Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K

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The densities of 1-chlorobutane, 1-chloropentane, 1-chloroheptane, 1-chlorooctane, 1-chlorodecane, and 1-chlorotetradecane have been measured within the temperature range from (253.15 to 423.15) K. The experimental results were used to calculate the isobaric thermal expansion coefficient α_p.

Introduction

The density is one of the most often-quoted properties of a substance, and its meaning is often required for prediction of the other properties of the one. 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 of condensed substances.

This work is a part of the project of the Molecular Acoustic Laboratory to investigate thermophysical properties of monohaloalkanes and their binary mixtures. In this work, we report the densities of some 1-chloroalkanes as a function of temperature at atmospheric pressure. Scientific and technical interests in these substances arise from their diverse applications and extensive use in practice. They are used in the petroleum, pharmaceutical, paint and varnish, textile, and paper industries, for the preparation of polymeric materials, and in many other fields. That is why representative international conferences on the thermochemical, thermodynamic, and transport properties of halogenated hydrocarbons and their mixtures were held in recent years in Pisa (Italy, 1999), Paris (France, 2001), and Rostock (Germany, 2002) under the auspices of IUPAC.

In our earlier work,[1−5] we have determined the speed of sound, density, relative permittivity, viscosity, and heat capacity of some 1-haloalkanes and their binary mixtures with *n*-alkanes. New measurements have been made for the density of 1-chlorobutane, 1-chloropentane, 1-chloroheptane, 1-chlorooctane, 1-chlorodecane, and 1-chlorotetradecane at temperature range from (253.15 to 423.15) K.

Experimental Section

Materials. The materials used in this study, 1-chlorobutane (1-ChlBu), 1-chloropentane (1-ChlPe), 1-chloroheptane (1-ChlHp), 1-chlorooctane (1-ChlOc), 1-chlorodecane (1-ChlDe), and 1-chlorotetradecane (1-ChlTetrade) (with a mole fraction purity of 0.999, 0.998, 0.999, 0.984, and 0.986, respectively) were supplied by Acros Organics. 1-Chloroheptane (1-ChlHp) with a mole fraction purity of 0.998 was obtained from Sigma-Aldrich.

Measurements. Density measurements were carried out using a 52.4890 cm^3 (at 298.15 K) pycnometer. The mass of the pycnometer was measured, using an analytical balance with an uncertainty of $\pm 3 \cdot 10^{-4}$ g. The pycnometer was calibrated with bidistilled water and other liquids (high *n*-alkanes). The position of the liquid level in the pycnometer was recorded with the traveling microscope, which could be read to ± 0.01 mm. A refrigerated thermostat (Kriovist, Termex Russia) was used to thermostat the pycnometer from (253.15 to 313.15) K. For measurements of liquid density from (323.15 to 423.15) K, a

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Table 1. Experimental Values of Density ρ of Liquid 1-Chlorobutane, 1-Chloropentane, 1-Chloroheptane, 1-Chlorooctane, 1-Chlorodecane, and 1-Chlorotetradecane at Various Temperatures

	ρ/(kg·m^{-3})					
T/K	1-ChlBu	1-ChlPe	1-ChlHp	1-ChlOc	1-ChlDe	1-ChlTetrade
253.15	925.8	917.5	908.3	905.5	899.9	
263.15	917.4	910.2	900.4	897.1	892.3	
273.15	907.3	900.7	891.7	889.0	884.2	
283.15	896.6	891.0	883.4	880.6	876.8	
288.15						868.5
293.15	885.9	881.3	874.5	872.3	868.9	864.9
298.15	880.4	876.2	870.4	868.3	865.0	861.0
303.15	874.9					857.5
313.15	863. 9					
323.15	852.1	851.3		847.4	845.6	843.3
323.65			848.2			
338.15	835.3					
343.15		830.6	830.6	830.5	830.0	829.0
363.15		809.1	812.6	813.2	814.2	814.3
393.15			784.4	786.8	789.5	792.5
423.15					764.6	770.1

