Densities, Molar Volumes, Cubic Expansion Coefficients, and Isothermal Compressibilities of 1-Alkanols from 323.15 to 373.15 K and at Pressures up to 10 MPa

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Densities of six alcohols, 1-pentanol, 1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, and 1-dodecanol, in the liquid state have been measured with a vibrating-tube densimeter from 323.15 to 373.15 K at pressures up to 10 MPa. Molar volumes (derived from the densities) have been fitted to polynomials as a function of temperature and pressure. Cubic expansion coefficients and isothermal compressibilities have been derived from molar volumes as a function of temperature and pressure. The results have also been compared with the available literature values.

Introduction

In continuation of our experimental investigations (*1*, *2*) of certain physical and thermodynamic properties of industrially important compounds under the National Data Program on Thermophysical Properties we report in this paper the densities for liquid alcohols 1-pentanol, 1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, and 1-dodecanol from 323.15 to 373.15 K and at pressures from 0.1 to 10 MPa. Molar volumes (derived from the observed densities) have been fitted to suitable polynomials as a power series in temperature and pressure. Cubic expansion coefficients and isothermal compressibilities have been evaluated as a function of temperature and pressure.

Experimental Section

Materials. Chemicals of the best available purity were used for investigation. 1-Pentanol (>99 mol%), 1-hexanol (>99 mol%), 1-heptanol (>99.5 mol%), 1-octanol (>99.5 mol%), 1-nonanol (>98 mol%), and 1-dodecanol (>99.5 mol%) were procured from Fluka and were used as such without any further purification. The purity of all the chemicals was checked by density measurement at 298.15 K; the values are presented in Table I. Good agreement was found between our values and the literature (*3*, *4*) values. Water which was used as reference, was distilled, deionized by passing it through a Cole-Parmer mixed-bed ion exchange resin column, and then degassed.

Density Measurements. Densities were measured with a vibrating tube digital densimeter (Model DMA 60/512, Anton Paar, Austria) which has been described elsewhere (*1*, *5*, *6*). The bath temperature was measured with a Leeds and Northrup thermometer accurate to ±0.03 K on IPTS-68 and was maintained with a proportional temperature controller (YSI Model 72). Pressure was measured with a static high-pressure unit obtained from Setaram of France accurate to ±0.01 MPa. This unit was calibrated by the National Physical Laboratory, New Delhi, against its transfer standard gauges (*7*). The reference pressure was taken as 10^5 Pa. Calibration of the densimeter was done with water and air, and all the measurements were made with reference to water. The estimated precision of the density measurements is ±0.03 kg m^{-3}. The densimeter was tested (*1*) by measuring the densities of cyclohexane and *n*-heptane as a function of temperature (from 303.15 to 333.15 K) at 0.1 MPa and of *n*-decane as a function of pressure (up to 9.7 MPa) and temperature (323.15–373.15 K). The results showed a good agreement with literature values. The differences between our and literature values are less than 0.05%.

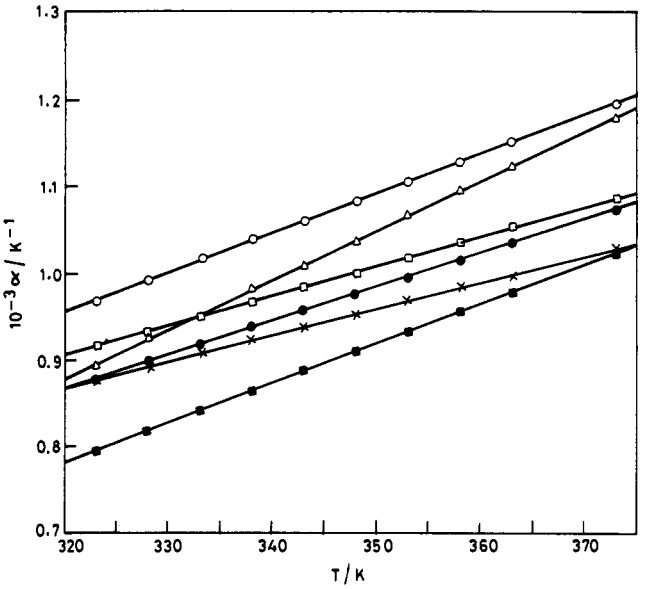

Figure 1. Cubic expansion coefficients versus temperature at 0.1 MPa: ○, 1-pentanol; △, 1-hexanol; □, 1-heptanol; ●, 1-octanol; ×, 1-nonanol; ■, 1-dodecanol.

