PVT Property Measurements for Some Aliphatic Esters from (298 to 393) K and up to 35 MPa

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The results of *PVT* measurements of the liquid phase within the temperature range of (298 to 393) K and up to 35 MPa are presented for some aliphatic esters. Measurements were made by means of a vibrating-tube densimeter, model DMA 512P from Anton Parr. The calibration of the densimeter was performed with water and *n*-heptane as reference fluids. The experimental *PVT* data have been correlated by a Tait equation. This equation gives excellent results when used to predict the density of the esters using the method proposed by Thomson et al. (*AIChE J*. **1982**, *28*, 671−676). Isothermal compressibilities, isobaric expansivities, thermal pressure coefficients, and changes in the isobaric heat capacity have been calculated from the volumetric data.

Introduction

PVT data of liquids are important for efficient design of chemical processes and to develop correlation and prediction methods applicable over wide temperature and pressure ranges. The aliphatic esters are important materials in manufacturing processes connected with flavor and fragrance industries.

Several studies of thermophysical properties (density, viscosity, surface and interfacial tension) of several esters have been performed at room temperature and atmospheric pressure in our research group.[1−3] However detailed investigation of these properties for pure esters, in large temperature and pressure ranges, are still very scarce in literature. As far as we know, the available literature density data in the high pressure domain are the measurements for propyl and butyl acetates from Malhotra and Woolf[4] in the temperature range of (278 to 338) K and those performed by Kumagai and Iwasaki[5] for ethyl acetate in the range of (253 to 313) K. This paper gives a valuable contribution in this direction presenting reliable density data for some alkyl esters (ethyl, propyl, *n*-butyl, and *n*-pentyl acetates) from (298.15 to 393.15) K and up to 35 MPa. In order to compare our data with those from Malhotra and Woolf, we have made some density measurements at the same (*P, T*) conditions. The agreement was very good with absolute average deviations (AAD) of the order of 0.1 %. To correlate our density data, a Tait equation was applied. From this equation, isothermal compressibilities, isobaric expansivities, thermal pressure coefficients, and changes in the isobaric heat capacity have been calculated. The method of Thomson et al.[6] was applied to the prediction of the density in the pressure and temperature ranges considered with absolute average deviations of the order of 0.2 %.

Experimental Section

Materials. All the materials used are pro analysis grade. Tridistilled water was used. *N*-Heptane was from Lab-Scan with a stated purity higher than 99 (mass %). The esters (ethyl, propyl, *n*-butyl, and *n*-pentyl acetates) were obtained from Aldrich with purities of >99.9, >99.0, >99.7, and >99.0 mass %, respectively. The purities were not measured and all liquids have been used without purification. The density data at different temperatures and at atmospheric pressure obtained in this work are compared with literature values in Table 1.

Table 1. Densities of Pure Liquids at Different Temperatures and at Atmospheric Pressure, Obtained in This Work and from the Literature

	ρ/kg·m^{-3}			ρ/kg·m^{-3}	
T/K	this work	literature	*T*/K	this work	literature
		Ethyl Acetate			
298.15	894.0	894.0,[a] 894.45[b]	323.15	862.7	861.9[a]
303.15	887.6	887.0[a]	333.15	850.4	848.8[a]
313.15	875.2	875.2[c]	343.15	837.5	835.6[a]
		Propyl Acetate			
298.15	882.0	882.76,[d] 882.6[a]	338.15	836.7	837.02[d]
303.15	876.2	876.9[a]	343.15	831.2	830.2[a]
313.15	864.9	865.87,[d] 865.4[a]	353.15	820.0	818.2[a]
323.15	853.6	853.7,[a] 854.47[d]	363.15	804.8	806.1[a]
333.15	842.5	842.0[a]			
		Butyl Acetate			
298.15	875.7	876.02,[d] 876.6[a]	343.15	829.5	828.2[a]
303.15	870.4	871.8[a]	353.15	819.3	815.6[a]
313.15	859.9	861.8,[a] 860.50[d]	363.15	806.1	802.2[a]
323.15	849.7	851.2,[a] 850.11[d]	373.15	795.8	787.8[a]
333.15	839.6	840.1[a]	383.15	785.2	772.4[a]
338.15	834.5	834.10[a]			
		Pentyl Acetate			
298.15	871.4	871.9[a]	333.15	837.8	838.1[a]
303.15	866.5	867.2[a]	343.15	828.3	828.2[a]
313.15	856.7	857.6[a]	353.15	818.7	818.2[a]
323.15	847.1	847.9[a]			

[a] Ref 7. [b] Ref 8. [c] Ref 9. [d] Ref 4.

