# Density of Some 1-Bromoalkanes within the Temperature Range from (243.15 to 423.15) K

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The density $\rho$ of 1-bromopropane, 1-bromobutane, 1-bromopentane, 1-bromohexane, 1-bromoheptane, 1-bromooctane, and 1-bromododecane have been measured within the temperature range from (243.15 to 423.15) K. The experimental results were used to calculate the isobaric thermal expansion coefficient $\alpha_p$.

## Introduction

Density is the most often-quoted property of a substance and the property most often required for prediction of other properties of the substance. Experimental liquid densities of pure hydrocarbons and their mixtures are needed for the design of chemical processes. Therefore, experimental measurements are needed to understand the fundamental behavior of this property and then to develop new models. In this work, we report the densities of some 1-bromoalkanes as a function of temperature at atmospheric pressure.

This work is part of a project of the Laboratory of Molecular Acoustics to provide thermophysical properties of monohaloalkanes and binary mixtures containing monohaloalkanes. The thermophysical properties of monohaloalkanes have been extensively studied with the aim of a better understanding of the intermolecular interactions. In our earlier work,[1−6] we have determined the speed of sound, density, relative permittivity, viscosity, and heat capacity some 1-haloalkanes and their binary mixtures with *n*-alkanes. New measurements have been made for the density for 1-bromopropane, 1-bromobutane, 1-bromopentane, 1-bromohexane, 1-bromoheptane, 1-bromooctane, and 1-bromododecane at temperatures from (293.15 to 423.15) K.

## Experimental Section

***Materials.*** The materials used in this study [1-bromopropane (1-BrPr), 1-bromobutane (1-BrBu), 1-bromohexane (1-BrHx), 1-bromoheptane (1-BrHp), 1-bromooctane (1-BrOc), and 1-bromododecane (1-BrDod) (with a mole fraction purity of 0.999, 0.997, 0.994, 0.993, 0.992, and 0.992, respectively)] were supplied by Acros Organics. 1-Bromopentane (1-BrPe) with a mole fraction purity of 0.989 was obtained from Sigma-Aldrich.

***Measurements.*** Measurements of density were carried out using a 52.4890 $cm^3$ (at 298.15 K) pycnometer. The mass of pycnometer was measured, using an analytical balance with a precision of $\pm$ $3\cdot10^{-4}$ g. The pycnometer was calibrated with bi-distilled water. The position of the liquid level in the pycnometer was recorded with the traveling microscope, which could be read to $\pm$ 0.01 mm. A refrigerated thermostat (Kriovist, Termex Russia) was used to thermostat the pycnometer from (253.15 to 313.15) K. For measurements from (323.15 to 383.15) K, a thermostat (VIS-T, Termex Russia) was used. The temperature was measured with a 100 Ω platinum resistance thermometer and a digital thermometer bridge (Terkon, Termex Russia) on the ITS-90 scale. The total uncertainty in the temperature measurement is within $\pm$ 0.01 K. The estimated uncertainty of the density measurements was $\pm$ 0.005 %. Experimental values of density for the investigated liquids at 298.15 K were

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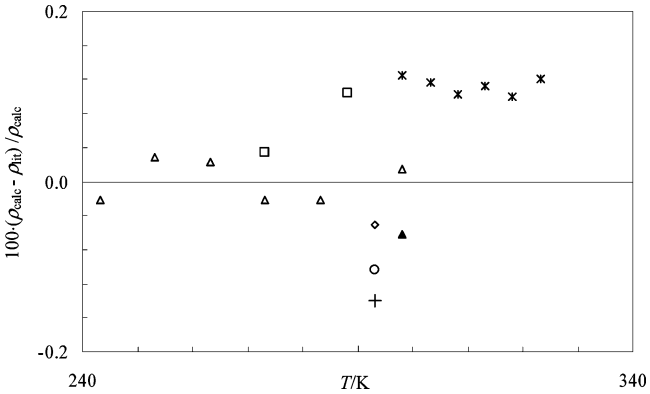


**Figure 1.** Deviation of literature density $\rho$ of 1-bromopropane from eq 1 as a function of temperature: △, this work; ▲, ref 10; □, ref 15; ◇, ref 16; +, ref 17; ○, ref 18; ∗, ref 29.