Table I. Experimental Densities ρ and Their Comparison with Literature Data at 298.15 K

		ρ/(kg·m^{-3})		
			literature	
compound	source	exptl	Diaz (*3*)	API (*4*)
1-pentanol	Fluka	810.92	810.97	811.5
1-hexanol	Fluka	815.50	815.65	815.9
1-heptanol	Fluka	818.91	819.42	818.6
1-octanol	Fluka	821.76	822.60	822.2
1-nonanol	Fluka	824.32	824.47	824.7
1-dodecanol	Fluka	829.85	829.95	

Results and Discussion

The measured densities for 1-pentanol, 1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, and 1-dodecanol from 323.15 to

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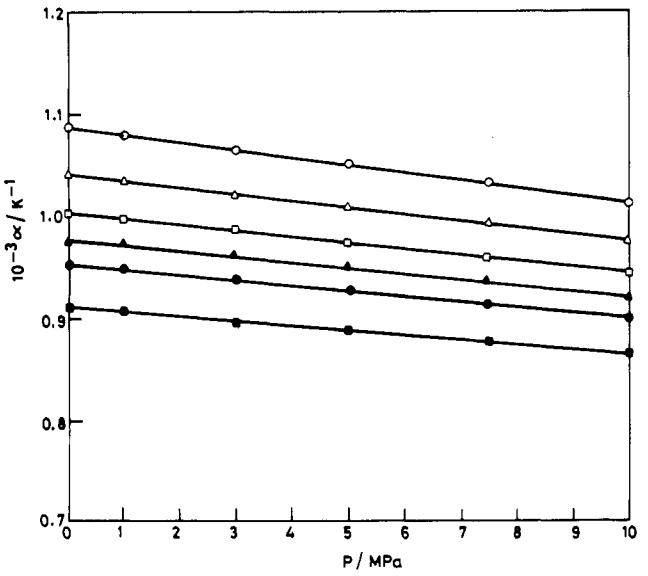

Figure 2. Cubic expansion coefficients versus pressure at 348.15 K: ○, 1-pentanol; △, 1-hexanol; □, 1-heptanol; ▲, 1-octanol; ●, 1-nonanol; ■, 1-dodecanol.

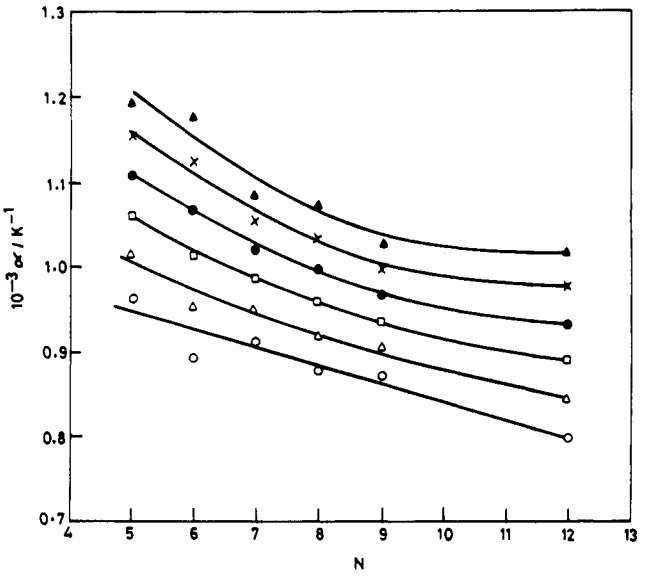

Figure 3. Cubic expansion coefficients versus N at 0.1 MPa. ○, 323.15 K; △, 333.15 K; □, 343.15 K; ●, 353.15 K; ×, 363.15 K; ▲, 373.15 K.

