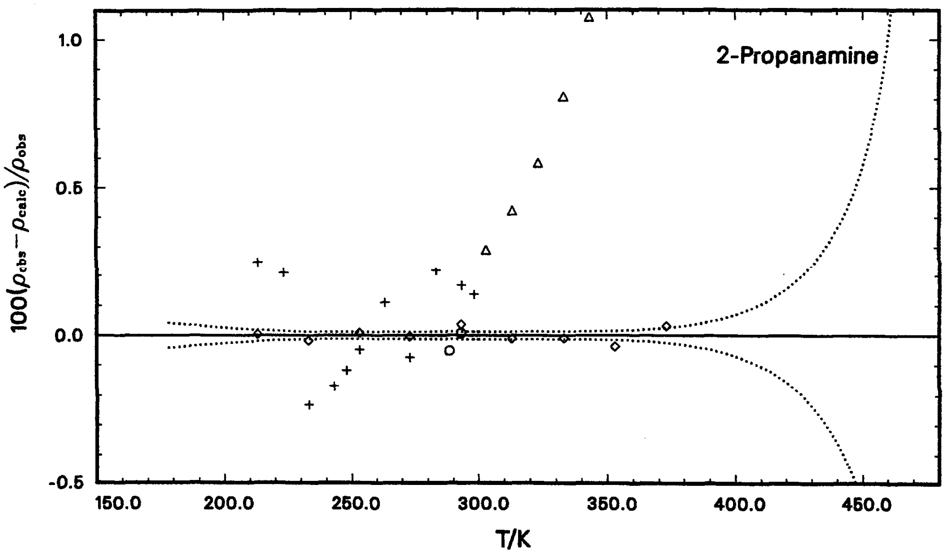

FIG. 12. Percent deviation of experimental saturated liquid densities for 2-propanamine from Eq. (6). ○ Bruhl (1895-49); △ Hough *et al.* (1950-523); + Shirai (1956-45); ◇ Costello and Bowden (1959-218)*; with * after reference number for data used in fitting.

289, 1962-363, 1963-325, 1965-333, 1967-225, 1975-33, 1985-372, 1987-70, and 1988-53). The selected values were within a few 0.01% of those from the fitting equation as shown in Fig. 13. The results from references (1953-611 and 1953-615) were much more inconsistent than were anticipated. Two extensive data sets published before 1900 (1887-59 and 1896-28) were persistently low by about 0.25%. The apparent precision of the results reported by Neubeck (1887-59) is enigmatic in light of the way his results have approximately constant deviations for each of the four benzenamines examined in this work. These deviations are not consistent with systematic errors in either temperature or density for the entire collection of data; they have been ascribed tentatively to impurities in his samples.

2-Methylbenzenamine. The temperature range of the available data was so limited that only two constants in the fitting equation could be obtained reliably. As indicated in Table 17, values from a number of sources were used for the fit; they were represented to within better than ±0.1%. Data at isolated points (1894-56, 1895-49, 1896-50, 1898-2, 1902-73, 1913-73, 1914-154, 1915-104, 1924-127, 1936-383, and 1960-288) were not indicated in Table 17. The results of Neubeck (1887-59) were persistently high by about 0.25% in the region of overlap with the remaining data; this precluded their use of the values reported near 472 K. All of the remaining values were represented with the fitting equation to within the experimental imprecisions. Deviations from the fitting equation for some of the experimental data are shown in Fig. 14.

3-Methylbenzenamine. 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, were represented with the fitting equation to better than ±0.1%. The values by Neubeck (1887-59), by Perkin (1896-28), and by Dessart (1926-22) were systematically higher than the accepted values by about 0.6%, 0.2%, and 0.4%, respectively. Those of Bingham and Spooner (1932-308) showed a statistically significant trend in their deviations, and those of Hatem (1949-488) were less precise than had been anticipated. Some isolated points considered (1895-49, 1898-2, 1924-127, 1913-163, and 1936-383) were not indicated in Table 17. Deviations from the fitting equation for some of the experimental data are shown in Fig. 15.

4-Methylbenzenamine. 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 fit to better than ±0.1%. The rejected values from sets over appreciable temperature ranges by Neubeck (1887-59) and Perkin (1896-28) showed significant trends in their deviations. Isolated points (1893-55, 1895-49, 1913-163, and 1913-178) were not indicated in Table 17. Deviations from the fitting equation for some of the experimental data are shown in Fig. 16.

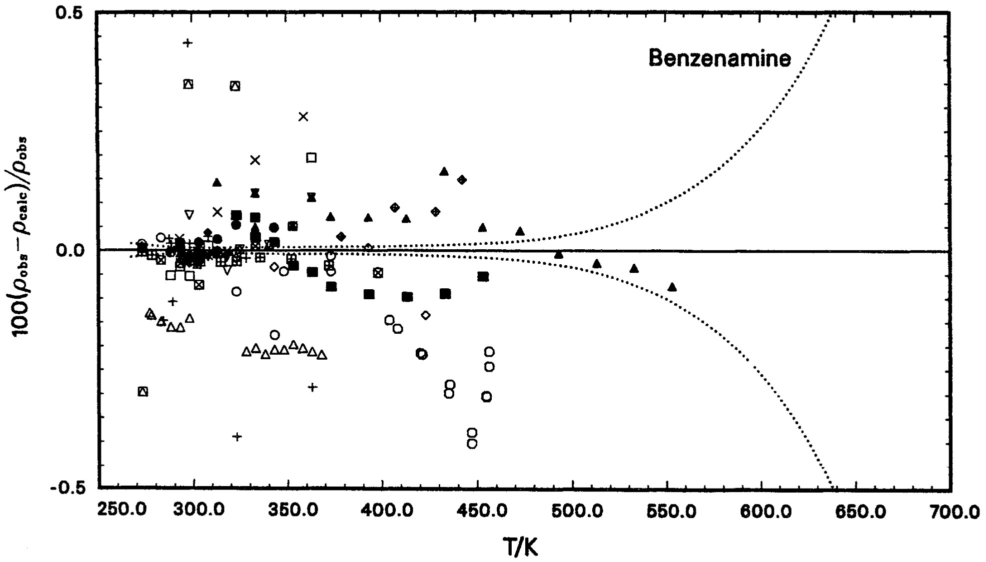

FIG. 13. Percent deviation of experimental saturated liquid densities for benzenamine from values calculated from Eq. (6). ○ Neubeck (1887-59); + Perkin (1892-22); + Jahn and Moeller (1894-43); △ Perkin (1896-28); △ Livingston *et al.* (1908-112); + Patterson and Findlay (1912-148)*; + Thole *et al.* (1913-178)*; + Herz (1914-137); □ Tyrer (1914-103)*; ⊗ Bramley (1916-233)*; ○ Bingham *et al.* (1920-95)*; ◇ Buehler *et al.* (1932-79); ● Azim *et al.* (1933-35)*; ⊕ Timmermans (1935-68)*; + Gibson and Loeffier (1939-114); ◇ Friend *et al.* (1937-125)*; × Vogel (1948-262); □ Hatem (1949-42)*; + Dreisbach and Martin (1949-120)*; Hough *et al.* (1950-523)*; ● Naumova (1953-615); + Tartakovskaya and Sukharev (1953-611); □ Naumova and Prokop'eva (1953-614); ▲ Kovalenko and Trifonov (1954-674)*; ▲ Costello and Bowden (1959-218)*; ∇ Lindberg and Stenholm (1966-203)*; ⊠ Sumer and Thompson (1967-58)*; × Deshpande and Bhatgadde (1968-223, 1971-17)*; ◆ Katz *et al.* (1971-157)*; ▼ Papepu *et al.* (1985-160)*; with * after reference number for data used in fitting.

TABLE 17. **Available saturated liquid density data.**

$\frac{\text{Range}}{\text{K}}$	$\frac{\sigma(T)^a}{\text{K}}$	$\frac{\text{Range}}{\text{kg·m}^{-3}}$	$\frac{10^2\sigma(\rho_l)/\rho_l^a}{\text{kg·m}^{-3}}$	sl^b	N^c	Author(s)	Ref.
			Methanamine				
190-293	0.05	778-663	0.01	1	15	Felsing and Thomas	1929-227
263-298	0.1	695-654	0.02	0	4	Le Fevre and Russell	1947-335
282-413	0.2	675-466	0.02	1	9	Isakova *et al.*	1966-198
			Ethanamine				
277-288	0.3	701-689	0.01	0	3	Perkin	1889-26
201-420	0.01	785-684	0.01	1	11	Pohland and Mehl	1933-369
273-288	0.01	706-688	0.005	1	4	Swift	1942-92

[a] See section 1.6.

[b] 1 for data selected and 0 for data not selected for least square fit.

[c] Number of experimental values.

TABLE 17. Continued.

Range K	$\sigma(T)^a$ K	Range kg·m^{-3}	$10^2\sigma(\rho_l)/\rho_l^a$ kg·m^{-3}	sl^b	N^c	Author(s)	Ref.
			1-Propanamine				
277-298	0.3	733-712	0.01	0	5	Perkin	1889-26
283-318	0.1	727-689	0.01	0	4	Turner and Merry	1910-66
292-315	0.1	718-695	0.03	1	8	Vogel	1948-262
213-413	0.2	797-577	0.04	1	11	Costello and Bowden	1959-218
			2-Propanamine				
303-343	0.003	680-638	0.01	0	5	Hough *et al.*	1950-523
213-298	0.02	773-684	0.02	0	11	Shirai	1956-45
213-373	0.2	771-592	0.04	1	9	Costello and Bowden	1959-218
			Benzenamine				
404-456	0.1	922-873	0.03	0	13	Neubeck	1887-59
284-363	0.1	1028-958	0.04	0	2	Perkin	1892-22
287-289	0.1	1027-1024	0.05	0	2	Jahn and Moeller	1894-43
277-368	0.2	1034-954	0.06	0	15	Perkin	1896-28
302-340	0.1	1013-981	0.03	0	3	Livingston *et al.*	1908-112
288-298	0.05	1026-1017	0.05	1	3	Patterson and Findlay	1912-148
298-323	0.2	1022-992	0.1	1	2	Thole *et al.*	1913-178
298-363	0.05	1017-962	0.03	0	3	Herz	1914-137
273-372	0.02	1030-952	0.01	1	9	Tyrer	1914-103
293-298	0.02	1021-1017	0.01	1	3	Hartung	1916-232
283-398	0.02	1039-929	0.02	1	9	Bramley	1916-233
273-373	0.02	1039-951	0.04	1	12	Bingham *et al.*	1920-95
323-423	0.03	996-905	0.02	0	5	Buehler *et al.*	1932-79
293-343	0.02	1022-978	0.01	1	6	Azim *et al.*	1933-351
273-303	0.01	1039-1013	0.01	1	3	Timmermans *et al.*	1935-68
305-333	0.04	1011-987	0.05	1	2	Weller	1935-369
273-328	0.02	1039-991	0.03	0	3	Gibson and Loeffler	1939-114
379-442	0.01	947-890	0.01	1	4	Friend *et al.*	1944-125
293-359	0.02	1022-967	0.05	0	4	Vogel	1948-262
288-308	0.001	1026-1009	0.05	1	5	Hatem	1949-42
293-298	0.01	1021-1017	0.02	1	2	Dreisbach and Martin	1949-120
323-453	0.003	996-878	0.01	1	10	Hough *et al.*	1950-523
303-333	0.03	1021-1004	0.05	0	3	Naumova	1953-615
298-398	0.03	1028-924	0.05	0	3	Tartakovskaya and Sukharev	1953-611
273-323	0.03	1036-999	0.05	0	3	Naumova and Prokop′eva	1953-614
293-363	0.03	1021-962	0.05	1	3	Kovalenko and Trifonov	1954-674
273-553	0.2	1039-779	0.04	1	15	Costello and Bowden	1959-218
298-318	0.01	1018-1000	0.03	1	3	Lindberg and Stenholm	1966-203
293-313	0.02	1022-1004	0.02	1	3	Sumer and Thompson	1967-58
298-318	0.01	1017-1000	0.02	1	3	Deshpande and Bhatgadde	1968-223
298-318	0.01	1017-1000	0.02	1	3	Deshpande and Bhatgadde	1971-17
298-313	0.01	1017-1005	0.01	1	4	Katz *et al.*	1971-157
298-318	0.01	1017-1000	0.03	1	5	Papepu *et al.*	1985-160

[a] See section 1.6.

[b] 1 for data selected and 0 for data not selected for least square fit.

[c] Number of experimental values.

TABLE 17. Continued.