Table 2. Values of the Parameters of Equation 1 for Density ρ and Standard Deviation σ for 1-Chloroalkanes from (243.15 to 423.15) K

liquid	A_0	A_1	A_2	σ
1-chlorobutane	1077.96	−0.2397	$-1.4165 \cdot 10^{-3}$	0.47
1-chloropentane	1077.88	−0.3761	$-1.0037 \cdot 10^{-3}$	0.54
1-chloroheptane	1088.04	−0.5967	$-4.4660 \cdot 10^{-4}$	0.16
1-chlorooctane	1093.64	−0.6788	$-2.5822 \cdot 10^{-4}$	0.14
1-chlorodecane	1076.03	−0.6393	$-2.2752 \cdot 10^{-4}$	0.17
1-chlorotetradecane	1063.57	−0.6431	$-1.1905 \cdot 10^{-4}$	0.15

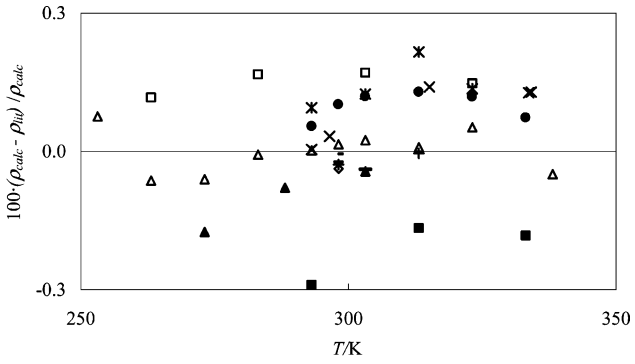

Figure 1. Deviation of literature density ρ of 1-chlorobutane from eq 1 as a function of temperature: Δ, this work; □, ref 7; ▲, ref 8; ×, ref 9; *, ref 29; ● , ref 11; —, ref 13, ref 14; -, ref 15; ■, ref 16; ◇, ref 12, ref 17; +, ref 18, ref 19; −, ref 20.

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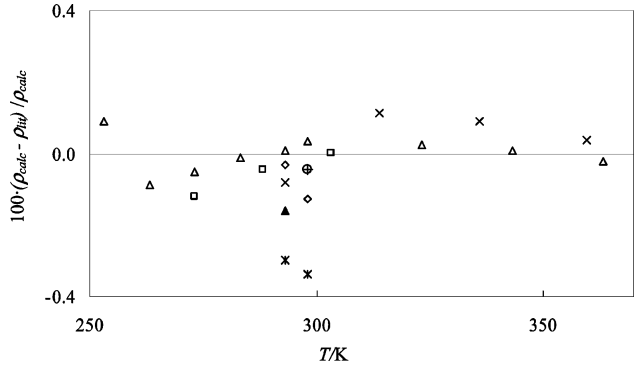

Figure 2. Deviation of literature density ρ of 1-chloropentane from eq 1 as a function of temperature: Δ, this work; □, ref 21; ▲, ref 22; ×, ref 9; *, ref 23; ◇, ref 24; +, ref 25; ○, ref 12, ref 20, ref 34, ref 35, ref 37.

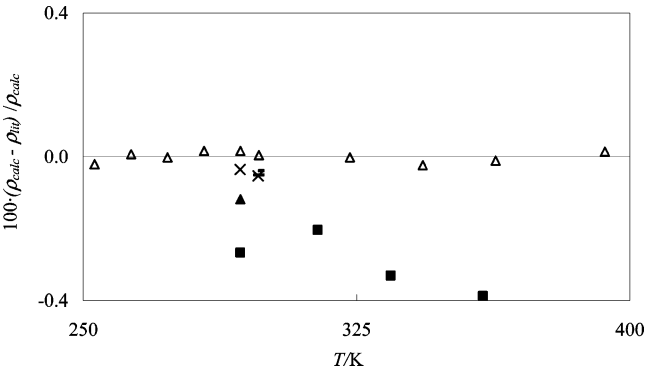

Figure 3. Deviation of literature density ρ of 1-chlorooctane from eq 1 as a function of temperature: Δ, this work; ■, ref 9; ▲, ref 23, ref 26; ×, ref 24; -, ref 25; −− , ref 12, ref 23, ref 34, ref 36, ref 38.