373.15 K at pressures of 0.1, 1.0, 3.0, 5.0, 7.5, and 10.0 MPa are reported in Table II. The density values for water, which has been taken as the standard reference, were taken from the literature (*8*). Except for 1-octanol, the densities of presently investigated fatty alcohols are reported in the literature only as a function of temperature (at 0.1 MPa).

The literature values are compared with our values in Tables III and IV. Our density values of fatty alcohols at different temperatures are in very good to excellent agreement with most of the reported values except with those of Efremov (*10*) for pentanol, Costello (*9*) and Singh (*12*) for hexanol, and Costello (*9*) for octanol. The density values of octanol

Table II. Experimental Densities ρ for Alcohols at Temperature T and Pressure P

	ρ/(kg·m^{-3})							ρ/(kg·m^{-3})					
T/K	0.1 MPa	1.0 MPa	3.0 MPa	5.0 MPa	7.5 MPa	10.0 MPa	T/K	0.1 MPa	1.0 MPa	3.0 MPa	5.0 MPa	7.5 MPa	10.0 MPa
					1-Pentanol								
323.15	792.18	792.99	794.63	796.15	797.90	799.73	348.15	771.92	772.71	774.65	776.46	778.57	780.59
328.15	788.92	789.55	790.75	792.65	794.48	796.29	353.15	768.08	769.06	771.03	772.76	774.80	776.88
333.15	784.39	785.20	786.97	788.54	790.42	792.28	358.15	763.64	764.57	766.52	768.41	770.67	772.73
338.15	780.59	781.37	783.10	784.67	786.51	788.36	363.15	759.36	760.31	762.39	764.29	766.55	768.69
343.15	776.19	777.06	778.93	780.48	782.55	784.42	373.15	750.46	751.49	753.43	755.52	757.84	760.28
					1-Hexanol								
323.15	797.34	798.06	799.57	801.04	802.71	804.41	348.15	777.68	778.41	780.37	782.02	783.98	785.93
328.15	794.09	794.74	795.91	797.71	799.49	801.15	353.15	773.89	774.78	776.54	778.24	780.26	782.28
333.15	789.67	790.36	792.01	793.57	795.41	797.17	358.15	769.75	770.62	772.51	774.30	776.42	778.30
338.15	786.02	786.72	788.35	789.94	791.72	793.64	363.15	765.47	766.39	768.32	770.17	772.30	774.34
343.15	781.78	782.59	784.27	785.76	787.75	789.97	373.15	757.03	758.07	759.78	761.77	763.92	766.26
					1-Heptanol								
323.15	801.09	801.85	803.38	804.77	806.41	808.12	348.15	781.91	782.65	784.43	786.04	787.93	789.83
328.15	797.68	798.53	799.59	801.35	803.07	804.75	353.15	778.40	779.25	780.98	782.54	784.50	786.39
333.15	793.62	794.39	795.99	797.46	799.20	800.86	358.15	774.25	775.04	776.80	778.50	780.61	782.51
338.15	790.17	790.81	792.37	793.84	795.55	797.27	363.15	770.31	771.18	773.01	774.75	776.84	778.73
343.15	786.06	786.83	788.48	789.91	791.77	794.02	373.15	762.00	762.94	764.62	766.46	768.57	770.73
					1-Octanol								
323.15	804.18	804.85	806.28	807.64	809.26	810.86	348.15	785.43	786.20	788.00	789.58	791.32	793.12
328.15	801.15	801.71	802.72	804.46	806.11	807.67	353.15	781.89	782.70	784.38	785.89	787.78	789.65
333.15	796.80	797.47	798.98	800.43	802.15	803.78	358.15	777.90	778.69	780.45	782.09	784.08	785.97
338.15	793.35	793.99	795.53	796.94	798.58	800.23	363.15	773.73	774.57	776.30	777.99	779.94	781.87
343.15	789.36	790.03	791.65	793.05	794.95	797.00	373.15	765.97	766.85	768.44	770.28	772.36	774.52
					1-Nonanol								
323.15	806.92	807.64	809.08	810.41	811.94	813.55	348.15	788.36	789.09	790.80	792.33	794.15	795.90
328.15	803.98	804.50	805.47	807.17	808.83	810.38	353.15	785.08	785.91	787.57	789.04	790.87	792.66
333.15	799.70	800.46	801.97	803.31	804.95	806.53	358.15	781.10	781.89	783.56	785.17	787.14	788.88
338.15	796.32	796.88	798.34	799.73	801.35	802.95	363.15	777.09	777.95	779.69	781.31	783.16	785.02
343.15	792.34	793.15	794.70	796.04	797.87	799.98	373.15	769.58	770.39	772.04	773.77	775.72	777.84
					1-Dodecanol								
323.15	812.71	813.31	814.64	815.94	817.43	818.89	348.15	794.85	795.44	797.05	798.52	800.22	802.00
328.15	809.82	810.33	811.29	812.90	814.39	815.90	353.15	791.66	792.34	793.85	795.24	796.93	798.67
333.15	805.78	806.34	807.74	809.08	810.66	812.16	358.15	787.79	788.49	790.10	791.61	793.42	795.14
338.15	802.46	803.00	804.39	805.72	807.23	808.83	363.15	784.06	784.80	786.38	787.94	789.80	791.53
343.15	798.60	799.30	800.66	801.99	803.68	805.68	373.15	776.69	777.58	778.92	780.54	782.43	784.52