$\frac{\text{Range}}{\text{K}}$	$\frac{\sigma(T)^a}{\text{K}}$	$\frac{\text{Range}}{\text{kg}\cdot\text{m}^{-3}}$	$\frac{10^2\sigma(\rho_l)/\rho_l^a}{\text{kg}\cdot\text{m}^{-3}}$	sl^b	N^c	Author(s)	Ref.
			2-Methylbenzenamine				
415-472	0.2	894-843	0.05	0	11	Neubeck	1887-59
277-328	0.5	1011-971	0.05	0	12	Perkin	1896-28
273-303	0.05	1015-990	0.06	1	3	Dutoit	1900-10
293-343	0.1	999-957	0.3	0	3	Kremann *et al.*	1914-108
273-373	0.02	1015-931	0.04	1	14	Bingham *et al.*	1920-95
323-423	0.03	974-889	0.03	0	5	Buehler *et al.*	1932-79
273-303	0.05	1015-990	0.01	1	3	Timmermans *et al.*	1935-68
398-466	0.03	907-845	0.05	1	7	Friend and Hargreaves	1944-125
293-298	0.01	998-994	0.03	1	2	Dreisbach and Martin	1949-120
291-308	0.05	1000-986	0.02	0	5	Hatem	1949-488
			3-Methylbenzenamine				
422-476	0.2	885-833	0.05	0	12	Neubeck	1887-59
277-298	0.1	1004-990	0.05	0	6	Perkin	1896-28
273-305	0.1	1009-983	0.03	0	5	Dessart	1926-22
273-373	0.05	1005-922	0.01	1	8	Bingham and Spooner	1932-308
298-423	0.03	985-881	0.03	0	6	Buehler	1932-79
273-303	0.05	1005-980	0.01	1	3	Timmermans *et al.*	1935-68
374-466	0.03	923-837	0.05	1	8	Friend and Hargreaves	1944-125
293-298	0.02	988-984	0.02	1	2	Dreisbach and Martin	1949-120
291-308	0.05	993-971	0.02	0	5	Hatem	1949-488
			4-Methylbenzenamine				
416-474	0.2	883-829	0.04	0	11	Neubeck	1887-59
323-343	0.1	952-946	0.01	0	4	Perkin	1896-28
323-333	0.05	961-953	0.06	1	2	Dutoit	1900-10
319-413	0.05	971-873	0.1	0	11	Beck	1907-112
313-448	0.01	970-850	0.03	1	7	Bramley	1916-233
350-383	0.05	940-904	0.05	0	3	Bernoulli and Veillon	1932-307
323-393	0.05	962-902	0.01	1	4	Buehler	1932-79
318-333	0.01	966-954	0.01	1	4	Timmermans *et al.*	1937-146
409-463	0.03	889-835	0.05	1	5	Friend and Hargreaves	1944-125

[a] See section 1.6.

[b] 1 for data selected and 0 for data not selected for least square fit.

[c] Number of experimental values.

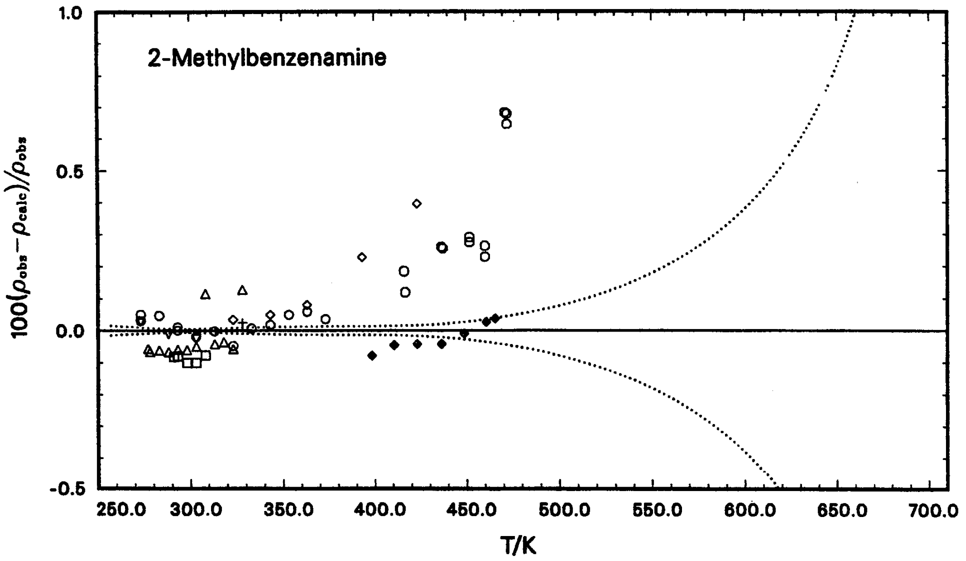

FIG. 14. Percent deviation of experimental saturated liquid densities for 2-methylbenzenamine from values calculated from Eq. 6. ○ Neuback (1887-59); △ Perkin (1896-28); ▽ Dutoit (1900-10)*; + Thole (1913-163); o Bingham *et al.* (1920-95)*; ◇ Buehler (1932-79); ◇ Friend and Hargreaves (1944-125)*; □ Hatem (1949-488); with * after reference number for data used in fitting.

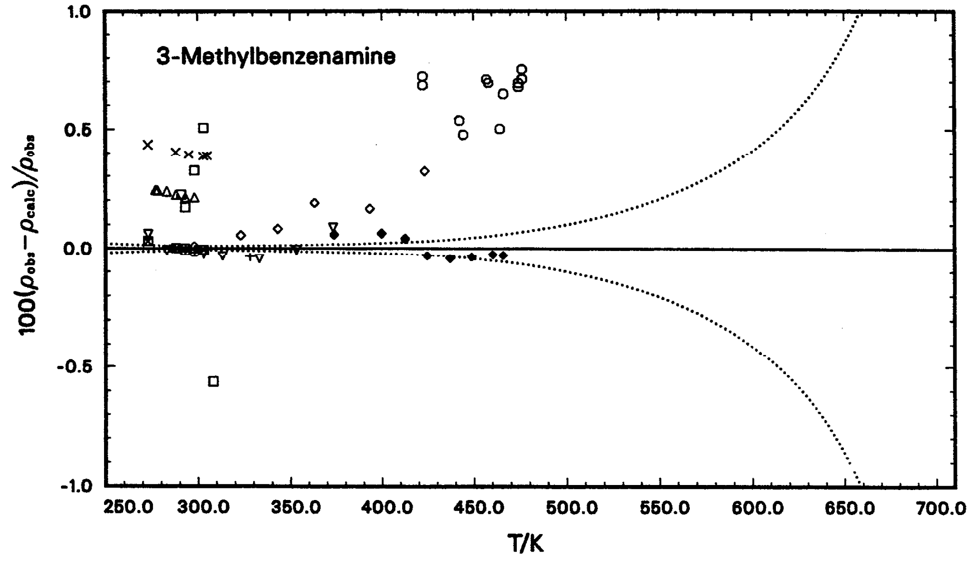

FIG. 15. Percent deviation of experimental saturated liquid densities for 3-methylbenzenamine from values calculated from Eq. (6). ○ Neuback (1887-59); △ Perkin (1896-28); + Thole (1913-163); × Dessart (1926-22); ▽ Bingham and Spooner (1932-308)*; ◇ Buehler (1932-79); □ Timmermans *et al.* (1935-67)*; ◇ Friend and Hargreaves (1944-125)*; ⊕ Dreisbach and Martin (1949-120)*; □ Hatem (1949-488); with * after reference number for data used in fitting.

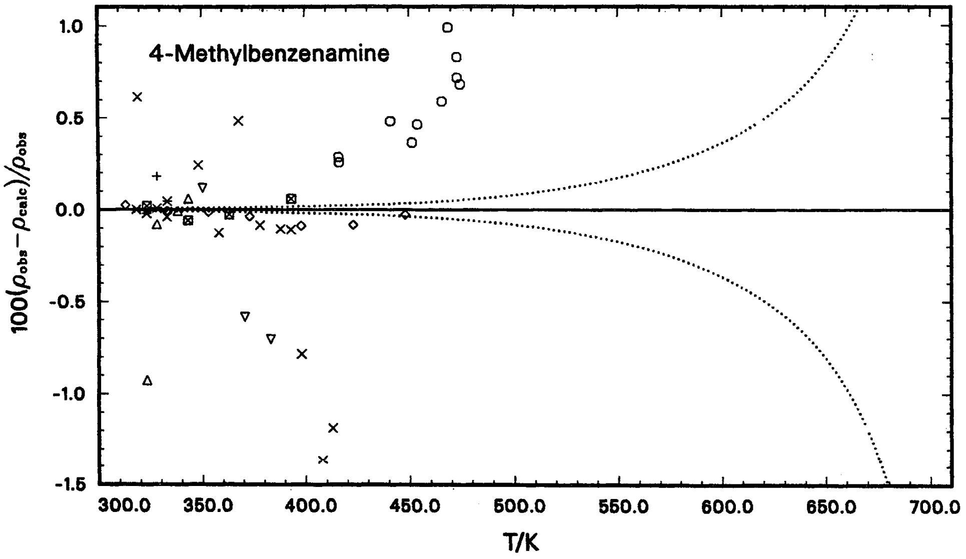

FIG. 16. Percent deviation of experimental saturated liquid densities for 4-methylbenzenamine from values calculated from Eq. (6). ○ Neuback (1887-59); △ Perkin (1896-28); ×Beck (1907-112); + Thole (1913-163); ◇ Bramley (1916-233)*; ▽ Bernoulli and Veillon (1932-307); □ Buehler (1932-79)*; ×Timmermans *et al.* (1937-146)*; with * after reference number for data used in fitting.

3.4. Second Virial Coefficients

The temperature ranges over which measurements of second virial coefficients have been made, along with the estimated uncertainties, are listed in Table 18.

Methanamine. The second virial coefficient data of Lambert and Strong (1950-430) were not used because of their high uncertainty. Only the values of Adam *et al.* (1976-113) were used to derive the recommended values from Eq. (9). Deviations of the experimental values from those calculated from the smoothing equation are shown in Fig. 17. The estimated uncertainties in the smoothed virial coefficients are ± 20 $cm^3\,mol^{-1}$ at 180 K, decreasing to ± 10 $cm^3\,mol^{-1}$ at 610 K.

Ethanamine. The values of Lambert and Strong (1950-430) were the only data available. The estimated uncertainty in the virial coefficients is ± 50 $cm^3\,mol^{-1}$. The parameter A_b in Eq. (9) was constrained to conform with Eq. (10) for methanamine. If this parameter was allowed to be freely adjustable, the remaining parameters were not consistent with those for methanamine. The deviations of the values from those calculated from the smoothing equation are shown in Fig. 18.

1-Propanamine. Second virial coefficients were derived from the Claperyon equation with the enthalpy of vaporization data of Majer *et al.* (1979-78) and the Cox equation constants from Table 2. The derived values at 298.15, 313.15, and 328.15 K were (-1053 ± 20), (-822 ± 10), and (-769 ± 10) $cm^3\,mol^{-1}$, respectively. The value at 313.15 K seemed inconsistent with the other two points and was given zero weight. The values of both A_b and D_b in Eq. (9) were determined from the constants for methanamine in Eq. (10), and the value of C_b was determined by a least-squares fit.

2-Propanamine. Values of the second virial coefficient derived from enthalpies of vaporization determined by Majer *et al.* (1979-78) were (-806 ± 10) and (-721 ± 10) $cm^3\,mol^{-1}$ at 298.15 and 313.15 K, respectively. These were used to determine the constant C_b in Eq. (9) in a manner similar to that described above for 1-propanamine.

Benzenamine. The only data available were reported by Lagutkin *et al.* (1973-167) who used a virial equation with the first four virial coefficients and the data derived by Seshadri *et al.* (1969-168) from an empirical equation of state. The latter work used the Martin-Hou (1955-712) equation of state without volumetric data essential as input to reliably specify second virial coefficients. For these reasons we did not consider these results; however, they are listed in a recent compilation (1986-782) of virial coefficients.

No second virial coefficients or direct enthalpy of vaporization measurements were available for the remaining compounds.

TABLE 18. Available second virial coefficient data.

Range K	Range cm^3·mol^{-1}	$\sigma(B)$ cm^3·mol^{-1}	sl[a]	Author(s)	Ref.
		Methanamine			
293 to 405	−535 to −220	50	0	Lambert and Strong	1950-430
296 to 550	−471 to −118	10	1	Adam *et al.*	1976-113
		Ethanamine			
293 to 405	−821 to −345	50	1	Lambert and Strong	1950-430
		1-Propanamine			
298 to 328	−1053 to −769	20	1	This work (derived)	
		2-Propanamine			
298 to 313	−806 to −721	20	1	This work (derived)	

[a] Selected if 1 and rejected if 0.