Experimental and Calibration Procedures. Densities of liquids were determined using a vibrating-tube densimeter (model DMA 512P from Anton Parr). Figure 1 shows the installation of the DMA 512P cell and the peripheral equipment used. The required pressure was generated and controlled with a HIP pressure generator model 50-6-15 from High Pressure Equipment Co., using acetone as the hydraulic fluid. Pressures

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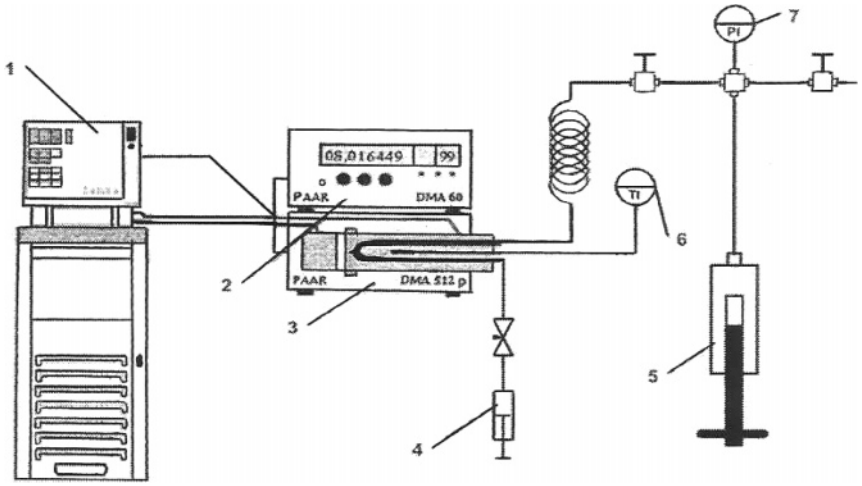

Figure 1. Experimental setup for the measurement of liquid densities at high pressures: 1, Julabo FP-50 thermostatic bath; 2, DMA 60 (Anton Paar) device for the measuring the period of oscilation; 3, measuring cell DMA 512P (Anton Paar); 4, syringe for sample introduction; 5, pressure generator model HIP 50-6-15; 6, PT probe; 7, pressure transducer WIKA, S-10.

Table 2. Experimental Density (ρ) Data for Ethyl Acetate as a Function of Temperature (T) and Pressure (P)

	ρ/kg·m^{-3} at P/MPa											
T/K	0.10	1.00	2.00	3.00	3.80	5.00	10.00	15.00	20.00	25.00	30.00	35.00
298.15	894.0	894.7	895.7	896.7	897.4	898.8	903.4	907.7	912.0	916.1	921.1	926.3
303.15	887.6	888.5	889.5	890.5	891.3	892.7	897.5	902.0	906.3	910.7	915.9	921.2
308.15	881.4	882.3	883.3	884.4	885.3	886.7	891.7	896.4	900.9	905.4	910.7	916.2
313.15	875.2	876.1	877.2	878.3	879.2	880.6	885.8	890.7	895.4	899.8	905.3	910.9
318.15	868.8	869.8	871.0	872.2	873.1	874.5	880.0	885.1	889.8	894.5	900.1	905.9
323.15	862.7	864.0	865.1	866.2	867.1	868.6	874.2	879.4	884.3	889.2	895.0	900.9
328.15	856.4	857.8	859.2	860.5	861.5	862.5	868.4	873.9	879.0	884.1	890.1	896.2
333.15	850.4	851.7	853.0	854.4	855.4	856.8	862.9	868.5	873.8	879.0	885.2	891.4
338.15	844.0	845.4	846.8	848.2	849.3	850.8	857.1	863.0	868.5	873.9	880.3	886.7
343.15	837.5	839.1	840.6	842.0	843.2	844.5	851.2	857.3	863.0	868.5	875.1	881.6
348.15	829.4	830.5	832.3	833.8	835.0	836.8	845.5	851.8	857.7	863.5	870.2	877.0
353.15		824.3	826.0	827.5	828.8	830.6	837.7	844.3	850.4	856.1	862.7	869.6
358.15		818.4	820.0	821.6	822.8	824.7	832.1	838.9	845.2	851.0	857.6	864.7
363.15		811.8	813.5	815.3	816.6	818.5	826.3	833.3	839.7	845.8	852.9	860.2
368.15		804.9	806.8	808.6	810.0	812.1	820.2	827.5	834.3	840.6	848.0	855.5
373.15		798.5	800.4	802.4	803.8	806.0	814.4	822.0	829.0	835.5	843.0	850.6
378.15		791.8	793.8	795.8	797.3	799.6	808.5	816.5	823.7	830.5	838.4	846.3
383.15		784.8	787.1	789.1	790.8	793.2	802.4	810.7	818.2	825.3	833.5	841.6
388.15		778.2	780.5	782.7	784.4	786.9	796.4	805.1	813.0	820.3	828.8	837.2
393.15		771.0	773.5	775.9	777.7	780.4	790.5	799.4	807.6	815.2	823.9	832.4