Table III. Experimental Densities of 1-Alkanols Compared with the Literature at Different Temperatures

	ρ/(kg·m^{-3})									
T/K	exptl	ref 3	ref 9	ref 10	ref 11	ref 12	ref 13	ref 14	ref 15	ref 16
					1-Pentanol					
323.15	792.18							792.19		792.00
333.15	784.39	784.44	783.40	780.00						784.40
353.15	768.08		768.00	784.00						
373.15	750.46		751.50	752.00						
					1-Hexanol					
323.15	797.34					806.50	796.86			
333.15	789.67	789.95	792.40	788.00		803.40			789.40	
353.15	773.89		776.60	773.00						
373.15	757.03		759.90	757.00						
					1-Heptanol					
333.15	793.62	794.05		794.00						
353.15	778.40			778.00						
373.15	762.00			762.00						
					1-Octanol					
323.15	804.18				804.20					
333.15	796.80	797.58	794.80	797.00	797.00				796.94	
353.15	781.89		780.40	782.00						
373.15	765.97		764.30	767.00						
					1-Nonanol					
333.15	799.70	799.91		800.00						
353.15	785.08			786.00						
373.15	769.58			771.00						
					1-Dodecanol					
333.15	805.78	806.06	805.70						805.81	
353.15	791.66		792.00							
373.15	776.69		777.40							

Table IV. Experimental Densities ρ of 1-Octanol Compared with the Literature at Different Temperatures T and Pressures P

	ρ/(kg·m^{-3})			
	P = 5.0 MPa		P = 10.0 MPa	
T/K	exptl	ref 17	exptl	ref 17
333.15	800.43	800.50	803.78	804.00
353.15	785.89	786.20	789.65	790.30
373.15	770.28	771.00	774.52	775.40