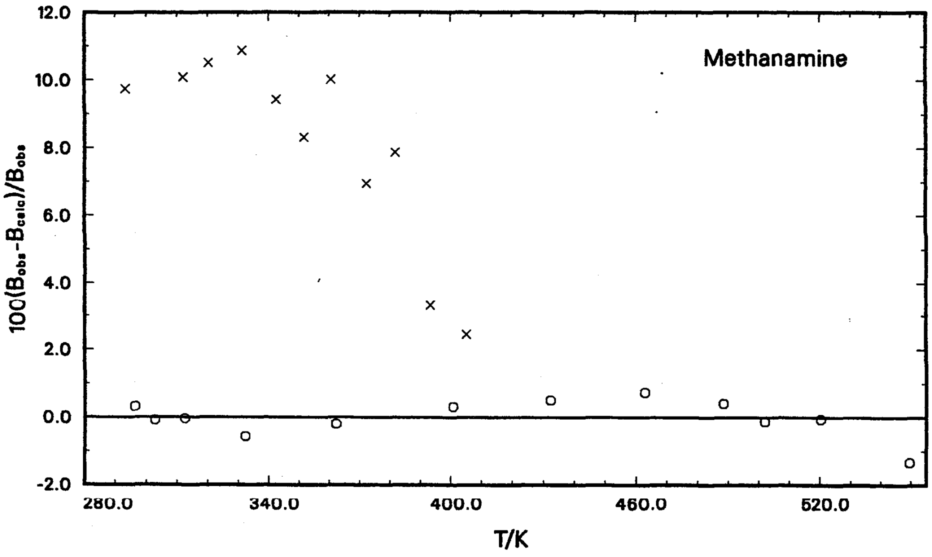

FIG. 17. Percent deviation of experimental second virial coefficients for methanamine from the smoothing equation. × Lambert and Strong (1950-430); ○ Adam *et al.* (1976-113)*; with * after reference number for data used in fitting.

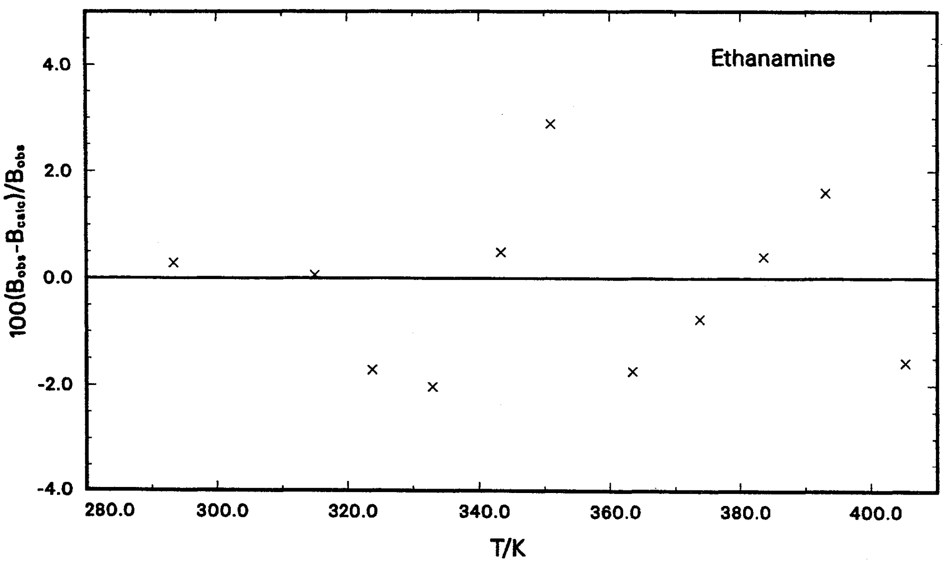

FIG. 18. Percent deviation of experimental second virial coefficients for ethanamine from the smoothing equation. ×Lambert and Strong (1950-430).

3.5. Enthalpies of Vaporization or Sublimation

Calorimetrically determined enthalpies of vaporization together with values calculated from vapor pressure data, along with estimated uncertainties are listed in Table 19.

Methanamine. Aston *et al.* (1937-248) determined calorimetrically the enthalpy of vaporization at 266.84 K. Using the enthalpies for the liquid and ideal gas and the second virial coefficients of this report, we corrected the value determined by Aston *et al.* (1937-248) to give the enthalpy of vaporization to the ideal gas state at 298.15 K reported in Table 10.

Ethanamine. No calorimetric value was available. The enthalpy of vaporization at 298.15 K was determined from vapor pressure data and corrected to the ideal gas state using the second virial coefficients of this report.

1-Propanamine. The enthalpy of vaporization was determined calorimetrically by Majer *et al.* (1979-78) at 298.15, 313.15, and 328.15 K and by Kusano and Saito (1976-127) at 298.15 K. We calculated the enthalpy of vaporization, corrected to the ideal gas state at 298.15 K, using the enthalpy of vaporization determined by Majer *et al.* (1979-78) at 298.15 K and the second virial coefficients of this report.

2-Propanamine. The enthalpy of vaporization was determined calorimetrically by Majer *et al.* (1979-78) at 298.15 and 313.15 K. Using the value at 298.15 K and the second virial coefficients of this report, we calculated the enthalpy of vaporization to the ideal gas state at 298.15 K.

Benzenamine. The enthalpy of vaporization of benzenamine was determined calorimetrically by Hatton *et al.* (1962-3) at 332.2 K and by Kusano and Wadsö (1971-2) at 298.15 K. These two determinations were consistent with those derived from the Claperyon equation. The value determined by Kusano and Wadsö was selected; corrections for gas imperfection were insignificant.

2-Methylbenzenamine. The enthalpy of vaporization to the ideal gas was calculated for 353.15 K from the Claperyon equation with the vapor pressure equation, and the value was corrected to 298.15 K using the enthalpies of the liquid and ideal gas. Corrections for gas imperfections were assumed to be insignificant.

3-Methylbenzenamine. The enthalpy of vaporization at 298.15 K was determined in a manner similar to that for 2-methylbenzenamine.

4-Methylbenzenamine. The enthalpy of vaporization at 353.15 K was calculated from the Claperyon equation with the vapor pressure equation of this report. This result was used to derive an enthalpy of sublimation to the ideal gas at 298.15 K. The value of the heat capacity of the liquid at 316.89 K compiled by Kudchadker and Wilhoit (1983-108) was used to calculate the enthalpy difference of the liquid to the triple-point temperature at 316.89 K. The enthalpy of fusion determined by Rastogi *et al.* (1963-367) and an estimated value of the heat capacity of the crystals $[C_{\text{sat}}(c)/R] \simeq C_{\text{sat}}(l)/R - 7$ was used to determine the enthalpy difference of the condensed phases from 316.89 to 298.15 K.

TABLE 19. Available enthalpy of vaporization and sublimation data at 298.15 K.

x[a]	$\frac{T}{\mathrm{K}}$	$\frac{\Delta_x^g H}{\mathrm{kJ \cdot mol^{-1}}}$	$\frac{\sigma(\Delta_x^g H)^b}{\mathrm{kJ \cdot mol^{-1}}}$	Method	sl	Author(s)	Ref.
				Methanamine			
l	263.84	25.81	0.10	Calorimetry	1	Aston *et al.*	1937–218
l	298.15	24.17	0.20	Vapor press.	0	TRC – this work	
				Ethanamine			
l	298.15	26.27	0.20	Vapor press.	1	TRC – this work	
				1-Propanamine			
l	298.15	30.34	0.10	Calorimetry	0	Kusano and Saito	1976–127
l	298.15	31.26	0.10	Calorimetry	1	Majer *et al.*	1979–78
l	313.15	30.14	0.10	Calorimetry	0	Majer *et al.*	1979–78
l	328.15	28.92	0.10	Calorimetry	0	Majer *et al.*	1979–78
l	298.15	31.28	0.10	Vapor press.	0	TRC – this work	
				2-Propanamine			
l	298.15	28.36	0.10	Calorimetry	1	Majer *et al.*	1979–78
l	313.15	27.19	0.10	Calorimetry	0	Majer *et al.*	1979–78
l	298.15	28.36	0.10	Vapor press.	0	TRC – this work	
				Benzenamine			
l	333.15	52.95	0.10	Calorimetry	0	Hatton *et al.*	1962–3
l	298.15	55.83	0.10	Calorimetry	1	Kusano and Wadsö	1971–2
l	298.15	56.13	0.20	Vapor press.	0	TRC – this work	
				2-Methylbenzenamine			
l	298.15	62.7	0.50	Vapor press.	1	TRC – this work	
				3-Methylbenzenamine			
l	298.15	62.7	0.50	Vapor press.	1	TRC – this work	
				4-Methylbenzenamine			
s	298.15	78.8	0.50	Vapor press.	1	TRC – this work	

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[a] Designation for condensed phase (x). [b] See section 1.6.

3.6. Enthalpies of Combustion and Formation

Several determinations for the enthalpies of combustion of these amino compounds were made near the turn of the century. Most of these measurements were made at room temperature which ranged from 15 °C to 20 °C. Thomsen (1905-2) made his measurements in the gas phase but for comparison we converted his values to the liquid state using the selected enthalpies of vaporization. All values were corrected to 25 °C with appropriate heat capacity data. In general, these old values were found to deviate appreciably from recent determinations. The older data are included primarily for completeness, and we do not give them significant weight in our evaluation. The available enthalpy of combustion data along with estimated uncertainties are listed in Table 20. Enthalpies of formation were calculated using the enthalpies

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

ph[a]	$\Delta_c U^\circ/M$ / $\mathrm{kJ \cdot g^{-1}}$	$2\sigma(\Delta_c U^\circ/M)^b$ / $\mathrm{kJ \cdot g^{-1}}$	$\Delta_c H^\circ$ / $\mathrm{kJ \cdot mol^{-1}}$	$2\sigma(\Delta_c H^\circ)^b$ / $\mathrm{kJ \cdot mol^{-1}}$	Author(s)	Ref.
			Methanamine			
l	−33.94[c]	0.10	−1056[c]	5	Thomsen	1905-223
l	−34.44	0.45	−1071	15	Lemoult	1907-116
l	−33.78	0.30	−1051	10	Muller	1910-127
l	−34.095	0.013	−1060.8	0.4	Jaffe	1958-350
			Ethanamine			
l	−37.99	0.10	−1716	5	Berthelot	1881-41
l	−37.92[c]	0.10	−1713[c]	5	Thomsen	1905-223
l	−37.85	0.30	−1710	15	Lemoult	1907-116
l	−37.933	0.011	−1713.3	0.3	Jaffe	1958-350
			1-Propanamine			
l	−40.14[c]	0.15	−2377[c]	10	Thomsen	1905-223
l	−39.45	0.25	−2336	15	Lemoult	1907-116
l	−39.940	0.005	−2365.3	0.3	Smith and Good	1967-60
			2-Propanamine			
l	−39.758	0.008	−2354.5	0.5	Smith and Good	1967-60
			Benzenamine			
l	−36.74	0.30	−3425	30	Petit	1889-4
l	−36.48	0.10	−3400	10	Stohman *et al.*	1890-2
l	−37.03[c]	0.60	−3452[c]	60	Thomsen	1905-223
l	−36.44	0.10	−3397	10	Lemoult	1907-116
l	−36.67	0.20	−3418	20	Swarts	1919-41
l	−36.398	0.010	−3392.8	1.0	Huffman[d]	1942-*
l	−36.401	0.010	−3393.1	1.0	Anderson and Gilbert	1942-5
l	−36.415	0.010	−3394.4	1.0	Cole and Gilbert	1951-259
l	−36.400	0.009	−3393.0	0.8	Hatton *et al.*	1962-3

TABLE 20. Continued.

ph[a]	$\frac{\Delta_c U^\circ/M}{\mathrm{kJ \cdot g^{-1}}}$	$\frac{2\sigma(\Delta_c U^\circ/M)^b}{\mathrm{kJ \cdot g^{-1}}}$	$\frac{\Delta_c H^\circ}{\mathrm{kJ \cdot mol^{-1}}}$	$\frac{2\sigma(\Delta_c H^\circ)^b}{\mathrm{kJ \cdot mol^{-1}}}$	Author(s)	Ref.
			2-Methylbenzenamine			
l	−37.62	0.10	−4035	10	Petit	1889-4
l	−37.61	0.02	−4034.5	2	TRC – this work[e]	
			3-Methylbenzenamine			
l	−37.68	0.10	−4040	10	Petit	1889-4
l	−37.59	0.02	−4032.7	2	TRC – this work[e]	
			4-Methylbenzenamine			
s	−37.39	0.10	−4011	10	Petit	1889-4
s	−37.45	0.02	−4017.3	2	TRC – this work[e]	

[a] phase of substances for which measurements were made. [b] See section 1.6.

[c] from original values for combustion of vapor at the boiling point.

[d] Anderson and Gilbert listed the unpublished value of the enthalpy of combustion of benzenamine determined by Huffman.

[e] estimated.

ormation of auxiliary substances listed in Table 21.

Methanamine. The value of Jaffe (1958-350) was pted. The early values reported by Thomsen (1905-2), Lemoult (1907-116), and by Muller (1910-127) agree the selected value within their estimated uncertainties.

Ethanamine. The value of Jaffe (1958-350) was adopt- For historical background we list those by Thomsen 05-2), Berthelot (1881-41) and Lemoult (1907-116) ch agree with the selected value within the estimated un- ainties.

1-Propanamine. The value by Smith and Good (1967- , determined with a high-purity sample was adopted. We d the early values determined by Thomsen (1905-2) and emoult (1907-116). The value of the latter is particular- oor.