Table 3. Experimental Density (ρ) Data for Propyl Acetate as a Function of Temperature (T) and Pressure (P)

	ρ/kg·m^{-3} at P/MPa											
T/K	0.10	1.00	2.00	3.00	3.30	5.00	10.00	15.00	20.00	25.00	30.00	35.00
298.15	882.0	882.5	883.4	884.3	884.6	886.4	890.7	894.8	898.7	902.5	906.9	911.7
303.15	876.2	876.8	877.7	878.8	879.0	880.8	885.3	889.5	893.5	897.4	902.0	906.9
308.15	870.5	871.2	872.2	873.2	873.4	875.3	879.9	884.3	888.4	892.4	897.2	902.3
313.15	864.9	865.5	866.6	867.6	867.9	869.9	874.7	879.2	883.5	887.6	892.6	897.7
318.15	879.3	859.8	860.9	862.1	862.4	864.4	869.4	874.1	878.5	882.8	887.9	893.2
323.15	853.6	854.8	855.8	856.9	857.1	859.0	864.1	869.0	873.5	877.9	883.2	888.8
328.15	848.0	848.7	849.9	851.0	851.3	853.7	859.0	864.0	868.7	873.3	878.8	884.4
333.15	842.5	843.6	844.8	845.9	846.2	848.3	853.9	859.0	863.9	868.6	874.3	880.1
338.15	836.7	838.0	839.2	840.5	840.8	842.8	848.6	853.9	859.0	863.8	869.6	875.5
343.15	831.2	832.3	833.7	834.9	835.3	837.6	843.6	849.1	865.3	859.2	865.0	871.2
348.15	825.6	826.8	828.1	829.5	829.9	832.2	838.3	844.1	849.5	854.5	860.6	866.8
353.15	820.0	821.2	8222.6	824.0	824.4	826.9	833.3	838.8	844.8	850.0	856.4	862.7
358.15	811.6	812.9	814.4	815.8	816.3	818.6	825.3	831.5	837.2	842.8		
363.15	804.8	806.9	808.4	810.0	810.4	812.9	819.9	826.2	832.1	837.7	844.4	
368.15		801.0	802.7	804.3	804.8	807.4	814.6	821.2	827.3	833.1		
373.15		795.5	797.2	798.9	799.5	802.3	809.8	816.6	822.9	833.9		
378.15		789.4	791.3	793.0	793.6	796.3	803.3	811.3	817.7	824.0	831.2	
383.15		783.6	785.5	787.3	788.2	791.2	799.2	806.6	813.2	819.7		
388.15		777.9	779.8	781.6	782.1	785.4	793.8	801.5	808.5	815.2	823.2	
393.15		771.8	7733.9	775.9	776.4	779.7	788.6	796.5	803.8	810.7		

were measured with a pressure transducer (WIKA, S-10) with a precision of ± 0.03 MPa. This uncertainty is not relevant since the mean value of the isothermal compressibility for the compounds studied here are on the order of 10^{-3} MPa^{-1}. The temperature in the vibrating-tube cell was measured with a platinum resistance probe with an uncertainty of ± 0.01 K coupled with a GW Instek Dual Display Digital Multimeter GDM-845. A Julabo P-50 thermostatic bath with silicone oil

Table 4. Experimental Density (ρ) Data for *N*-Butyl Acetate as a Function of Temperature (T) and Pressure (P)