**Table 1. Comparison of Density $\rho$ of Liquid 1-Bromopropane, 1-Bromobutane, 1-Bromopentane, 1-Bromohexane, 1-Bromooctane, and 1-Bromododecane at 298.15 K**

| | $\rho$/(kg·m$^{-3}$) | |
|---|---|---|
| liquid | this work | lit. |
| 1-bromopropane | 1344.67 | 1345.5[10] |
| | | 1343.0[29] |
| 1-bromobutane | 1265.71 | 1268.9[8] |
| | | 1268.9[11] |
| | | 1268.6[13] |
| | | 1268.7[29] |
| 1-bromopentane | 1208.54 | 1211.4[8] |
| | | 1211.31[9] |
| | | 1212.3[13] |
| 1-bromohexane | 1166.71 | 1169.0[8] |
| | | 1168.95[9] |
| | | 1166.4[12] |
| | | 1168.8[13] |
| 1-bromooctane | 1106.04 | 1107.84[9] |
| | | 1107.7[13] |
| 1-bromododecane | 1035.58 | 1036.2[14] |

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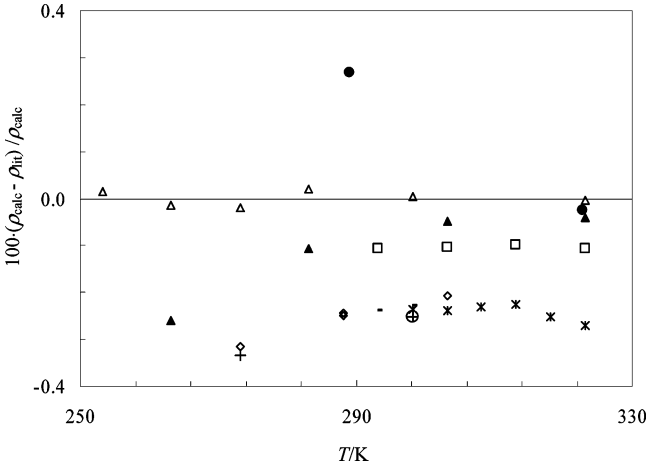


**Figure 2.** Deviation of literature density $\rho$ of 1-bromobutane from eq 1 as a function of temperature: △, this work; +, ref 8; ○, ref 11; −, ref 13; ◇, ref 15; ▲, ref 19; □, ref 20; ●, ref 21; ∗, ref 29.

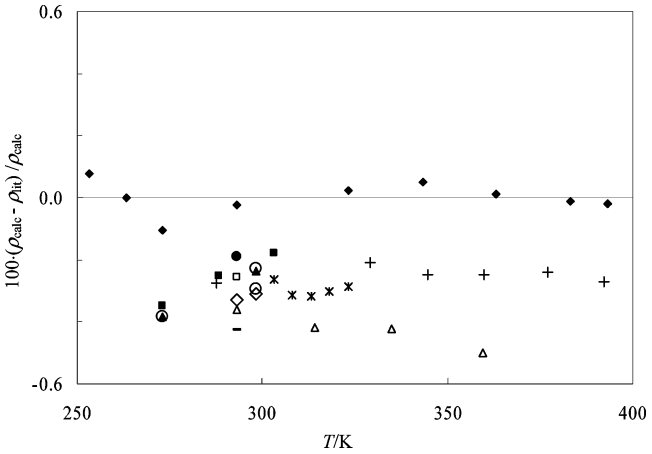


**Figure 3.** Deviation of literature density $\rho$ of 1-bromopentane from eq 1 as a function of temperature: ◆, this work; ▲, ref 8; ○, ref 9; ◇, ref 13; □, ref 16; △, ref 17; +, ref 21; ■, ref 22; ●, ref 23; −, ref 24; ∗, ref 29.

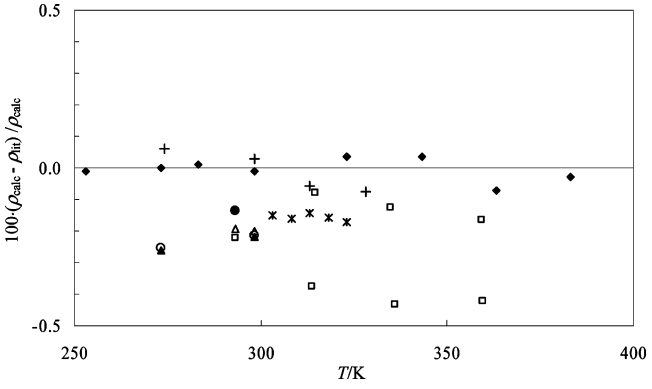


**Figure 4.** Deviation of literature density $\rho$ of 1-bromohexane from eq 1 as a function of temperature: ◆, this work; ▲, ref 8; ○, ref 9; +, ref 12; △, ref 13; □, ref 17; ●, ref 23; ∗, ref 29.

compared with those found in the literature and were in fairly good agreement, as shown in Table 1.