2-Propanamine. The selected value was determined by th and Good (1967-60) on a high-purity sample.

Benzenamine. There are several older determinations he enthalpy of combustion of benzenamine. They are se by Petit (1889-4), by Stohmann, (1890-2), by Thom- (1905-2), by Lemoult (1907-116), and by Swarts (1919- . An unpublished value determined by Huffman was listed by Anderson and Gilbert (1942-5).

The measurements of Anderson and Gilbert (1942-5), Cole and Gilbert (1951-259), and Hatton *et al.* (1962-3) on high-purity samples at 298.15 K agree. The value determined by Hatton *et al.* (1962-3) was selected.

2-Methylbenzenamine. Petit (1889-4) determined the enthalpy of combustion of 2-methylbenzenamine in the liquid state at 298.15 K. The purity of the sample was stated to be above 99%. Owing to questions concerning the accuracy of these measurements, we deemed that estimated values would be more reliable. The enthalpy of combustion was estimated in the ideal gas state at 298.15 K using the enthalpies of formation of benzenamine, methylbenzene, and 1,2-dimethylbenzene as shown below:

$$\begin{aligned}\Delta_f H^\circ&(\text{2-methylbenzenamine})\\ &= \Delta_f H^\circ(\text{benzenamine}) + \Delta_f H^\circ(\text{1,2-dimethylbenzene})\\ &\quad - \Delta_f H^\circ(\text{methylbenzene}).\end{aligned}$$

This enthalpy of combustion was converted to a value for a liquid. Petit's value was 0.5 kJ mol^{-1} more negative than our selected value. This agreement is probably fortuitous in

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

Compound	phase	$\Delta_f H^\circ/\mathrm{kJ \cdot mol^{-1}}$[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
Methylbenzene	g	50.17 ± 0.42	TRC tables
1,2-Dimethylbenzene	g	19.08 ± 1.08	TRC tables
1,3-Dimethylbenzene	g	17.32 ± 0.75	TRC tables
1,4-Dimethylbenzene	g	18.03 ± 1.00	TRC tables

[a] Uncertainties are two standard errors, see section 1.6.

view of his poor value for benzenamine.

3-Methylbenzenamine. Petit (1889-4) determined the enthalpy of combustion of 3-methylbenzenamine in the liquid state at 298.15 K. The purity of the sample was stated to be above 99%. We estimated its enthalpy of formation in the ideal gas state at 298.15 K using the enthalpies of formation of benzenamine, methylbenzene, and 1,2-dimethylbenzene in a manner similar to that used for 2-methylbenzene. Our estimated value is 7.3 kJ mol^{-1} less negative than Petit's result.

4-Methylbenzenamine. Petit (1889-4) determined the enthalpy of combustion of 3-methylbenzenamine in the solid state at 298.15 K. The purity of the sample was stated to be above 99%. We estimated its enthalpy of formation in the ideal gas state at 298.15 K using the enthalpies of formation of benzenamine, methylbenzene, and 1,4-dimethylbenzene in a manner similar to that used for 2-methylbenzene. Our estimated value is 6.3 kJ mol^{-1} more negative than Petit's result.

3.7. Condensed Phase Calorimetric Properties

The available heat capacity and phase transition data for the condensed phases, along with estimated uncertainties, are listed in Table 22. Evaluation of thermodynamic properties of the substances in the condensed phases, i.e., crystals and liquid, required low-temperature heat-capacity measurements (C_{sat}) in each condensed phase and temperatures and enthalpies of phase transitions (T_{tr} and $\Delta_{\mathrm{tr}}H$). Because the results for the solid phase were dependent upon thermal histories, sets of data were chosen to best represent the measurements on the equilibrium forms of the crystals. Weighted combinations of the liquid phase data were used in smoothing and integrating the heat capacity data. The integrations were performed with a spline function method which used six points at a time in least-squares fits to cubic functions with the constraints that the contiguous cubic functions have continuity in value, slope, and curvature at their point of junction. The results were extrapolated to 0 K with fits of the data between 10 and 25 K to the Debye heat capacity function (1912-160). Corrections for heterophase premelting were made to the data prior to making the integrations. Where heat capacity and related enthalpy of transition data in the condensed phase did not extend to temperatures low enough to apply the third law of thermodynamics, the limited data were evaluated without attempts to derive related thermodynamic properties by integration. The calculated results are presented as C_{sat}/R, $\Delta_0^T S/R$, $-\Delta_0^T G/R$, and $\Delta_0^T H/RT$. The data selections are discussed below.

Methanamine. The low-temperature heat capacity C_{sat} for crystal (12.71 to 176.91 K) and liquid (186.61 to 259.28 K) methanamine were measured by Aston *et al.* (1937-248). Aston and Eidinoff (1939-396) used a newly constructed adiabatic calorimeter to redetermine the heat capacity of the liquid over the temperature range 185 to 260 K. Their values, reported graphically, are in good agreement with the previous ones. The C_{sat}, T_m, and $\Delta_{\mathrm{tr}}H$ values reported by Aston *et al.* (1937-248) were adopted for evaluation of the thermodynamic properties in the condensed phases. The heat capacities were recomputed on IPTS-68 and integrated by procedures described in the first paragraph of this section (3.7). Their data from series III, series IV, series VI at 259.3 K, series VII, series XIII, series XIV up to 102.6 K, and series XVIII were used in determining smoothed heat capacities. They were extended to 298.15 K [above the highest measurement temperature of 260.5 K by Aston *et al.* (1939-396)] with a graphical extrapolation. The data from series I at 101.2 K and series XIV at 102.6 and 106.7 K were used to determine the enthalpy and entropy of transition at 101.469 K. The entropy of transition, 0.160 R, is 0.045 R higher than the value reported by Aston *et al.* (1939-396) owing to slightly different methods of subtracting the background heat capacity. The enthalpy of fusion

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

	Heat Capacity					Phase Transition				Author(s)	Ref.
ph.	$\frac{\text{Range}}{\text{K}}$	$\frac{\sigma(T)^a}{K}$	$\frac{\sigma_c(C_{sat})^a}{R}$	$\sigma_f(C_{sat})^a$	Pts.	Trans.	$\frac{T}{K}$	$\frac{\Delta_{tr}H}{J \cdot mol^{-1}}$	$\frac{\sigma(\Delta_{tr}H)^a}{J \cdot mol^{-1}}$		
Methanamine											
cII	12.71-101.20	0.05	0.025	0.005[c]	59	cII⇌ cI	101.469	134.14	10	Aston *et al.*	1937-248
cI	101.83-176.91	0.01	0	0.01[c]	44	cI⇌ *l*	179.708	6133.6	42		
l	186.61-259.28	0.01	0	0.01	25		–	–	–		
l	185.0-260.0	0.01	0	0.01	–[b]		–	–	–	Aston and Eidinoff	1939-396
Ethanamine											
	–	–	–	–	–	*c* ⇌ *l*	192.65	–	–	Timmermans	1913-137
	–	–	–	–	–	*c* ⇌ *l*	192.15	–	–	Pohland and Mehl	1933-369
1-Propanamine											
l	298.15	–	–	0.001	1		–	–	–	Smith and Good	1967-60
l	298.15	–	–	0.005	1		–	–	–	Konicek and Wadsö	1971-11
c	10-188.36	0.01	0.01	0.01[c]	19	*c* ⇌ *l*	188.36	10625	50	Vasil′ev *et al.*	1971-154
l	188.36-300	0.01	0	0.01	15		–	–	–		
c	11.65-181.81	0.002	0.014	0.005[c]	44	*c* ⇌ *l*	188.389	10975	4	Finke *et al.*	1972-140
l	189.96-334.56	0.002	0	0.001	19		–	–	–		
2-Propanamine											
l	313.15-343.15	0.003	0	0.004	4		–	–	–	Hough *et al.*	1950-523
l	298.15	–	–	0.001	1		–	–	–	Smith and Good	1967-60
l	298.15	–	–	0.005	1		–	–	–	Konick and Wadsö	1971-11
c	11.56-172.50	0.002	0.023	0.005[c]	45	*c* ⇌ *l*	178.011	7326.3	1	Finke *et al.*	1972-140
l	181.48-318.16	0.002	0	0.001	18		–	–	–		

[a] See section 1.6.

[b] Data reported graphically.

[c] Values for solid within 20 K of phase transition temperature is three times as large.

TABLE 22. Continued.

	Heat Capacity					Phase Transition					
ph.	$\frac{\text{Range}}{\text{K}}$	$\frac{\sigma(T)^a}{\text{K}}$	$\frac{\sigma_c(C_{\text{sat}})^a}{R}$	$\sigma_f(C_{\text{sat}})^a$	Pts.	Trans.	$\frac{T}{\text{K}}$	$\frac{\Delta_{\text{tr}}H}{\text{J}\cdot\text{mol}^{-1}}$	$\frac{\sigma(\Delta_{\text{tr}}H)^a}{\text{J}\cdot\text{mol}^{-1}}$	Author(s)	Ref.
						Benzenamine					
l	290-465	0.01	0	0.05	4		–	–	–	von Reis	1881-5
l	293.15-449.15	–	0	0.05	1		–	–	–	Louguinine	1902-9
l	293.15	–	0	0.02	1		–	–	–	Timofeev	1905-94
l	291.15	–	0	0.01	1		–	–	–	Hartung	1915-94
l	291.15-298.15	0.02	0	0.01	3		–	–	–	Hartung	1916-232
l	274.23-332.02	0.01	0	0.01	12		–	–	–	Lang	1928-196
l	303.15-412.75	0.01	0	0.04	22		–	–	–	Blacet *et al.*	1931-211
l	293.23-319.97	0.03	0	0.01	6		–	–	–	Ferguson and Miller	1933-387
c	93.50-236.30	0.15	0.06	0.01	12	$c \rightleftharpoons l$	266.8	10556	84	Parks *et al.*	1933-94
l	275.70-298.20	0.15	0	0.01	3						
l	288	–	0	0.01	1		–	–	–	Radulescu and Jula	1934-351
l	298.15-351.15	0.01	0	0.005	3		–	–	–	Ellyett	1937-435
	–	–	–	–	–	$c \rightleftharpoons l$	267.3	10920	200	Ziegler and Andrews	1942-126
l	323.15-453.15	0.003	0	0.006	10					Hough *et al.*	1950-523
l	293	–	–	–	1		–	–	–	Crützen *et al.*	1957-486
c	13.49-257.83	0.005	0.02	0.002[b]	94	$c \rightleftharpoons l$	267.13	10540	5	Hatton *et al.*	1962-3
l	270.22-313.06	0.005	0	0.005	17		–	–	–		
l	298-318	–	–	–	–		–	–	–	Deshpande and Bhatagadde	1971-17
l	298.15	–	0	0.005	1					Nichols and Wadsö	1975-49
c	190-260	–	–	–	–[b]	$c \rightleftharpoons l$	267	–		Lesbats and Lichanot	1987-147
l	270-310	–	–	–	–[b]		–	–	–		

[a] See section 1.6.

[b] Data reported graphically.

[c] Values for solid within 20 K of phase transition temperature is three times as large.

TABLE 22. Continued.

	Heat Capacity					Phase Transition					
ph.	$\frac{\text{Range}}{\text{K}}$	$\frac{\sigma(T)^a}{\text{K}}$	$\frac{\sigma_c(C_{\text{sat}})^a}{R}$	$\sigma_f(C_{\text{sat}})^a$	Pts.	Trans.	$\frac{T}{\text{K}}$	$\frac{\Delta_{\text{tr}}H}{\text{J}\cdot\text{mol}^{-1}}$	$\frac{\sigma(\Delta_{\text{tr}}H)^a}{\text{J}\cdot\text{mol}^{-1}}$	Author(s)	Ref.
2-Methylbenzenamine											
l	294-485	0.1	0	0.1	4		–	–	–	von Reis	1881-5
l	293.15-469.15	–	0	0.05	1		–	–	–	Louguinine	1902-9
l	302.4-302.7	–	0	0.005	1		–	–	–	Kolossowsky and Udowenko	1934-365
l	288	–	0	0.02	1		–	–	–	Radulescu and Jula	1934-351
3-Methylbenzenamine											
l	302.4-302.9	–	0	0.005	1		–	–	–	Kolossowsky and Udowenko	1934-365
4-Methylbenzenamine											
l	293	–	–	0.02	1		–	–	–	Campbell and Campbell	1940-332
	–	–	–	–	–	$c \rightleftharpoons l$	316.85	18912	126	Rastogi *et al.*	1963-367

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[a] See section 1.6.

reported by Aston *et al.* (1939-396) was adopted in these calculations. The results are listed in Table 12.

The recalculated value of the entropy of the liquid at 298.15 K, 35.952 J K^{-1} mol^{-1}, is slightly higher than the value reported by Aston *et al.* (1937-248), 35.90 J K^{-1} mol^{-1}.