	ρ/kg·m^{-3} at P/MPa											
T/K	0.10	1.00	2.00	3.00	3.10	5.00	10.00	15.00	20.00	25.00	30.00	35.00
298.15	875.7	876.3	877.2	878.0	878.1	879.9	883.8	887.6	891.3	894.9	899.1	903.7
303.15	870.4	871.1	872.0	872.9	873.0	874.7	878.8	882.8	886.5	890.2	894.4	899.1
308.15	865.1	865.9	866.9	867.8	867.8	869.6	873.9	878.0	881.9	885.6	890.0	894.8
313.15	859.9	860.8	861.7	862.7	862.7	864.6	869.0	873.2	877.2	881.0	885.6	890.5
318.15	854.9	855.7	856.7	857.8	857.9	859.6	864.2	868.5	872.6	876.5	881.3	886.3
323.15	849.7	851.0	852.0	853.0	853.1	854.6	859.4	863.9	868.1	872.3	877.3	882.4
328.15	844.6	845.7	846.8	847.9	848.0	849.7	854.6	859.3	863.6	867.8	872.5	877.7
333.15	839.6	840.7	841.8	842.9	842.9	844.9	850.0	854.8	859.3	863.6	868.6	873.9
338.15	834.5	835.6	836.7	837.9	838.0	840.1	845.5	850.1	855.0	859.5	864.6	870.1
343.15	829.5	830.5	831.7	832.9	833.0	835.2	840.7	845.7	850.5	855.1	860.7	866.3
348.15	824.4	825.4	826.7	827.9	828.0	830.5	836.1	841.3	846.2	850.9	856.6	862.4
353.15	819.3	820.4	821.7	822.9	823.0	825.5	831.3	836.7	841.8	846.7	852.5	858.4
358.15	811.6	813.2	813.9	810.3	815.3	817.7	823.6	829.1	835.5			
363.15	806.1	807.5	808.8	810.1	810.3	812.8	819.2	824.9	830.4			
368.15	800.3	802.1	803.6	804.8	805.0	807.7	814.3	820.3	825.9			
373.15	795.8	797.2	798.7	800.2	800.4	803.1	809.9	815.9	821.3			
378.15	790.4	791.9	793.7	795.2	795.4	798.0	804.7	810.8	817.1			
383.15	785.2	786.7	788.3	789.9	790.0	792.9	800.1	806.7	812.8			
388.15	779.9	781.6	783.2	785.2	785.4	788.4	795.8	802.4	808.6			
393.15	775.2	776.4	778.1	779.5	779.7	782.8	790.6	797.7	804.2			

Table 5. Experimental Density (ρ) Data for *N*-Pentyl Acetate as a Function of Temperature (T) and Pressure (P)

	ρ/kg·m^{-3} at P/MPa											
T/K	0.10	1.00	2.00	2.70	3.00	5.00	10.00	15.00	20.00	25.00	30.00	35.00
298.15	871.4	871.9	872.7	873.3	873.5	875.3	879.1	882.7	886.2	889.6	893.6	897.9
303.15	866.5	867.1	867.9	868.5	868.7	870.5	874.4	878.1	881.6	885.1	889.4	893.8
308.15	861.6	862.2	863.1	863.7	863.9	865.8	869.8	873.6	877.3	880.8	885.2	889.7
313.15	856.7	857.4	858.3	858.9	859.2	861.0	865.2	869.0	872.8	876.4	880.9	885.5
318.15	851.9	852.6	853.5	854.2	854.4	856.4	860.7	864.7	868.5	872.3	876.9	881.7
323.15	847.1	847.7	848.7	849.3	849.6	851.7	856.1	860.2	864.2	868.1	872.8	877.6
328.15	842.3	843.2	844.4	845.2	845.5	847.1	851.6	855.9	860.0	864.1	869.0	874.0
333.15	837.8	838.7	839.8	840.5	840.8	842.7	847.4	851.8	856.0	860.1	865.1	870.2
338.15	832.9	834.0	835.1	835.8	836.1	838.1	842.9	847.5	851.9	856.2	861.3	866.5
343.15	828.3	829.3	830.4	831.2	831.5	833.5	838.5	843.2	847.7	852.1	857.3	862.7
348.15	823.2	824.6	825.7	826.5	826.9	828.8	834.0	838.9	843.5	847.9	853.3	858.8
353.15	818.7	819.9	821.1	821.9	822.3	824.4	829.8	835.0	839.7	844.3	849.8	855.4
358.15	811.3	812.2	813.4	814.1	814.5	816.9	822.5	827.7	832.5	838.0	843.9	849.7
363.15	806.3	807.4	808.7	809.6	809.9	812.4	818.1	823.4	828.3	833.9	839.9	845.6
368.15	801.2	802.3	803.7	804.6	805.0	807.5	813.4	818.8	824.0	829.8	835.9	841.4
373.15	795.5	796.4	797.7	799.5	799.0	802.5	808.2	813.9	819.8	826.3	831.3	832.4
378.15	790.4	791.6	793.1	794.0	794.4	797.1	803.5	808.9	813.2	817.7	822.3	823.6
383.15	786.8	788.1	789.6	790.7	791.1	793.9	800.5	806.6	811.7	816.5	824.0	830.0
388.15	781.9	783.4	785.0	786.0	786.5	789.4	796.3	802.5	808.1	813.7	819.7	826.2
393.15	777.2	778.7	780.3	781.4	781.9	784.9	791.9	798.4	803.9	809.7	815.7	822.2