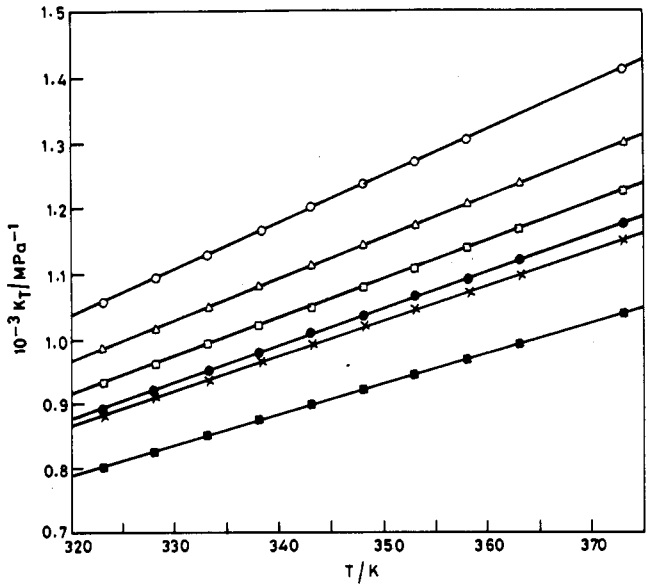

Figure 4. Isothermal compressibilities versus temperature at 0.1 MPa: ○, 1-pentanol; △, 1-hexanol; □, 1-heptanol; ●, 1-octanol; ×, 1-nonanol; ■, 1-dodecanol.

given in the literature (*17*) at different pressures are also in very good agreement with our experimental densities.

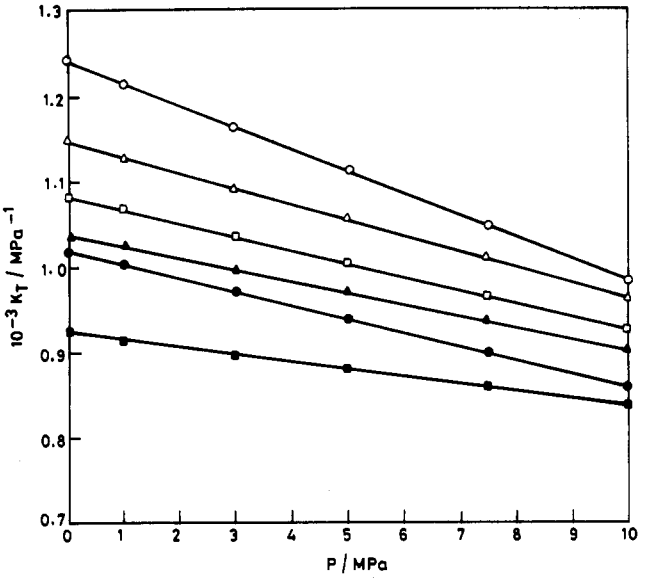

Figure 5. Isothermal compressibilities versus pressure at 348.15 K: ○, 1-pentanol; △, 1-hexanol; □, 1-heptanol; ▲, 1-octanol; ●, 1-nonanol; ■, 1-dodecanol.

The densities of presently investigated fatty alcohols are found to increase with the decrease in temperature, increase in pressure, and increase in chain length.

The molar volumes derived from observed densities by ordinary mathematics were fitted to the following second-degree polynomial in T and P:

$$V_m(T,P)/(\text{cm}^3\cdot\text{mol}^{-1}) = v_0 + v_1(T/\text{K}) + v_2(T/\text{K})^2 + v_3(P/\text{MPa}) + v_4(P/\text{MPa})^2 + v_5(P/\text{MPa})(T/\text{K}) \quad (1)$$

The values for the constants v_0, v_1, v_2, v_3, v_4, and v_5 are given in Table V.