Ethanamine. No low-temperature thermal measurements have been reported. The only property data reported were $T_m = -80.5$ °C (1913-137) and -81 °C (1933-369); and $C_p(l, 298.15\ K) = 130$ J K^{-1} mol^{-1} (1958-350).

1-Propanamine. The heat capacity of liquid 1-propanamine at 298.15 K was reported by Smith and Good (1967-60) [preliminary value from (1972-140)] and Konicek and Wadsö (1971-11). Using an adiabatic calorimeter, Vasil'ev *et al.* (1971-154) determined the heat capacity over the temperature range 60 to 300 K. They reported the enthalpy of fusion as 10625 J mol^{-1} and the triple-point temperature as 188.36 K. The thermodynamic functions were calculated from 10 to 300 K.

Finke *et al.* (1972-140) determined the low-temperature calorimetric quantities for 1-propanamine from 12 K to near the normal boiling temperature. Values of C_{sat}, T_m, and $\Delta_{tl}H$ were measured by adiabatic calorimetry. Using integration procedures identical to those described in the preface to this section, they calculated the thermodynamic function for the crystal and liquid states. Their property values determined on IPTS-48 with the 1960 revision (1961-165) were corrected to those based on IPTS-68 and then were converted to dimensionless quantities for this work. They are presented in Table 12. The reported values of C_{sat} and S at 298.15 K (in J K^{-1} mol^{-1}) are compared with those adopted in this work as follows: 162.51, 227.44 (1972-140); 166.4, 228.2 (1971-154); 160,—(1971-11); 162.3,—(1967-60); and 162.54, 227.43 (this work).

2-Propanamine. Hough *et al.* (1950-523) determined the isobaric heat capacities (C_p) of this compound in the temperatures range of 40 to 70 °C (313-343 K). The heat capacity at 298.15 K was reported by Smith and Good (1967-60) [preliminary value from (1972-140)] and by Konicek and Wadsö (1971-11), respectively. Finke *et al.* (1972-140) made low-temperature thermal measurements for 2-propanamine from 12 to 350 K, using adiabatic calorimetry. From these data they evaluated the thermodynamic quantities for this substance in the crystal and liquid states. Their values were adopted after making temperature scale corrections and converting to dimensionless units. Table 12 lists the results. A comparison of the values of heat capacity and entropy at 298.15 between the literature values and those adopted in this work is given below (in J K^{-1} mol^{-1}): 163.85, 218.32 (1972-140); 164, — (1971-11); 165.3, — (1967-60); 164.0, — (1950-523); and 163.88, 218.31 (this work).

Benzenamine. Heat capacities of benzenamine have been measured by many investigators: von Reis, 290 to 465 K (1881-5); Louguinine, 293.15 to 449.15 K (1902-9); Lang, 278.15 to 333.15 K (1928-196); Ferguson and Miller, 293 to 323 K (1933-387); Parks and Huffman, 94 to 298 K (1933-94); Radulescu and Jula, 288 K (1934-351); Hough *et al.*, 323 to 453 K (1950-523); Crutzen *et al.*, 293 K (1957-486); Hatton *et al.*, 13.49 to 313.06 K (1962-3); Deshpande and Bhatgadde, 298 to 318 K (1971-17); Nichols and Wadsö, 298.15 K (1975-49); and Lesbats and Lichanot, 200 to 310 K (1987-147). Lesbats and Lichanot reported their results at temperatures other than 298.15 K in graphical form only. Lesbats and Lichanot (1987-38) calculated the constant volume heat capacity of solid benzenamine from 203 to 263 K by adding Einstein functions associated with the internal modes of vibration to the Debye contributions for the crystal vibrations. We selected the data reported by Hatton *et al.* (1962-3) and Hough *et al.* (1950-523) for evaluation of the thermodynamic properties of benzenamine in the condensed phases.

The C_p data of Hough *et al.* (1950-523) were reconverted to C_{sat} with the vapor pressure equation and density equation of this report with the assumption that the coefficient of thermal expansion along the liquid saturation line was not significantly different than the coefficient of thermal expansion at constant pressure. The enthalpy of fusion of Hatton *et al.* (1962-3) was adopted.

The measurements were corrected to those based on the IPTS-68 in the evaluation procedures described above. The value of C_{sat} (l, 298.15 K) obtained was 191.91 J K^{-1} mol^{-1}. The values reported in the literature for the same conditions were (in J K^{-1} mol^{-1}): 192.5 (1881-5); 193.38 (1928-196); 190.92 (1933-94); 178.8 (1933-387); 191.05 (1962-3); 193.7 (1971-17); and 194.1 (1987-147). Our entropy at 298.15 K for benzenamine(l) is compared with the reported values as follows (in J K^{-1} mol^{-1}): 191.6 (1933-94), 191.30 (1962-3), and 191.06 (this work). The calculated results are listed in Table 12.

2-Methylbenzenamine. No low-temperature thermal measurements have been reported in the literature. The heat capacity of 2-methylbenzenamine(l) at 288 K (1934-351) and 302.5 K (1934-150, 1934-365) was determined to be 201.7 and 209.6 J K^{-1} mol^{-1}, respectively.

3-Methylbenzenamine. Low-temperature data were not available for evaluation of the thermodynamic properties of 3-methylbenzenamine in the condensed phases. The heat capacity of this compound at 302.7 K was reported as 216.9 J K^{-1} mol^{-1} by Kolosovskii and Udovenko (1934-150, 1934-365).

4-Methylbenzenamine. No low-temperature thermal measurements for this compound were reported in the literature. The heat capacity at 293 K was determined as 124.3 J K^{-1} mol^{-1} (1940-332) and tabulated as 178.9 J K^{-1} mol^{-1} (1965-314). Both of these values seem low when compared with the values for the other two isomers. Temperature extrapolation of other data (1884-48, 1895-59) also give discordant values.

3.8. Ideal Gas Thermodynamic Properties

The statistical mechanical methods used for calculating of the ideal gas thermodynamic properties in the temperature range 0 to 1500 K at 1 bar are similar to those discussed in a previous article (1986-87), where several textbooks and pertinent review articles on statistical mechanics are cited. The molecular symmetry classifications used here follow those of Wilson, Decius, and Cross (1955-691) and are cogently discussed by Cotton (1963-378).

Evaluations of translational, molecular rotational, and vibrational contributions to the thermodynamic properties of each compound were based on a rigid-rotor and harmonic-oscillator molecular 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 -NH$_2$ and -CH$_3$ groups, and in some cases, those from inversion about the nitrogen atom were evaluated separately. Good general discussions concerning 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

$$V_r(\theta)=\frac{1}{2}V_n(1-\cos n\theta), \tag{11}$$

where $n=2$ for the -NH$_2$ rotation and $n=3$ for the -CH$_3$ rotation, and θ is the angle of internal rotation. For the -CH$_3$ rotation in CH$_3$NH$_2$ the potential function

$$V_r(\theta)=\frac{1}{2}V_3(1-\cos 3\theta)+\frac{1}{2}V_6(1-\cos 6\theta)$$

was employed.

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 one was unavailable, it was calculated from the reduced moment of inertia (I_r) of the rotating group, from

$$F=h/8\pi^2cI_r, \tag{12}$$

where the value of I_r was calculated from molecular structural parameters. These parameters were either taken from experimental values obtained from other spectroscopic data or estimated by comparison with those for the other 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 with procedures developed by Lanne (1970-13) for the following double-minimum-potential function

$$V_w=A_d(z^4+B_dz^2), \tag{13}$$

where z is the relative motion displacement coordinate. Some of the constants for the potential function were available in the literature. For methanamine they were redetermined by a least-squares adjustment to reproduce the spectroscopically determined lowest transition frequencies. For ethanamine, 1-propanamine, and 2-propanamine, available information was not adequate for determining the constants of Eq. (13); therefore, only a simple-harmonic-wagging (vibrational) motion was considered.

When vibrational frequency assignments and structural data were available for each rotational conformer arising from rotation about bonds between secondary or tertiary carbon atoms, the conformers were treated as different species with differing reduced moments of inertia and with contributions from the amine and methyl rotations. 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 in determining the composition of the mixture. The thermodynamic properties for the equilibrium mixtures of the conformers were calculated by conventional thermodynamic equilibrium calculations.

For evaluation of $\Delta_fH°(T)$ and $\Delta_fG°(T)$, the values of $\Delta_fH°$ (298.15 K) were those of Table 11. The thermal functions for the elements C(graphite), H$_2$(g), and N$_2$(g) were values 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 data in this report.

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

Methanamine. The molecular structure of methanamine has been studied extensively by electron diffraction (1938-385, 1950-13), microwave (1947-355, 1952-615, 1953-626, 1954-678, 1954-681, 1955-612, 1956-575, 1957-497, 1957-498, 1971-167) and infrared (1964-409, 1967-261, 1968-228, 1982-85, 1987-94) spectroscopy. Takagi and Kojima (1971-167) determined the rotational, torsional, and inertial constants from microwave spectroscopy. Based upon the data of Lide (1957-497) and of Takagi and Kojima (1971-167), Harmony *et al.* (1979-155) evaluated the bond distances and angles. The ground state rotational constants from far-infrared spectroscopy by Ohashi *et al.* (1987-94) were used to calculate $I_aI_bI_c$, see Table 23. Based on the molecular structure reported by Itoh (1956-575), we calculated $I_r=1.852\times10^{-40}$ g cm^2.

Methanamine has point symmetry C_s with a symmetry number (σ) of 1. All fifteen normal vibrations are both Raman and infrared active. There are nine A′ species (ν_1–ν_9) and the remaining six are A″ species (ν_{10}–ν_{15}). There are numerous reports of infrared (1938-378, 1939-392, 1939-393, 1939-395, 1940-330, 1940-335, 1955-88) and Raman (1939-394, 1955-626, 1964-373, 1968-239, 1970-180) spectra. Gray and Lord (1957-496) used their carefully measured infrared spectra of methanamine and its deuterated derivatives to assign the fundamental vibrational frequencies. Later, Shimanouchi (1972-110) critically reviewed the reported vibrational assignments for this molecule. For evaluation of the vibrational contributions (except those for in-

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

					Internal rotation[e]							NH$_2$ inversion[f]			
Molecule	M[a]	$I_aI_bI_c$[b]	σ_{total}[c]	E$_0$	bond	I_r	$\nu(0\leftarrow1)$	m	V_m	n	V_n	A_w	B_w	$\nu(0\leftarrow1)$	V_{inv}
methanamine	31.05744	12.1387	6	—	C$_1$-N	1.852	262.8	3	8.203	6	−0.0293	46.19	12.09	780.1	20.19
ethanamine (trans)	45.08432	272.736	3	0.0	C$_1$-C$_2$	4.368	264.5	3	16.238	-	—			793[g]	
					C$_1$-N	2.706	236.7	3	8.909						
ethanamine (gauche)	45.08432	260.489	3	1.196	C$_1$-C$_2$	4.327	258.8	3	15.456	-	—			773[g]	
					C$_1$-N	2.709	218.0	3	7.737						
1-propanamine	59.11120	1788.2	3	—	C$_2$-C$_3$	4.698	252.0	3	15.807	-	—			775[g]	
					C$_1$-C$_2$	17.353	104.0	1	3.670	3	8.590				
					C$_1$-N	2.813	210.0	3	7.456						
2-propanamine (trans)	59.11120	1917.7	9	0.0	C$_1$-C$_2$	5.126	258.0	3	17.877	-	—			785[g]	
					C$_2$-C$_3$	5.126	236.0	3	15.089	-	—				
					C$_2$-N	2.946	267.0	3	11.801						
2-propanamine(gauche)	59.11120	1866.6	9	1.749	C$_1$-C$_2$	5.123	263.0	3	18.519	-	—			785[g]	
					C$_2$-C$_3$	5.123	201.0	3	11.155	-	—				
					C$_2$-N	2.947	221.0	3	8.422						
benzenamine	93.12828	22846.3	4	—	C$_1$-N	2.663	277.3	2	23.64	-	—	45.00	6.80	40.08	6.22
2-methylbenzenamine	107.15516	62963.0	6	—	C$_2$-C$_6$	5.259	99.70	3	6.230	-	—	45.85	6.83	40.05	6.40
					C$_1$-N	2.316	296.5	2	23.64						
3-methylbenzenamine	107.15516	74531.0	6	—	C$_3$-C$_6$	5.253	5.329	-	—	-	—	45.38	6.80	40.40	6.28
					C$_1$-N	2.314	296.6	2	23.64						
4-methylbenzenamine	107.15516	63970.0	12	—	C$_4$-C$_6$	5.175	5.410	-	—	-	—	45.13	7.20	30.93	7.00
					C$_1$-N	2.300	297.4	2	23.64						

[a] M = molar mass, g·mol^{-1}.

[b] $I_aI_bI_c$ = product of the three principal moments of inertia, 10^{-117}g^3 · cm^6.

[c] σ_{total} =total symmetry number.