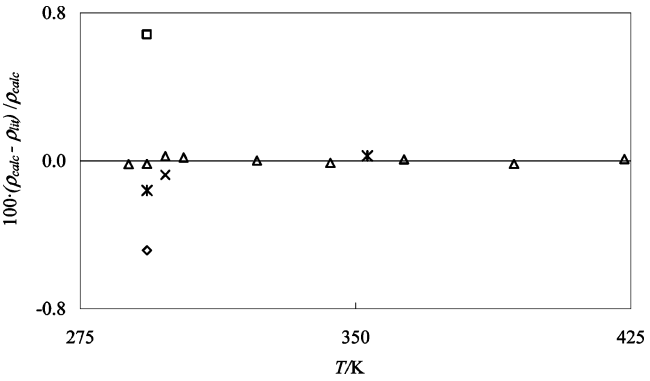

Figure 4. Deviation of literature density ρ of 1-chlorotetradecane from eq 1 as a function of temperature: Δ, this work; □, ref 27; ◇, ref 28; ×, ref 12, ref 34, ref 35; *, ref 29.

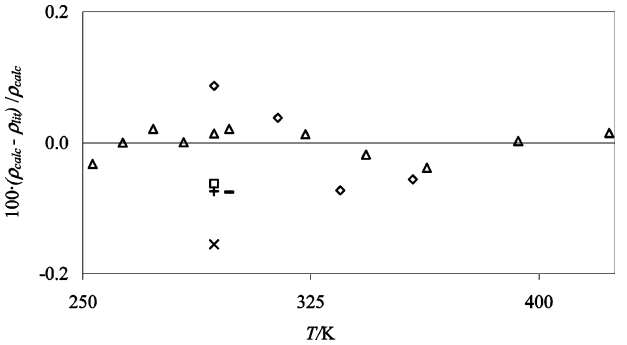

Figure 5. Deviation of literature density ρ of 1-chlorodecane from eq 1 as a function of temperature: Δ, this work; ◇, ref 9; □, ref 30, ref 39, ref 40; ×, ref 31; +, ref 28; -, ref 12, ref 34.

thermostat (VIS−T, Termex Russia) was used. The temperature was measured with a 100 Ω platinum resistance thermometer by a digital thermometer bridge (Terkon, Termex Russia) on the ITS-90 scale. The total uncertainty in the temperature measurement is within ± 0.01 K. The estimated uncertainty of the density measurements was ± 0.01 %. Experimental values of density for the investigated liquids were compared with those found in the literature.[6−40]

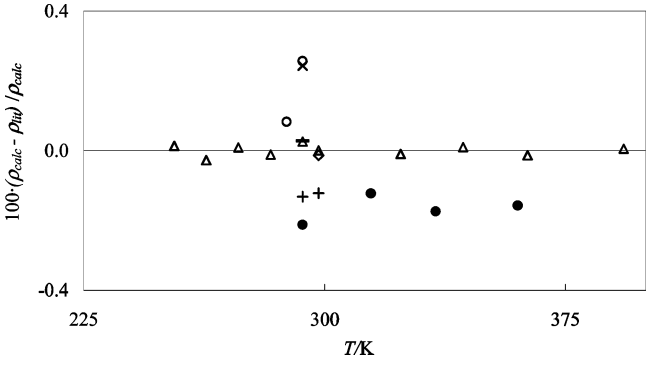

Figure 6. Deviation of literature density ρ of 1-chloroheptane from eq 1 as a function of temperature: Δ, this work; ●, ref 9; +, ref 23; ◇, ref 25; ×, ref 26; ○, ref 32; −, ref 33.