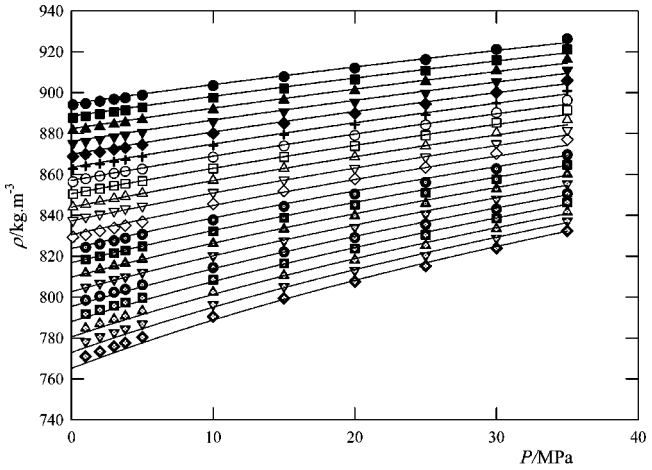

Figure 2. Isotherms of the density (ρ) for ethyl acetate. The symbols refer to the experimental data: from 298.15 K (●) up to 393.15 K with increments of 5 K. The curves are calculated with eq 6.

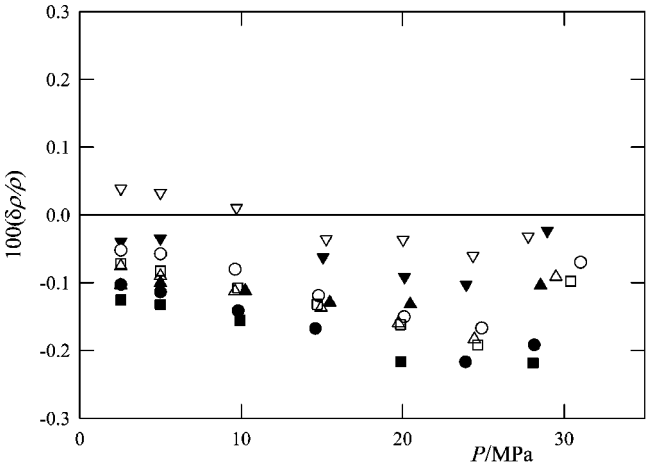

Figure 3. Percentage deviations between experimental data of this work and from Malhotra and Woolf[4] at the temperatures of (●, ○) 298.14 K; (■, □) 313.14 K; (▲, △) 323.14 K; and (▼, ▽) 338.13 K. The solid symbols refer to the propyl acetate, and the open symbols refer to *n*-butyl acetate. The quantity $100(\delta\rho/\rho)$ means $100(\rho_{eq\,6} - \rho_{lit})/\rho_{lit}$.

as circulating fluid was used in the thermostatic circuit of the measuring cell, which was held constant to ± 0.01 K. The diameter of tube is 1/16 in., and the buffer is more than 1 m in length, which guarantees the inexistence of diffusion of the hydraulic liquid in the liquid contained in the cell of densimeter.

Water and *n*-heptane have been used as reference fluids for the calibration of the vibrating-tube densimeter. The density of these substances were used to fit the calibration

Table 6. Critical Constants (T_c, P_c) and Parameters of Wagner Equation (eq 7)

			parameters of eq 7				
ester	T_c/K	P_c/kPa	n_1	n_2	n_3	n_4	m
ethyl acetate	523.3[a]	3882[a]	−7.73565	1.35123	−3.73614	−3.22368[a]	3
propyl acetate	549.4[b]	3360[b]	−7.78603	1.19822	−3.82058	−3.82058[b]	3
n-butyl acetate	576[b]	3050[b]	−7.98310	1.22855	−3.91728	−3.91728[b]	3
n-pentyl acetate	600[c]	2685[c]	−8.09753	1.60398	−3.37406	−5.04594[c]	2.5

[a] Ref 18. [b] Ref 19. [c] Ref 20.

Table 7. Density of the Saturated Liquid, $\rho^{/\sigma}$

T/K	$\rho^{/\sigma}$/kg.m^{-3}	T/K	$\rho^{/\sigma}$/kg.m^{-3}	T/K	$\rho^{/\sigma}$/kg.m^{-3}	T/K	$\rho^{/\sigma}$/kg.m^{-3}
			Ethyl Acetate				
298.15	893.9000	323.15	862.6	348.15	829.3	373.15	796.8
303.15	887.5000	328.15	856.3	353.15	822.9	378.15	790.2
308.15	881.3000	333.15	850.4	358.15	817.0	383.15	783.1
313.15	875.1000	338.15	844.0	363.15	810.2	388.15	776.6
318.15	868.8000	343.15	837.5	368.15	803.3	393.15	769.4
			Propyl Acetate				
298.15	881.8	323.15	853.5	348.15	825.5	373.15	793.9
303.15	876.0	328.15	847.8	353.15	819.9	378.15	787.5
308.15	870.3	333.15	842.4	358.15	811.6	383.15	781.9
313.15	864.7	338.15	836.6	363.15	804.7	388.15	776.4
318.15	859.0	343.15	831.2	368.15	799.5	393.15	770.0
			n-Butyl Acetate				
298.15	875.6	323.15	849.6	348.15	824.3	373.15	795.7
303.15	870.3	328.15	844.5	353.15	819.2	378.15	790.3
308.15	865.1	333.15	839.5	358.15	811.5	383.15	785.1
313.15	859.8	338.15	834.4	363.15	806.0	388.15	779.8
318.15	854.7	343.15	829.4	368.15	800.2	393.15	775.1
			n-Pentyl Acetate				
298.15	871.3	323.15	846.9	348.15	823.1	373.15	795.2
303.15	866.4	328.15	842.2	353.15	818.6	378.15	790.3
308.15	861.5	333.15	837.7	358.15	811.1	383.15	786.7
313.15	856.6	338.15	832.8	363.15	806.2	388.15	781.8
318.15	851.8	343.15	828.1	368.15	801.1	393.15	777.1