[d] E$_0$ = energy of lowest state relative to ground state, kJ·mol^{-1};

[e] Bond is the axis of relative rotation and the subscripts denote carbon numbers; I_r = reduced moment of inertia, 10^{-40} g·cm^2;
ν $(0\leftarrow1)$ = torsional wavenumber, cm^{-1}; V_m and V_n in kJ·mol^{-1} for the internal rotation potential function: $V_r = \frac{1}{2}[V_m(1-\cos m\theta) + V_n(1-\cos n\theta)]$ with θ = angle of internal rotation.

[f] A_w and B_w = coefficients in -NH$_2$ inversion potential function, Eq. 13; V_{inv} = inversion potential barrier height, kJ·mol^{-1}.

[g] Treated as a wagging vibration, see Table 24.

TABLE 24. Fundamental vibrational wavenumbers.

Compound	Fundamental vibrational wavenumber (cm^{-1})
Methanamine	3427, 3361, 2985, 2961, 2820, 1623, 1476, 1473, 1430, 1335, 1130, 1044, 945
Ethanamine (trans)	3754, 3656, 3400, 3307, 3270, 3243, 3240, 1600, 1524, 1510, 1459.1, 1433, 1408, 1349.8, 1177, 1118.7, 1090, 1055, 881.9, 793, 789.1, 387
Ethanamine (gauche)	3741, 3641, 3341, 3302, 3241, 3176, 3075, 1621.7, 1487.3, 1464.8, 1455.3, 1397.2, 1377.9, 1292.8, 1238.2, 1116.8, 1085.5, 1015.6, 892.5, 816.2, 773.1, 403
1-Propanamine	3347, 3244, 2972, 2954, 2954, 2943, 2902, 2892, 2885, 1626, 1475, 1466, 1460, 1437, 1400, 1354, 1316, 1302, 1275, 1220, 1142, 1087, 1077, 1023, 887, 878, 775, 722, 454, 323
2-Propanamine (trans)	3411, 3342, 2968, 2965, 2950, 2945, 2932, 2878, 2860, 1618, 1460, 1469, 1469, 1449, 1375, 1360, 1343, 1245, 1240, 1170, 1130, 1029, 976, 942, 919, 819, 785, 472, 404, 369
2-Propanamine (gauche)	3393, 3328, 2968, 2965, 2950, 2945, 2918, 2878, 2860, 1618, 1460, 1469, 1469, 1449, 1375, 1360, 1343, 1245, 1240, 1170, 1130, 1029, 976, 942, 919, 826, 781, 459, 407, 369
Benzenamine	3500, 3418, 3088, 3072, 3053, 3037, 3025, 1618, 1603, 1590, 1503, 1468, 1324, 1276, 1190, 1173, 1152, 1090, 1050, 1028, 990, 968, 957, 874, 825, 812, 745, 690, 619, 526, 500, 415, 390, 233
2-Methylbenzenamine	3470, 3430, 3080, 3060, 3060, 3025, 2940, 2940, 2920, 1622, 1622, 1585, 1470, 1445, 1445, 1445, 1382, 1301, 1280, 1260, 1218, 1200, 1155, 1062, 1033, 1033, 985, 985, 927, 845, 845, 750, 750, 713, 651.3, 535, 515, 435.5, 435.4, 398.5, 263.2, 251.6
3-Methylbenzenamine	3480, 3430, 3065, 3055, 3055, 3040, 2940, 2940, 2920, 1625, 1610, 1585, 1498, 1470, 1470, 1470, 1375, 1312, 1295, 1295, 1171, 1160, 1143, 1075, 1030, 1030, 999, 960, 930, 930, 875, 780, 690, 690, 664.7, 545, 520, 475, 431.3, 395.7, 282.2, 275.1
4-Methylbenzenamine	3480, 3440, 3060, 3060, 3045, 3045, 2940, 2940, 2920, 1645, 1627, 1585, 1515, 1445, 1445, 1445, 1380, 1325, 1270, 1270, 1177, 1177, 1120, 1085, 1045, 1045, 980, 950, 925, 845, 845, 815, 740, 651.3, 651.3, 651.3, 499.4, 434, 410, 382.6, 273, 273

nal rotation and inversion), the frequencies (ν_1–ν_8, ν_{10}, d ν_{11}) recommended by Shimanouchi (1972-110) and se determined by Woltt *et al.* (ν_{12}) (1964-496) and Hada *et al.* (ν_{13} and ν_{14}) (1982-82) were used, see Table 24.

The interactions among the vibration, inversion, internal rotation, and molecular rotation in methylamine has been the subject of spectral investigations which include microwave (1954-679, 1954-681, 1955-612, 1956-575, 1957-

TABLE 25. Potential barriers to internal rotation in methanamine.

V_3	V_6	Author(s)	Ref.
kJ· mol^{-1}			
11.96		Aston *et al.*	1937-248
6.36		Aston and Doty	1940-325
8.85		Lassettre and Dean	1949-506
7.56		Lide	1954-678
8.14		Shimoda *et al.*	1954-681
7.95		Aston and Gittler	1955-602
8.27		Itoh	1956-575
8.19		Lide	1957-497
8.27		Nishikawa	1957-503
8.25		Gray and Lord	1957-496
8.190	−0.038	Tsubor *et al.*	1966-408
8.27		Tsubor *et al.*	1967-261
8.173	−0.024	Tamagake *et al.*	1968-228
8.173	−0.024	Tsubor *et al.*	1968-229
8.203[a]	−0.130[a]	Takagi and Kojima	1971-167
8.180	−0.002	Belorgeot *et al.*	1982-85

[a] Adopted in this work.

497, 1957-498, 1957-503, 1971-167, 1974-202, 1974-203), infrared (1957-496, 1964-409, 1967-261, 1968-228, 1969-192, 1974-199, 1982-82, 1982-85, 1984-175) and ultraviolet (1969-193, 1982-134) studies.

Mathematical models for the internal rotation and inversion in methanamine, using microwave spectral data, have been developed by Itoh (1956-575), Kivelson and Lide (1957-497), and Nishikawa (1957-503). Table 25 summarizes the potential barriers to internal rotation in CH_3NH_2 reported in the literature. The reported torsional wavenumbers of the -CH_3 top in CH_3NH_2 are summarized in Table 26.

TABLE 26. Torsional wavenumber in methanamine.

Torsional Wavenumber/cm^{-1}	Method of Determination	Ref.
270	Infrared spectroscopy	1940-325
269.5	Far infrared spectroscopy	1954-693
264	Theoretical calculation	1957-496
263.9	Infrared spectroscopy	1968-228
270, 271	Theoretical calculation	1968-235
268	Selected value	1972-110
269.8, 270.2	Theoretical calculation	1978-98
262.8	Calculated value	this work

TABLE 27. Inversion wavenumber and potential barrier in methanamine

Inversion Wavenumber cm^{-1}	Inversion potential barrier $\mathrm{kJ \cdot mol}^{-1}$	Method of Determination	Ref.
780		Infrared spectroscopy	1957-496
780.1		Infrared spectroscopy	1964-409
780		Raman spectroscopy	1964-496
	20.19 ± 0.12	Theoretical calculation	1967-261
776.16, 783.83	21.82	Theoretical calculation	1978-98
	19.09	Theoretical calculation	1978-100
	24.89[a]	Theoretical calculation	1987-94
780.1	20.19	Selected and calculated	this work

[a] Quoted value.

Takagi and Kojima (1971-167) used their microwave spectra of methanamine and its deuterated species to determine the molecular constants including the V_3 and V_6 terms for the -CH_3 internal rotation and potential function $V_r(\theta) = \frac{1}{2}[V_3(1-\cos 3\theta) + V_6(1-\cos 6\theta)]$. This potential function was adopted together with the calculated reduced moment of inertia (I_r) listed in Table 23. Draeger *et al.* (1983-12) employed the potential function $V_r = \frac{1}{2}V_3(1-\sin 3\theta)$, where $V_3 = 8267$ kJ mol^{-1}, for calculating the restricted rotor contributions.

Shimoda *et al.* (1954-681) calculated the version splittings for CH_3NH_2. Tsuboi *et al.* (1964-409, 1967-261) used the fine structure of their 780.1 cm^{-1} infrared band to calculate the potential barrier height for methanamine inversion as (1688 ± 10) cm^{-1} [(20.19 ± 0.12) kJ mol^{-1}]. Kreglewski (1978-98) developed a Hamiltonian for vibration, inversion, internal rotation, and rotation of CH_3NH_2 and used the data of Tsuboi *et al.* (1967-261) to calculate the potential constants and energy levels for inversion and internal rotation. Diallo *et al.* (1985-335) used a spectrometer with improved resolving power to obtain new details in the central region of the amino wagging band of CH_3NH_2 at 780 cm^{-1}. The reported inversion wavenumbers and potential barriers are listed in Table 27.

Draeger *et al.* (1983-12) employed a variation of Eq. (13) to calculate the inversion energy levels for evaluating the inversion contributions to the thermodynamic properties of CH_3NH_2. The potential function was derived from the observed transitions and barrier heights of the inversion mode. However, we could not reproduce the transition frequencies with his parameters. His parameters gave $\nu_{\mathrm{inv}}(1_v \leftarrow 0_v) = 825.7$ cm^{-1} which is not consistent with the accepted value of 780 cm^{-1}. We redetermined the constants in Eq. (13) to reproduce the experimentally observed (1964-409) value $\nu_{\mathrm{inv}} = 780.1$ cm^{-1}. Thirty-six generated energy levels (0 to 24100 cm^{-1}) were employed for calculating the inversion contributions to the thermodynamic properties of CH_3NH_2.

Tables 23 and 24 summarize the molecular constants used for calculation of the ideal gas thermodynamic properties of methanamine. The results are listed in Table 13.

The calculated values are compared with experimental values where possible. Felsing and Jessen (1933-392) used a constant-flow calorimeter to determine the vapor heat capacities (C_p) of methanamine at 273.15, 298.15, and 323.15 K as 49.02, 54.02, and 57.70 J K^{-1} mol^{-1}, respectively. Their measurement imprecision was about 2%. Aston and Doty (1940-325) subsequently used the Berthelot equation of state to convert these values to ideal gas heat capacities (C_p°) as 47.91, 53.18, and 57.03 J K^{-1} mol^{-1}. Evidently, the C_p° values quoted by Draeger *et al.* (1983-12) for CH_3NH_2 are for the real gas (1933-392) rather than for the ideal gas. We assumed the C_p measurements of Felsing and Jessen (1933-392) were at atmospheric pressure and used the second virial coefficients of this work to derive values of C_p° at 273.15, 298.15, and 323.15 K as 46.78, 52.43, and 56.53 J K^{-1} mol^{-1}, respectively. Our values from spectroscopic data for the same respective temperatures are 47.81, 50.05, and 52.43 J K^{-1} mol^{-1}. It is very unlikely that the computed values can be in error by as much as the differences from the experimental values. Stull and Sinke (1969-147) speculated that the experimental values may be too high because corrections for hydrogen bonding could not be adequately made. Draeger *et al.* reproduced these experimental values much more closely in their statistical mechanical calculations; however, they used a single term, $n = 3$, in Eq. (11) for the methyl rotation. We could not reproduce the derivation of their Eq. (12) from their Eqs. (8) and (11) for internal rotation, and we had problems with their inversion potential as discussed above.

There are several reports of the ideal gas thermodynamic properties of methanamine calculated from statistical mechanics. The values of C_p° and S° ($p = 1$ atm) at 298.15 K were reported as (in J K^{-1} mol^{-1}): 51.71, 241.63 (1954-117); 49.25, 242.84 (1961-264); 49.83, 242.38 (1965-395); 50.08, 242.59 (1969-147); and 53.01, 243.38 (1983-12), respectively. The values obtained in this work are 50.05 and 242.9 (1 atm) J K^{-1} mol^{-1}, respectively. The entropy at 298.15 K derived in this work from the third law (241.77 ± 1.26) J K^{-1} mol^{-1} agrees within the accuracy of the two values.

Aston and Gittler (1955-602) (1955-621) derived a value of (243.6 ± 1.3) J K^{-1} mol^{-1} from chemical equilibrium studies of methanamine with hydrogen chloride at temperatures from 276.15 to 313.15 K. They determined the activity of the hydrogen chloride from emf measurements involving HCl with mercury and with silver.