## Results and Discussion

The experimental values of density for 1-BrPr (Figure 1), 1-BrBu (Figure 2), 1-BrPe (Figure 3), 1-BrHx (Figure 4), 1-BrHp (Figure 5), 1-BrOc (Figure 6), and 1-BrDod (Figure 7) as a function of temperature are listed in Table 2. These data were fitted by the method of least-squares with the following equation:

$$\rho/(\mathrm{kg\cdot m^{-3}}) = A_0 + A_1(T/\mathrm{K}) + A_2(T/\mathrm{K})^2 \qquad (1)$$

where $A_0$, $A_1$, and $A_2$ are the adjustable parameters. The standard deviation $\sigma(\rho)$ is defined by

$$\sigma(\rho) = [\sum_{i=1}^{n} (\rho_{\mathrm{obs}} - \rho_{\mathrm{cal}})^2/(n-p)]^{1/2} \qquad (2)$$

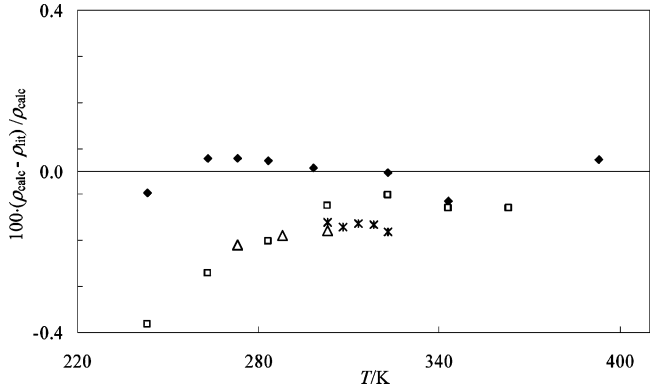


**Figure 5.** Deviation of literature density $\rho$ of 1-bromoheptane from eq 1 as a function of temperature: ◆, this work; □, ref 19; △, ref 25; ∗, ref 29.

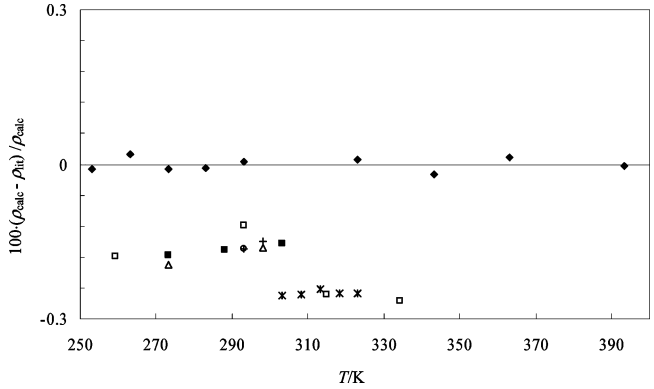


**Figure 6.** Deviation of literature density $\rho$ of 1-bromooctane from eq 1 as a function of temperature: ◆, this work; △, ref 9; +, ref 13; □, ref 17; ■, ref 25; ○, ref 26; ∗, ref 29.

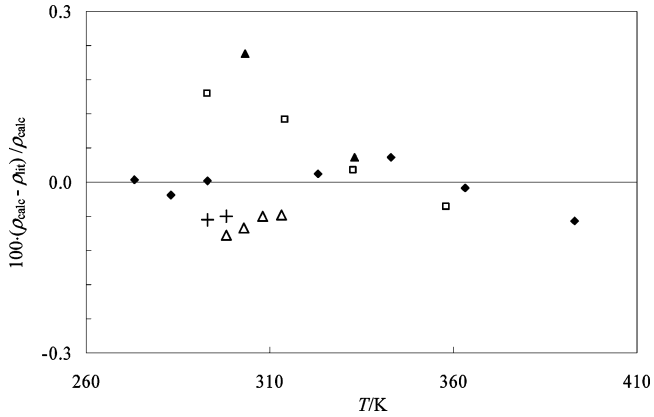


**Figure 7.** Deviation of literature density $\rho$ of 1-bromododecane from eq 1 as a function of temperature: ◆, this work; +, ref 14; □, ref 17; ▲, ref 27; △, ref 28.