The cubic expansion coefficients (α) and isothermal compressibilities (k_T) were derived from eq 1 using the

Table V. Coefficients of Equation 1 and Standard Deviations (σ)

compound	v_0	v_1	v_2	v_3	v_4	v_5	σ
1-pentanol	$0.110\,169 \times 10^3$	−0.101 133	$0.323\,332 \times 10^{-3}$	0.193 478	$0.152\,337 \times 10^{-2}$	$-0.963\,025 \times 10^{-3}$	0.03
1-hexanol	$0.137\,266 \times 10^3$	−0.170 855	$0.441\,701 \times 10^{-3}$	0.190 582	$0.127\,268 \times 10^{-2}$	$-0.980\,670 \times 10^{-3}$	0.04
1-heptanol	$0.136\,215 \times 10^3$	−0.078 322	$0.326\,804 \times 10^{-3}$	0.198 281	$0.122\,322 \times 10^{-2}$	$-0.103\,188 \times 10^{-2}$	0.03
1-octanol	$0.158\,201 \times 10^3$	−0.119 009	$0.404\,081 \times 10^{-3}$	0.214 453	$0.120\,092 \times 10^{-2}$	$-0.111\,120 \times 10^{-2}$	0.04
1-nonanol	$0.165\,901 \times 10^3$	−0.077 043	$0.361\,502 \times 10^{-3}$	0.213 461	$0.154\,104 \times 10^{-2}$	$-0.114\,978 \times 10^{-2}$	0.04
1-dodecanol	$0.235\,784 \times 10^3$	−0.222 221	$0.626\,119 \times 10^{-3}$	0.231 795	$0.108\,382 \times 10^{-2}$	$-0.128\,795 \times 10^{-2}$	0.08

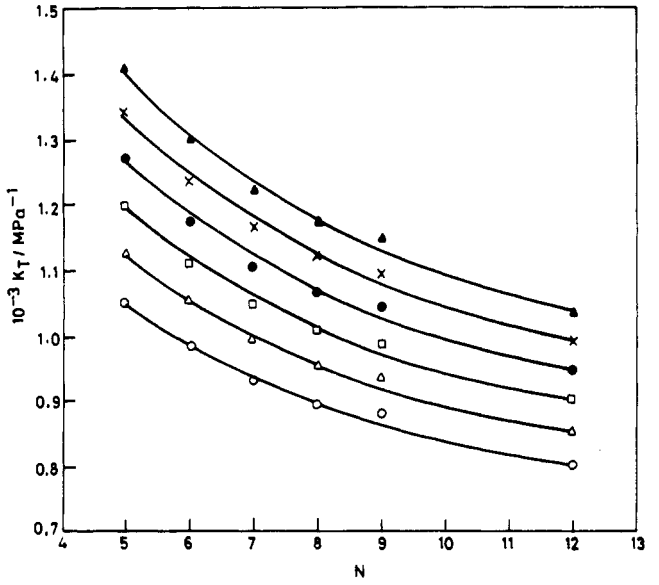

Figure 6. Isothermal compressibilities versus N at 0.1 MPa: ○, 323.15 K; △, 333.15 K; □, 343.15 K; ●, 353.15 K; ×, 363.15 K; ▲, 373.15 K.

following relations:

$$\alpha = V^{-1}(\partial V/\partial T)_P$$

$$k_T = -V^{-1}(\partial V/\partial P)_T$$

Our results of isothermal compressibility are found to be in good agreement with those of Diaz (*3*) and Carlson (*18*) at 333.15 K and 0.1 MPa and are compared in Table VI, but we have not found any data in the literature on cubic expansion coefficients and isothermal compressibilities for these alcohols at other temperatures and pressures to compare with our results.

Cubic expansion coefficients and isothermal compressibilities of alcohols as a function of temperature (at 0.1 MPa), pressure (at 348.15 K), and the number N of carbon atoms have been plotted in Figures 1–6. Our results show that the cubic expansion coefficient and isothermal compressibility increase with an increase in temperature (at a fixed pressure), decrease with an increase in pressure (at a fixed temperature), and decrease with an increase in the chain length of the alcohol over the whole temperature range.

Table VI. Comparison of Compressibilities with the Literature at 0.1 MPa and 333.15 K

	k_T/MPa^{-1}		
compound	this work	ref 3	ref 18
1-pentanol	1130	1095	
1-hexanol	1050	1042	1042
1-heptanol	992	989	989
1-octanol	951	954	954
1-nonanol	938	923	923
1-dodecanol	852	864	864

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