Ethanamine. Rotation of the -NH_2 group about the C–N axis of ethanamine produces one trans and two gauche conformers where the relative conformations are for the unshared pair of *p* electrons on the nitrogen atom with respect to the terminal methyl group. Wolff and Ludwig (1964-496) noted the differences in the Raman spectra of the trans and gauche isomers. Molecular orbital calculations by Radom *et al.* (1972-30) predicted that the gauche conformer was more stable than the trans by (182 cm^{-1} or 2218 J mol^{-1}). Manocha *et al.* (1974-186) analyzed the far-infrared spectra of gaseous $CH_3CH_2ND_2$ and $CH_3CD_3ND_2$ to predict that the gauche form is more stable than the trans by 104 cm^{-1} (1243 J mol^{-1}). Contrary to the foregoing investigations, others have indicated that the trans isomer is more stable. From examination of the infrared absorption spectra of eight isotopic ethanamine molecules, Tsuboi *et al.* (1975-118) assigned the torsional oscillational frequencies of the methyl and amino groups for the trans and gauche isomers. They made the energy level calculations on the basis of a coupled two-top system and reported that the trans form was more stable by 230 cm^{-1} (2753 J mol^{-1}). Durig and Li (1975-168) used their observed Raman spectra of gaseous $CH_3CH_2NH_2$ and $CH_3CH_2ND_2$ to determine that the trans conformer is more stable by 207 cm^{-1} (2477 J mol^{-1}). Hamada *et al.* (1983-92) used the difference in intensity of the -NH_2 vibrations observed in matrix isolation spectroscopy with varied nozzle temperatures to determine that the trans conformer was more stable by (100 ± 10) cm^{-1} $(1197 \pm 120$ J $mol^{-1})$. Fischer and Botskor (1984-145) compared the relative intensities from the microwave spectra for several temperatures to determine that the trans conformer is more stable by (110 ± 50) cm^{-1}. We adopted the value of Hamada *et al.* (1983-92) in this work.

Both *trans*- and *gauche*-ethanamine were studied by Fischer and Botskor (1982-83, 1984-145) with microwave spectroscopy to determine the rotational constants. Their values were adopted to obtain the product of the three principal of inertia ($I_aI_bI_c$) and the reduced moments of inertia (I_r), listed in Table 23. Some of the reported molecular structural parameters of *trans*- and *gauche*-ethanamine (1971-156, 1974-186, 1975-188, 1975-168, 1982-83) were estimated.

Investigations of the vibrational spectra of ethanamine include: Raman spectra by Wolff and Ludwig (1964-496, 1972-198), Durig and Li (1975-168) and Manocha and Fateley (1976-119); and far-infrared spectra by Tsuboi *et al.* (1968-229) and Manocha *et al.* (1974-186). The infrared absorption spectra of the two rotamers and eight deuterated species were examined by Scott (1971-155) and Tsuboi *et al.* (1975-118). Recently, Hamada *et al.* (1983-92) studied the infrared and Raman spectra of $CH_3CH_2NH_2$ and five deuterated species. They assigned a complete set of normal vibrational wavenumbers for the gaseous trans and gauche conformers. Their vibrational assignments for each conformer were used (except for the torsional wavenumbers for the -CH_3 and -NH_2 rotations, see Table 24).

From the internal rotation constants (F) and torsional wavenumbers (1975-168, 1976-119) for -CH_3 and -NH_2 rotations, the respective barrier heights (V_3 and V_2) were calculated. Ninety-six energy levels (0 to 15300 cm^{-1}) for the -CH_3 rotation and seventy-eight energy levels (0 to 16000 cm^{-1}) for the -NH_2 rotor were used in calculating the contributions to thermodynamic properties.

The results for the two conformers were combined with their enthalpy of isomerization to calculate the thermodynamic properties of the equilibrium mixtures. The results are presented in Table 13.

Experimental values for ethanamine are not available for comparison with our calculations. Some statistical mechanically derived values of C_p° and S° at 298.15 K and 1 atm, are compared with our results as follows (in J K^{-1} mol^{-1}): 72.63, 284.85 (1969-147); 72.63, 284.64 (1971-156); and 71.54, 283.77 (this work). A methylene increment method (1968-224) gave 71.25 and 271.29 for C_p° and S° at 298.15 K.

1-Propanamine. 1-Propanamine has five possible conformations: *T–T*, *G–T*, *G–G'*, *T–G*, and *G–G* where the first letter (*T* or *G*) refers to the trans or gauche orientation of the C–C–C–N chain, and the second letter (*T*, G, or *G'*) refers to the trans or one of the two nonequivalent gauche orientations of the C–C–N–: chain. The symbol : is for the unshared pair of *p* electrons on the nitrogen atom. The observed spectra of this compound are too complex to interpret as arising from a single conformation (1971-155). Theoretical calculations (1980-110, 1985-281) show that the *T–G* form is the most stable and that the *G–G* form (formed from the *T-G* form by rotation of 120° about the C_1–C_2 bond) is 2.72 kJ higher in potential energy than the *T–G* conformer. These conformers define the path of minimum potential energy for rotation about the C_1–C_2 bond.

Wolff and Ludwig (1964-496, 1972-198) determined the Raman spectrum of 1-propanamine(*g*) and gave a partial vibrational assignment. Based on the observed far-infrared spectrum (1968-227), Scott (1971-155) satisfactorily showed that the observed wavenumbers cannot be uniquely assigned to his calculated normal vibrational frequencies for the five possible conformations of this compound.

The molecular structure of 1-propanamine has not been experimentally determined. Estimated molecular structural parameters (1971-155) of the *T–G* conformer were used to calculate the values of I_a, I_b, and I_c and reduced moments of inertia (I_r) for the -CH_3 and -NH_2 rotations (see Table 23).

We adopted the normal vibrational wavenumbers of the

-G conformer assigned by Scott. If observed wavenumbers ere not available, calculated values were used. The barriers o rotation, V_3 in Eq. (11), were calculated from torsional avenumbers [252 cm^{-1} for CH$_3$ and 210 cm^{-1} for -NH$_2$ 1971-155)] and the corresponding F values. Rotation bout the C_1–C_2 bond was treated as hindered with a tor- onal wavenumber of 104 cm^{-1}, and the potential function as used in the semiclassical approximation of Pitzer and winn (1942-175). Inversion was treated as a harmonic os- illator.

The internal rotational contributions to thermodynam- properties were determined from 96 and 78 internal rota- on energy levels for -CH$_3$ and -NH$_2$, respectively. We orced approximate agreement between the calculated en- opy at 298.15 K (325.44 J mol^{-1} K^{-1}) with our evaluated hird-law value $S° = (325.93 \pm 0.84)$ J mol^{-1} K^{-1} by ad- sting the skeletal torsion of T–G conformer to 106 cm^{-1}. he calculated thermodynamic properties are listed in Table 3.

The vapor heat capacity of this compound has not been easured. Previous statistical-mechanically calculated val- es of C_p° and $S°$ at 298.15 K and 1 atm compare with our alues as follows: (in J K^{-1} mol^{-1}) 91.21, 325.93 (1971- 55); and 91.17, 325.44 (this work, at 1 atm). The following stimated values of C_p° and $S°$ at 298.15 K calculated by roup additivity have been reported: 94.14, 301.08 (1968- 24); 95.77, 324.18 (1969-147).

There was some concern with assuming that the prop- rties could be reliably calculated from a single conformer nd with a torsional mode about the bond between number 1 nd 2 carbon atoms. This approximation was tested by per- orming a similar calculation for the trans isomer of butane. he fundamental torsional frequency was adjusted to fit the recisely calculated entropy with those from the more exact ethod of Chen *et al.* (1975-63) at 298.15 K and was 45 m^{-1}. It was not feasible to transfer these differences for utane to values for 1-propanamine because the barrier to otation for the latter is apparently much larger than for utane as evidenced by the difference in torsional frequen- ies required to reproduce the entropies at 298.15 K.

2-Propanamine. For 2-propanamine rotation of -NH$_2$ bout the C–N bond produces three possible staggered con- ormations. The orientation with the unshared pair of elec- ons on the N atom trans to the C–H bond is denoted as s- ans with C_s symmetry. The unshared pair of electrons ans to one of the C–C bonds results in two equivalent auche conformations with C$_1$ symmetry. We treated 2-pro- anamine as an equilibrium mixture of s-trans and gauche onformers in methods similar to the calculations for 2-eth- amine, described above.

Krueger and Jan (1970-181) investigated the infrared ectrum of (CH$_3$)$_2$CDNH$_2$ in a dilute solution with CCl$_4$ nd determined the energy difference between the two con- ormations as (0.50 ± 0.08) kJ mol^{-1}. A theoretically cal- ulated value of 2.80 kJ mol^{-1} was reported by Lathan *et al.* 1973-187). The gauche conformers are more stable than e s-trans.

From analysis of microwave spectrum of *trans*-2-pro- anamine(*g*), Mehrotra *et al.* (1977-105) determined the rotational constants and moments of inertia (I_a, I_b, I_c) which were used to obtain the values of $I_aI_bI_c$ listed in Table 23. Durig *et al.* (1979-100) studied the Raman spectra of gas, liquid, and solid, and the infrared spectra of gas and solid 2-propanamine-d_0 and -d_2. They assigned 33 vibrational wavenumbers for both s-trans and gauche conformers. Their vibrational assignments (except the two -CH$_3$ torsional wavenumbers for gauche conformer) were adopted. Their numerical values are listed in Table 24. Scott (1971-155) assigned similar vibrational wavenumbers for these two conformers from analysis of far-infrared spectra of 2-propanamine in solution and vapor states (1968-227). He interpreted the observed spectra of 2-propanamine as arising from a single conformation; gauche with C$_1$ symmetry. His torsional assignments, as listed in Table 23, for the two -CH$_3$ rotations in the gauche conformer were selected for determining V_3 in Eq. (11).

For both the gauche and s-trans conformers, estimated molecular structural parameters were used to calculate the principal moments of inertia (I_a, I_b, and I_c) and the reduced moments of inertia (I_r) for the -CH$_3$ and -NH$_2$ rotors. See Table 23 for their values.

The internal rotational contributions to thermodynamic properties for each conformer were determined from 102 and 78 internal rotation energy levels for -CH$_3$ and -NH$_2$, respectively.

The selected value $H°(\text{gauche},0\ \text{K}) - H°(\text{s-trans}, 0\ \text{K}) = 1.749$ kJ mol^{-1} (1979-100) was used with the properties calculated for the conformers to compute the thermodynamic properties of 2-propanamine which are listed in Table 13.

Vapor heat capacities of 2-propanamine are not available for comparison with our results. Calculated thermodynamic properties of 2-propanamine have been reported by Scott (1971-155) and Durig *et al.* (1979-100). Scott (1971-155) adopted his vibrational assignments for gauche conformer and the calculated principal moments of inertia based on an assumed molecular structure to evaluate the thermodynamic properties for 2-propanamine. He disregarded the presence of rotational conformers; his calculated thermodynamic property values are generally lower than either ours or those of Durig *et al.* (1979-100). Durig *et al.* (1979-100) employed a molecular model composed of s-trans and gauche conformers. For -NH$_2$ torsion, they used a potential function of the form

$$V_r = \frac{1}{2} \sum_i V_i (1 - \cos i\theta), \tag{14}$$

where $i = 1$ to 6 and the internal rotational constant of the form

$$F = F_0 + \sum_i F_i \cos i\theta, \tag{15}$$

where $i = 1$ to 4, and F is a function of the angle of internal rotation (θ) and F_0 is defined for the s-trans conformer. For -CH$_3$, a complicated internal rotational Hamiltonian was used to account for interaction of the methyl rotations. They selected a value of 1749 J mol^{-1} for the energy difference between s-trans and gauche conformers to compute the compositions of the equilibrium mixture of 2-propanamine.

The reported statistical-mechanical values of C_p° and S° at 298.15 K and 1 atm are compared with ours as follows (in J K^{-1} mol^{-1}): 95.8, 311.8 (1979-100); 94.56, 312.54 (1971-155); and 97.55, 312.24 (this work). The entropy derived from condensed phase heat capacity measurements in section 3.7, (311.6 ± 0.8) J K^{-1} mol^{-1}, adequately agrees with the value derived from spectroscopic data.

Benzenamine. Benzenamine has symmetry C_s ($\sigma = 1$). The nonplanar configuration of this molecule has been discussed by Evans (1960-296). From an investigation of the microwave spectra of $C_6H_5NH_2$ and C_6H_5NHD, Lister and Tyler (1966-402) established that $C_6H_5NH_2(g)$ has a nonplanar structure in which the -NH_2 plane (containing the nitrogen atom and its two attached hydrogens) makes an angle of 40° with the plane of the C_6H_5- group. The same result was obtained from uv studies by Brand *et al.* (1966-403). Lister *et al.* (1974-79) determined the molecular structure from microwave spectra of thirteen deuterated species of benzenamine and found that the C–H distance is (1.402 ± 0.002) Å and that the -NH_2 group adopts an out-of-plane angle of 37°29′ ± 2° with the angle HNH 113°6′ ± 2°. They also reported the values of I_a, I_b, and I_c. These values were adopted to calculate the $I_aI_bI_c$ (see Table 23). Similar moments of inertia values were reported by Hatta *et al.* (1973-164).