Table 8. Coefficient Z_{RA} in Rackett Equation (eq 6), Standard Deviation of the Fit (σ), and Average Absolute Deviation (AAD)

				ρ_c/kg·m^{-3}	
ester	Z_{RA}	σ/kg·m^{-3}	AAD %	eq 6	lit.
ethyl acetate	0.25620 ± 0.00010	1.4	0.13	307	308[a]
propyl acetate	0.25445 ± 0.00004	1.0	0.09	295	296[a]
n-butyl acetate	0.25572 ± 0.00001	0.9		289	281[b]
n-pentyl acetate	0.25074 ± 0.00001	0.8	0.08	279	277[c]

[a] Ref 21. [b] Ref 16. [c] Ref 20.

Table 9. Coefficients of Equations 6 and 9, Standard Deviation of the Fit (σ), and Average Absolute Deviation (AAD)

ester	C	b_1/MPa	b_2/MPa·K	σ/kg·m^{-3}	AAD %
ethyl acetate	0.105	−179.70	82534.5	1.0	0.10
propyl acetate	0.119	−187.53	90764.9	0.9	0.09
n-butyl acetate	0.176	−271.56	137730.9	0.8	0.07
n-pentyl acetate	0.128	−162.42	89612.7	1.2	0.10

equation proposed by Niesen,[10] which has a solid theoretical basis as discussed by Holcomb and Outcalt.[11] The calibration equation is

$$\rho(T, P, \tau) = \left[\frac{\tau^2(T, P)(A_1 + A_2T + A_3T^2)}{\tau^2(T_0, P_0 = 0)}\right] + A_4 + A_5T + A_6P \quad (1)$$

where $\rho(T, P)$ and $\tau(T, P)$ are the density and the vibration period, respectively, which are both function of temperature (T) and of pressure (P). The vibration period $\tau(T_0, P_0 = 0)$ is measured at a reference temperature (T_0) and vacuum. In this work $T_0 = 303.15$ K, and the measured period at $P = 0$ is $\tau(T_0, P_0) = 0.388074\ \mu$s. The parameters A_i in eq 1 are $A_1 = 10287.83$ kg·m^{-3}, $A_2 = -4.048$ kg·m^{-3}·K^{-1}, $A_3 = 5.701 \times 10^{-4}$ kg·m^{-3}·K^{-2}, $A_4 = -9531.03$ kg·m^{-3}, $A_5 = 1.3846$ kg·m^{-3}·K^{-1}, and $A_6 = -1.4423 \times 10^{-1}$ kg·m^{-3}·MPa^{-1}. For water, density data due to Saul et al.[12] and from the National Institute of Science and Technology (NIST)[13] in the temperature range of (293.15 to 393.15) K and pressures from 0.1 MPa up to 35 MPa were used. For *n*-heptane, the density data compiled by Nichols and Reamer[14] and from NIST[15] were taken in the same range of pressure and temperature. The standard deviation of the fitting (σ)

$$\sigma = [\sum_{i=1}^{N_p} (\rho_{cal} - \rho_{exp})_i^2/(N_p - k)]^{1/2} \quad (2)$$

was 1 kg·m^{-3} and gives the uncertainty assigned to the calibration of the densimeter. In eq 2, ρ_{cal} and ρ_{exp} are respectively the density data from eq 1 and the value for the ith experiment; N_p represents the number of points ($N_p = 436$); and k is the number of adjusted parameters ($k = 6$). The AAD defined as

$$\text{AAD (\%)} = \frac{\sum_{i=1}^{N_p} |(\rho_{cal} - \rho_{exp})/\rho_{exp}|_i}{N_p} \quad (3)$$

was equal to 0.1 %.