Table 3. Calculated Isobaric Thermal Expansion Coefficient of Liquid 1-Chlorobutane, 1-Chloropentane, 1-Chloroheptane, 1-Chlorooctane, 1-Chlorodecane, and 1-Chlorotetradecane at Various Temperatures

	$\alpha_P \cdot 10^3/K^{-1}$					
T/K	1-ChlBu	1-ChlPe	1-ChlHp	1-ChlOc	1-ChlDe	1-ChlTetrade
243.15	0.991	0.931	0.888	0.880	0.827	
248.15	1.011	0.946	0.897	0.887	0.833	
253.15	1.032	0.962	0.906	0.894	0.839	
258.15	1.052	0.977	0.915	0.901	0.845	
263.15	1.073	0.993	0.924	0.908	0.851	
268.15	1.095	1.009	0.933	0.915	0.857	
273.15	1.116	1.026	0.942	0.922	0.863	
278.15	1.138	1.042	0.952	0.929	0.870	
283.15	1.161	1.059	0.962	0.936	0.876	0.815
288.15	1.183	1.076	0.971	0.944	0.882	0.819
293.15	1.206	1.093	0.981	0.951	0.889	0.824
298.15	1.230	1.111	0.991	0.959	0.896	0.829
303.15	1.254	1.128	1.001	0.966	0.902	0.834
308.15	1.278	1.146	1.011	0.974	0.909	0.839
313.15	1.303	1.165	1.022	0.982	0.916	0.844
318.15	1.328	1.183	1.032	0.990	0.923	0.849
323.15	1.353	1.202	1.043	0.998	0.930	0.854
328.15	1.379	1.221	1.054	1.006	0.937	0.859
333.15	1.406	1.241	1.064	1.014	0.944	0.864
338.15		1.261	1.076	1.022	0.951	0.869
343.15		1.281	1.087	1.031	0.958	0.874
348.15		1.301	1.098	1.039	0.966	0.880
353.15		1.322	1.110	1.048	0.973	0.885
358.15		1.343	1.121	1.056	0.981	0.890
363.15			1.133	1.065	0.988	0.896
368.15			1.145	1.074	0.996	0.901
373.15			1.157	1.083	1.004	0.907
378.15			1.169	1.092	1.012	0.912
383.15			1.182	1.102	1.020	0.918
388.15			1.195	1.111	1.028	0.924
393.15					1.036	0.930
398.15					1.044	0.936
403.15					1.053	0.941
408.15					1.061	0.947
413.15					1.070	0.953
418.15					1.079	0.960
423.15						

Results and Discussion

The experimental values of density for 1-chlorobutane, 1-chloropentane, 1-chloroheptane, 1-chlorooctane, 1-chlorodecane, and 1-chlorotetradecane as a function of temperature are listed in Table 1. These results were fit as a function of temperature by

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

where the coefficients A_0, A_1, and A_2 were determined by regression to minimize the standard deviation σ, defined by

$$\sigma(\rho) = [\sum_{i=1}^{n}(\rho_{obsd} - \rho_{calcd})^2/(n - p)]^{1/2} \quad (2)$$

where ρ_{obsd} and ρ_{calcd} are the observed and calculated quantities; n is the total number of experimental points; and p is the power of the used polynomial. The values of parameters A_0, A_1, and A_2 of eq 1 and the standard deviation $\sigma(\rho)$ for all investigated liquids are given in Table 2. Deviation of literature density for investigated 1-chloroalkanes from eq 1 as a function of temperature is presented in Figures 1 to 6.

The most complete information about the density of 1-chloroalkanes can be found in ref 6. An analysis of these data[6] shows that the temperature dependences are lacking for most 1-chloroalkanes. There are a few exceptions. Data for 1-chlorobutane from (293.15 to 334.15) K, 1-chloropentane from (293.15 to 359.65) K, 1-chloroheptane from (293.15 to 360.15) K, 1-chlorooctane from (293.15 to 359.65) K, and 1-chlorodecane from (293.15 to 358.55) K were reported by Vogel.[9] Reference 11 contains values for 1-chlorobutane from (293.10 to 333.10) K.

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 the isobaric thermal expansion coefficient was 1 %. The calculated values of the isobaric thermal expansion coefficient α_P for investigated liquids are presented in Table 3.

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