The infrared and Raman spectra of benzenamine have been the subject of several investigations. Williams *et al.* (1939-411) investigated the near infrared spectrum. Evans (1960-296) studied the Raman spectra (liquid phase) and infrared spectra (vapor, solution and liquid phases) of $C_6H_5NH_2$, C_6H_5NHD, and $C_6H_5ND_2$. Complete vibrational assignments for $C_6H_5NH_2$ were made. Tsuboi (1960-211) examined isotopic effects on the vibrational wavenumbers and made assignments for modes involving the -NH_2 group. Kuwae and Machida (1978-112) studied the CH out-of-plane deformation vibrations of monosubstituted benzenes. Their assignments of the vibrational wavenumbers for benzenamine agreed with those reported by Evans (1960-296). Vibrational assignments of Evans were adopted for calculating the thermodynamic properties of this compound by Draeger (1984-19) and Hussein *et al.* (1985-203). Recently, Niu *et al.* (1985-127) proposed a number of reassignments of the spectra of $C_6H_5NH_2$ and its deuterated analogs. The values reported by Niu *et al.* (1985-127), except those for -NH_2 internal rotation and inversion modes, were employed here.

Larsen *et al.* (1976-13) used far infrared spectroscopy to investigate the inversion and torsion of the -NH_2. They used the molecular structure determined by microwave spectroscopy (1974-79) with $V_r(\theta) = (1/2)\Sigma_i V_i \times (1 - \cos i\theta)$ ($i = 1$ and 2) for the potential function to calculate the wavenumbers for the inversion mode. The potential barrier 524.4 cm^{-1} used for their calculation is larger than the 454 cm^{-1} barrier found by Quack and Stockburger (1972-193), and the potential minimum at 42.17° is in agreement with the value of 42° (1972-193) but larger than the value 37.5° reported by Lister *et al.* (1974-79).

Kydd and Krueger (1977-91) observed the vapor phase infrared spectra of $C_6H_5NH_2$, C_6H_5NHD and $C_6H_5ND_2$ from 12 to 650 cm^{-1}. They assigned several inversion transitions due to $C_6H_5NH_2$, which were in excellent agreement with those proposed by Larsen *et al.* (1976-13). Kydd and Krueger (1977-91) chose a simple double-minimum potential with a gaussian barrier to describe the inversion motion. The calculated inversion transitions were in perfect agreement with the observed energy levels. The barrier height, 525.9 cm^{-1}, compares favorably with the value 524.4 cm^{-1}, reported by Larsen *et al.* (1976-13).

Based on the inversion transitions 40.8, 423.8, and 700.1 cm^{-1} observed by Kydd and Krueger (1977-91), Draeger (1984-19) derived a reduced potential function $V_w/\text{cm}^{-1} = 45.00[(r/r_o)^4 - (r/r_o)^2]$ for inversion in $C_6H_5NH_2$. This potential function was used to generate 30 inversion energy levels (0 to 19500 cm^{-1}) for evaluation of the inversion contributions to thermodynamic properties.

The torsional wavenumber of 277.3 cm^{-1} for benzenamine was determined by Larsen *et al.* (1976-13) from far-infrared spectrum. We adopted this torsional wavenumber and calculated $F = 10.512$ cm^{-1} to evaluate the internal rotation barrier height (V_2) in Eq. (11) as 23.637 kJ mol^{-1} for the -NH_2 rotation. The adopted value of I_r was based on the molecular structure determined by Lister *et al.* (1974-74) from microwave spectroscopy. We generated 72 internal rotation energy levels (0 to 14500 cm^{-1}) for evaluation of internal rotational contributions to thermodynamics properties.

The computed thermodynamic properties of benzenamine are listed in Table 13. The value of S° (298.15 K) = 317.87 J K^{-1} mol^{-1} obtained at 1 bar pressure or 317.76 J K^{-1} mol^{-1} at 1 atm is in agreement with the third law value (318.67 ± 0.84) J K^{-1} mol^{-1}. Our calculated C_p° and S° at 298.15 K and 1 atm are compared with statistical mechanically derived values as follows (in J K^{-1} mol^{-1}): 108.41, 319.16 (1962-3, 1969-147); 108.11, 318.40 (1983-12); 111.21, 319.78 (1985-203); and 107.94, 317.87 (this work).

2-Methylbenzenamine. An assumed molecular structure of 2-methylbenzenamine was used to calculate the values of $I_aI_bI_c$ and the reduced moments of inertia (I_r) for -CH_3 and -NH_2 rotors. The structural parameters of the ring were assumed to be the same as those of benzenamine (1974-79). The bond distances and angles in the -CH_3 group were the same as those in alkanes. The calculated results are given in Table 23.

Based on reported infrared spectra of 2-methylbenzenamine, Draeger (1984-19) obtained the vibrational wavenumbers of this compound which were adopted in this work (see Table 24). Partial vibrational assignments for the compound were reported by Sverdlov *et al.* (1974-117). The barrier for -CH_3 rotation, $V_3 = 6230$ J mol^{-1}, was taken from Rudolph *et al.* (1973-66), assuming the barrier for the adjacent methyl groups in 1,2-dimethylbenzene molecule is the same as that for the adjacent -CH_3 group in 2-methylbenzenamine. From the far-infrared vapor phase spectra of the 2-, 3-, and 4-methylbenzenamines, Kydd and Krueger (1980-76) observed the first three -NH_2 inversion vibration energy levels for each isomer. Draeger (1984-19) derived a reduced potential function $V_w(r/r_o) = \{a(r/r_o)^4$

$- b(r/r_o)^2\}$ where $a = 45.85$ cm^{-1} and $b = 6.83$ cm^{-1} for fitting the -NH$_2$ inversion energy levels reported by Kydd and Krueger (1980-76) for 2-methylbenzenamine. We adopted this reduced potential function to generate 24 inversion energy levels (0 to 14400 cm^{-1}) for calculation of inversion contributions to thermodynamic properties of this compound.

The contributions to thermodynamic properties due to internal rotations of -CH$_3$ and -NH$_2$ group were evaluated by using 102 and 66 internal rotation energy levels, respectively. The I_r and barrier height values employed for generating levels are presented in Table 23. The value of F was computed, and the value of V_2 for the -NH$_2$ group was taken from that of -NH$_2$ in benzenamine.

The calculated thermodynamic properties of 2-methylbenzenamine are given in Table 13. There are no experimental vapor heat capacity or third-law entropy measurements available for comparison. Our calculated values of C_p° and S° at 298.15 K and 1 atm are compared with other calculated values in the literature as follows (in J K^{-1} mol^{-1}): 133.9, 349.3 (1983-108); 134.94, 355.20 (1984-19); and 130.21, 351.05 (this work). The differences between our values and those of Draeger (1984-19) result from differing computational methods because the differences persisted when his choice of molecular constants and vibrational frequencies were used as input to our computational procedure; the differences appear to arise from internal-rotational contributions to the heat capacity. The differences from those of Kudchadkar *et al.* (1983-108) arise from differences in choices of input data.

3-Methylbenzenamine. Molecular structural parameters for 3-methylbenzenamine were estimated by procedures similar to those for 2-methylbenzenamine to calculate values of $I_aI_bI_c$ and reduced moments of inertia for the -CH$_3$ and the -NH$_2$ rotor. They are listed in Table 23.

The fundamental vibrational wavenumbers reported by Draeger (1984-19) were adopted (see Table 24). The -CH$_3$ group was assumed to rotate freely. Based on $V_2 = 23.64$ kJ mol^{-1} and $F = 12.095$ cm^{-1}, 66 -NH$_2$ internal rotation energy levels were generated for calculating the internal rotational contributions. The reduced potential function derived by Draeger (1984-19) for 3-methylbenzenamine was adopted to generate 24 inversion energy levels. The calculated inversion energy levels (40.4, 422.0, and 706.4 cm^{-1}) are in good agreement with those (40.2, 423.2, and 705.2 cm^{-1}) observed by Kydd and Krueger (1980-76).

The evaluated thermodynamic properties for 3-methylbenzenamine are listed in Table 13. There are no experimental C_p° and S° values available for comparison with our calculated results. A comparison of C_p° and S° at 298.15 K and 1 atm between other calculated values and ours are given here (in J K^{-1} mol^{-1}): 128.9, 354.3 (1983-108); 130.04, 355.69 (1984-19); and 125.47, 352.49 (this work). The differences have explanations similar to those for 3-methylbenzenamine.

4-Methylbenzenamine. The values of $I_aI_bI_c$ for 4-methylbenzenamine and of I_r and V_n for the -CH$_3$ and the -NH$_2$ groups were determined by estimation procedures similar to those for the other benzenamine methyl derivatives described above. The vibrational assignments of Draeger (1984-19) for this substance were employed for statistical calculation of vibrational contributions to thermodynamic properties. The -CH$_3$ group was assumed to be a free rotor. Sixty-six energy levels were generated for the -NH$_2$ internal rotation. Kydd and Krueger (1980-76) observed the first three -NH$_2$ vibration wavenumbers for this compound. We employed the reduced potential function derived by Draeger (1984-19) from these observed inversion energy levels to generate 24 inversion energy levels calculating -NH$_2$ inversion contributions to thermodynamic properties. The evaluated thermodynamic properties are presented in Table 13.

No experimental C_p° and S° have been reported in the literature. Our calculated C_p° and S° at 298.15 K and 1 atm are compared with other calculated values reported in the literature as follows (in J K^{-1} mol^{-1}): 128.5, 353.4 (1983-108); 130.79, 352.37 (1984-19); and 126.16, 347.02 (this work). The comments on the differences for 2-methylbenzenamine apply here.

4. Discussion

The eight primary amines selected in this study of their thermodynamic and thermophysical properties are the lowest members of the primary alkanamine and alkylbenzenamine homologous series of compounds. These results serve as a basis in empirical correlations for estimating properties of the higher members of these homologous series. However, the reliability of the estimated quantities depends on the accuracy and reliability of the basic values used for the estimation. It would be beneficial to obtain new data to improve the reliability of the thermodynamic properties of the amines selected for this work.

Predictive methods were used to derive recommended values of the critical properties of the methyl substituted benzenamines because measurements for these were absent or of poor quality; measurement of the critical properties for these is recommended. For 2-propanamine, the vapor pressure data above atmospheric pressure appears inconsistent. There are few reliable density values at high temperature for ethanamine, and the methylbenzenamines. Second virial coefficient data were measured for methanamine and ethanamine, but the values for ethanamine are of low quality. Second virial coefficient measurements would be informative for the higher alkanamines and benzenamines; however, these could be derived from enthalpy of vaporization values which are absent for these same substances. Reliable enthalpy of combustion measurements for the methylbenzenamines should receive high priority. There are no low temperature heat capacity measurements for ethanamine and the three methylbenzenamines. Liquid heat-capacity measurements on these compounds are either nonexistent or unreliable. For any of the properties considered here, measurements of properties for 2-methylbenzenamine would be more informative than they would be for the other two isomers.

We are not completely satisfied with the methods used for computing the ideal gas thermodynamic functions by statistical mechanics. The greatest deficiencies lie in the computational methods for compounds with compound internal rotations such as those in ethanamine and the propanamines.

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6. 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 Eq. (3a) and (3b)
sat	for value of C_{sat} or p_{sat} determined with an infinite amount of vapor(here) in equilibrium with the condensed phase (l or c)
tr	for value of T or Δ of H at a transition temperature

Superscripts (see other variables and notations, and functional notation below)

Other variables and designations

$A_a,B_a,\ldots,F_a$	coefficients in extended Antoine Eq. (5)
A_d,A_d	coefficients in Eq. (13) for -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) and (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_{cnd}	heat capacity determined at constant *cnd* (sat or p)
D_r	coefficient to (T_c/T) in expontential term of Eq. (10)
F	$= h/8\pi^2 cI_r$, function for internal rotation
F_i	coefficient in $\Sigma_i F_i \cos i\theta$ 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 degree Celsius at which the vapor pressure is 130 kPa in the extended Antoine 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 or r/r_o)	potential function for inversion of -NH$_2$ where z and r/r_o are the relative motion displacements
X_a	in the extended Antoine Eq. (5)
a,b	coefficients in potential function for -NH$_2$ inversion
c	crystal
g	gas
l	liquid
n	exponent to X_a in extended Antoine Eq. (5)
p	pressure
p_{sat}	vapor pressure
p_{tp}	triple point pressure
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
$\nu_{\mathrm{tor}}(0\rightarrow 1)$	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

°C	degree celsius, temperature
J	joule, energy
K	kelvin, temperature
Pa	pascal = newton/(meter)^2, pressure
R	$= 8.3145\,10\ \mathrm{J\,K^{-1}\,mol^{-1}}$, gas constant
c	$= 2.997\,924\,58\times10^8\ \mathrm{m\,s^{-1}}$, speed of light
cm^{-1}	$\cong$29 979.2458 MHz, wavenumber
e	= 2.71828,..., Napierian base
h	$= 6.6260755\times10^{-34}$ J Hz, Planck's constant
m	meter
mol	$= 6.0221367\times10^{23}$ molecules, mole
s	second
π	= 3.1415...

Functional notation

$\cos(\theta)$	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
$Y(A_1,A_2,...)$	variable Y as a function of the parameters, $A_1,A_2,...$
Z°	value of $Z(C,H,S,G)$ at 100 kPa, standard state
$Z(ph,T)$	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 (f or tr)
$\Delta_{s1}^{s2} Z$	change in variable $Z(G,H,S)$ in passing between states $s1$ to $s2$

7. References

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