Due to the very low viscosity of the esters studied in this work (less than 1 mPa·s at 298.15 K and 0.1 MPa), the density correction ($\Delta\rho$) due to viscosity is less than 0.005 kg·m^{-3}, which

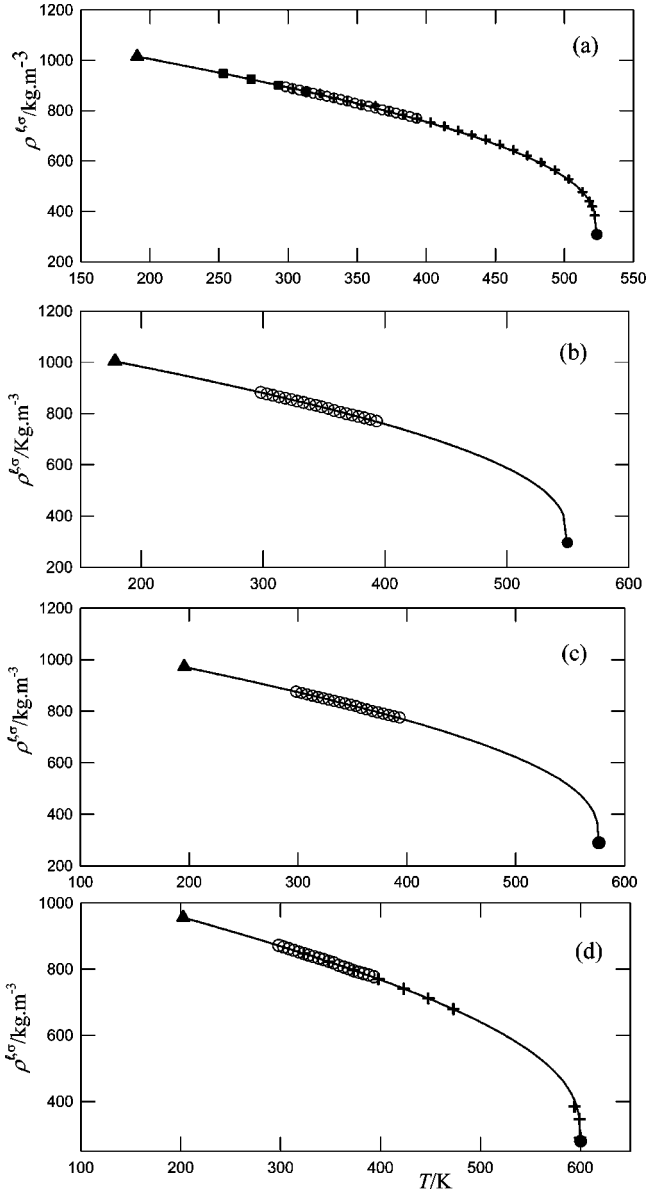

Figure 4. Density of saturated liquid of the alkyl esters ($\rho^{\prime\sigma}$) as a function of temperature. Full curves are calculated from eq 8 with the value Z_{RA} from this work: ▲, triple point; ●, critical point. (a) Ethyl acetate: +, ref 22; ■, ref 5. (b) Propyl acetate. (c) *n*-Butyl acetate. (d) *n*-Pentyl acetate: +, ref 20; ○, this work.

can be considered negligible. This conclusion can be obtained using the equation recommended by Anton Parr for the densimeter DMA 512P:

$$\frac{\Delta\rho}{\rho} = (-0.5 + 0.45\sqrt{\eta}) \times 10^{-4} \quad (4)$$

where η is the dynamic viscosity (in mPa·s). This equation can be applied for liquids with viscosities less than 100 mPa·s. We have not found in the literature viscosity data for the acetates at high pressure. The effect of pressure on liquid viscosity can be predicted with good accuracy from the corresponding states method proposed by Lucas:[16]

$$\frac{\eta}{\eta_{low}} = \frac{1 + D(\Delta P_r/2.118)^A}{1 + C\omega\Delta P_r} \quad (5)$$

where η_{low} is the viscosity at $P = 0.1$ MPa; ω is the acentric factor; ΔP_r ($= (P - P^\sigma)/P_c$) is the change in reduced pressure at fixed temperature (P^σ is the saturation pressure at the same temperature); and A, C, and D are functions of the reduced temperature ($T_r = T/T_c$). Applying eq 5 to the alkyl esters at $T = 298.15$ K and $P = 30$ MPa, the values obtained for the viscosity are less than 1 mPa·s with the exception of the *n*-pentyl acetate substance for which η(298.15 K, 30 MPa) = 1.07mPa.s.