**Table 2. Experimental Values of Density $\rho$ of Liquid 1-Bromopropane, 1-Bromobutane, 1-Bromopentane, 1-Bromohexane, 1-Bromooctane, and 1-Bromododecane at Various Temperatures**

| | $\rho$/(kg·m$^{-3}$) | | | | | | |
|---|---|---|---|---|---|---|---|
| $T$/K | 1-BrPr | 1-BrBu | 1-BrPe | 1-BrHx | 1-BrHp | 1-BrOc | 1-BrDod |
| 243.15 | 1431.1 | | | | 1191.0 | | |
| 253.15 | 1415.4 | 1326.5 | 1260.3 | 1218.0 | | 1151.1 | |
| 263.15 | 1400.3 | 1313.8 | 1249.9 | | 1169.6 | 1140.9 | |
| 273.15 | 1385.3 | 1300.5 | 1239.6 | 1195.3 | 1159.2 | 1131.2 | 1056.5 |
| 283.15 | 1369.4 | 1286.4 | | 1183.8 | 1148.7 | 1121.2 | 1048.5 |
| 293.15 | | | 1214.9 | | | 1111.0 | 1039.8 |
| 298.15 | 1344.5 | 1265.7 | | 1166.8 | 1132.9 | | |
| 323.15 | | 1229.5 | 1177.1 | 1137.3 | 1106.0 | 1080.6 | 1014.0 |
| 343.15 | | | 1151.0 | 1113.7 | 1084.5 | 1060.5 | 996.2 |
| 363.15 | | | 1124.7 | 1090.8 | | 1039.5 | 979.0 |
| 383.15 | | | 1097.4 | 1066.1 | | | |
| 393.15 | | | 1083.4 | | 1026.6 | 1008.4 | 952.4 |
| 403.15 | | | | 1040.9 | | | |
| 423.15 | | | | | | | 923.7 |

**Table 3. Values of the Parameters of Equation 1 for Density $\rho$ and Standard Deviation $\sigma$ for 1-Bromoalkanes from (243.15 to 423.15) K**

| liquid | $A_0$ | $A_1$ | $A_2$ | $\sigma$ |
|---|---|---|---|---|
| 1-bromopropane | 1692.91 | −0.6809 | $-1.63 \times 10^{-3}$ | 0.4 |
| 1-bromobutane | 1568.21 | −0.6139 | $-1.34 \times 10^{-3}$ | 0.2 |
| 1-bromopentane | 1476.64 | −0.5801 | $-1.07 \times 10^{-3}$ | 0.7 |
| 1-bromohexane | 1475.90 | −0.9206 | $-3.90 \times 10^{-4}$ | 0.4 |
| 1-bromoheptane | 1409.26 | −0.7821 | $-4.84 \times 10^{-4}$ | 0.4 |
| 1-bromooctane | 1388.28 | −0.8848 | $-2.07 \times 10^{-4}$ | 0.2 |
| 1-bromododecane | 1257.52 | −0.6399 | $-3.51 \times 10^{-4}$ | 0.4 |

**Table 4. Calculated Isobaric Thermal Expansion Coefficient of Liquid 1-Bromopropane, 1-Bromobutane, 1-Bromopentane, 1-Bromohexane, 1-Bromooctane, and 1-Bromododecane at Various Temperatures**

| | $\alpha_p$·10$^3$/K$^{-1}$ | | | | | | |
|---|---|---|---|---|---|---|---|
| $T$/K | 1-BrPr | 1-BrBu | 1-BrPe | 1-BrHx | 1-BrHp | 1-BrOc | 1-BrDod |
| 243.15 | 1.031 | 0.946 | 0.865 | 0.904 | 0.855 | 0.849 | 0.749 |
| 248.15 | 1.048 | 0.961 | 0.877 | 0.911 | 0.863 | 0.855 | 0.756 |
| 253.15 | 1.065 | 0.976 | 0.890 | 0.918 | 0.870 | 0.860 | 0.762 |
| 258.15 | 1.082 | 0.991 | 0.902 | 0.926 | 0.878 | 0.866 | 0.768 |
| 263.15 | 1.100 | 1.006 | 0.915 | 0.933 | 0.886 | 0.871 | 0.774 |
| 268.15 | 1.118 | 1.021 | 0.928 | 0.941 | 0.895 | 0.877 | 0.780 |
| 273.15 | 1.136 | 1.037 | 0.941 | 0.949 | 0.903 | 0.882 | 0.787 |
| 278.15 | 1.154 | 1.053 | 0.954 | 0.956 | 0.911 | 0.888 | 0.793 |
| 283.15 | 1.173 | 1.069 | 0.967 | 0.964 | 0.919 | 0.894 | 0.800 |
| 288.15 | 1.192 | 1.085 | 0.981 | 0.972 | 0.928 | 0.900 | 0.806 |
| 293.15 | 1.211 | 1.101 | 0.994 | 0.980 | 0.937 | 0.906 | 0.813 |
| 298.15 | 1.231 | 1.118 | 1.008 | 0.989 | 0.945 | 0.912 | 0.820 |
| 303.15 | | 1.135 | 1.022 | 0.997 | 0.954 | 0.918 | 0.827 |
| 308.15 | | 1.152 | 1.036 | 1.005 | 0.963 | 0.924 | 0.833 |
| 313.15 | | 1.170 | 1.051 | 1.014 | 0.972 | 0.930 | 0.840 |
| 318.15 | | 1.188 | 1.065 | 1.022 | 0.981 | 0.936 | 0.847 |
| 323.15 | | 1.206 | 1.080 | 1.031 | 0.990 | 0.943 | 0.854 |
| 328.15 | | | 1.095 | 1.040 | 1.000 | 0.949 | 0.862 |
| 333.15 | | | 1.111 | 1.049 | 1.009 | 0.956 | 0.869 |
| 338.15 | | | 1.126 | 1.058 | 1.019 | 0.962 | 0.876 |
| 343.15 | | | 1.142 | 1.067 | 1.028 | 0.969 | 0.883 |
| 348.15 | | | 1.158 | 1.076 | 1.038 | 0.976 | 0.891 |
| 353.15 | | | 1.174 | 1.086 | 1.048 | 0.982 | 0.898 |
| 358.15 | | | 1.190 | 1.095 | 1.058 | 0.989 | 0.906 |
| 363.15 | | | 1.207 | 1.105 | 1.068 | 0.996 | 0.914 |
| 368.15 | | | 1.224 | 1.114 | 1.079 | 1.003 | 0.922 |
| 373.15 | | | 1.241 | 1.124 | 1.089 | 1.010 | 0.929 |
| 378.15 | | | 1.258 | 1.134 | 1.100 | 1.017 | 0.937 |
| 383.15 | | | 1.276 | 1.144 | 1.111 | 1.025 | 0.945 |
| 388.15 | | | 1.294 | 1.155 | 1.121 | 1.032 | 0.954 |
| 393.15 | | | 1.313 | 1.165 | 1.133 | 1.039 | 0.962 |
| 398.15 | | | | 1.176 | 1.144 | 1.047 | 0.970 |
| 403.15 | | | | 1.186 | 1.155 | 1.054 | 0.979 |
| 408.15 | | | | | 1.167 | 1.062 | 0.987 |
| 413.15 | | | | | 1.178 | 1.070 | 0.996 |
| 418.15 | | | | | 1.190 | 1.078 | 1.005 |
| 423.15 | | | | | 1.202 | 1.086 | 1.014 |

where $\rho_{obs}$ and $\rho_{cal}$ are the observed and calculated quantities, $n$ is the total number of experimental points, and $p$ is the number of estimated parameters. The values of parameters $A_0$, $A_1$, and $A_2$ of eq 1 and standard deviation $\sigma(\rho)$ for all investigated liquids are given in Table 3.

The most complete information about the density of 1-bromoalkanes can be found in ref 7. An analysis of these data[7] shows that the temperature dependences are lacking for most 1-bromoalkanes. There are a few exceptions. Data for 1-BrHx from (293.15 to 359.45) K, 1-BrOc (293.15 to 359.35) K, and 1-BrDod from (293.15 to 358.05) K were reported by Vogel.[17] Ref 19 contains values for 1-BrBu from (183.15 to 363.15) K and 1-BrHp from (203.15 to 363.15) K. Data for 10 1-bromoalkanes (1-bromoethane to 1-bromoundecane) from (292.35 to 323.15) K were presented in ref 29.

We have compared our results with Bridgman's data[30] for 1-BrPr (1377.7 kg·m$^{-3}$ at 0 °C), 1-BrBu (1268.5 kg·m$^{-3}$ at 25 °C), and 1-BrPe (1250.5 kg·m$^{-3}$ at 0 °C and 1182.73 at 50 °C) extrapolated from single-phase area on a line of saturation. The average deviation of these data from our values is ± 0.5 %.

The isobaric thermal expansion coefficient

$$\alpha_p = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_p \quad (3)$$

was calculated from numerical differentiation of the density fitting equation. The estimated uncertainty of calculated values for isobaric thermal expansion coefficient was 1 %. The calculated values of isobaric thermal expansion coefficient $\alpha_p$ for investigated liquids are presented in Table 4.

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