Results and Discussion

Density measurements were carried out in wide ranges of temperature (298 to 393) K and pressure (0.1−35) MPa. Particular attention was given to the subcritical data; therefore, we have measured the density in the above-mentioned temperature domain for several subcritical pressure values. The experimental data for ethyl, propyl, *n*-butyl, and *n*-pentyl acetates are reported in Tables 2 to 5 . In Figure 2, a graphical representation for the ethyl acetate is given. As usual, the density of each ester decreases with the rise of temperature along isobars and increases when pressure increases at constant temperature. Moreover the densities of the alkyl esters decrease with the increase of the alkyl chain length. This behavior was observed also in complex ester molecules like polyol esters.[17] This is the opposite of what is observed with alkanes. In this family the molecules interact only through dipole-induced forces proportional to the length of the carbon chain, and the increasing in the density is due to the reduction of the free volume. In the case of the esters, the adding of -CH_2- groups disrupts the local configurational order of -COO- group causing a lower molecular packing efficiency (decrease in the density).[17]

The density data due to Malhotra and Woolf[4] for propyl acetate and for *n*-butyl acetate at temperatures of (298.14, 313.14, 323.14, and 338.13) K have been compared with our own measurements at the same temperatures and pressures. The results of comparison are shown in Figure 3. The AAD is 0.1 % for both substances.

The Tait equation

$$\rho = \frac{\rho^{ref}}{\left\{1 - C\ln\frac{(B + P)}{(B + P^{ref})}\right\}} \quad (6)$$

was fitted to the measured density data in the ranges of pressure and of temperature mentioned above. The reference state (^{ref}) must be carefully selected. As reference state we could take the liquid at a given temperature and atmospheric pressure, $\rho^{ref} = \rho(\ell, T, P = 0.1$ MPa) or the saturated (σ) liquid, $\rho^{ref} = \rho^{\prime\sigma} = \rho(\ell, T, P^\sigma)$. The vapor pressure ($P^\sigma$) of the aliphatic esters studied here can be described accurately by the Wagner equation:

$$\ln(P^\sigma/\text{kPa}) = \ln(P_c/\text{kPa}) + (T_c/T)(n_1\tau + n_2\tau^{1.5} + n_3\tau^m + n_4\tau^{2m}) \quad (7)$$

where $m = 2.5$ or 3 and $\tau = 1 - T_r$. The critical constants (T_c, P_c) and the parameters n_i are listed in Table 6. From the Wagner equation, we can see that the vapor pressure range corresponding to the temperature range of (298.15 to 393.15) K extends from (12.6 to 346.8) kPa for ethyl acetate, from (4.50 to 173) kPa for propyl acetate, from (1.54 to 85.0) kPa for *n*-butyl acetate, and from (0.5 to 41.8) kPa for *n*-pentyl acetate. This means

Table 10. Isothermal Compressibility (κ_T), Isobaric Expansivity (α_P), Thermal Pressure (γ_V), and Change in Molar Heat Capacity ($\Delta C_{P,m}$) for Ethyl Acetate

	P/MPa											
	0.10	1.00	2.00	3.00	3.80	5.00	10.00	15.00	20.00	25.00	30.00	35.00
						$T = 298.150$ K						
$k_T \times 10^3$/MPa^{-1}	1.080	1.071	1.061	1.052	1.044	1.033	0.990	0.950	0.914	0.881	0.850	0.821
$\alpha_P \times 10^3$/K^{-1}	1.358	1.349	1.339	1.329	1.321	1.309	1.264	1.223	1.184	1.148	1.115	1.084
γ_V/MPa·K^{-1}	1.258	1.260	1.262	1.264	1.265	1.267	1.277	1.286	1.295	1.304	1.313	1.321
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.3	−0.5	−0.6	−0.8	−1.6	−2.2	−2.8	−3.4	−3.8	−4.2
						$T = 303.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.133	1.123	1.112	1.102	1.094	1.082	1.034	0.991	0.952	0.916	0.882	0.851
$\sigma_P \times 10^3$/K^{-1}	1.380	1.370	1.359	1.349	1.341	1.329	1.281	1.237	1.196	1.159	1.124	1.092
γ_V/MPa·K^{-1}	1.218	1.220	1.222	1.224	1.226	1.228	1.238	1.248	1.257	1.266	1.274	1.282
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.5	−0.7	−0.9	−1.7	−2.4	−3.0	−3.5	−4.0	−4.4
						$T = 308.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.190	1.179	1.167	1.156	1.147	1.133	1.082	1.035	0.992	0.953	0.917	0.883
$\alpha_P \times 10^3$/K^{-1}	1.403	1.393	1.381	1.370	1.361	1.348	1.298	1.251	1.209	1.169	1.133	1.099
γ_V/MPa·K^{-1}	1.179	1.181	1.183	1.186	1.187	1.190	1.200	1.209	1.219	1.228	1.236	1.245
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.6	−0.7	−0.9	−1.8	−2.5	−3.1	−3.7	−4.2	−4.6
						$T = 313.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.250	1.238	1.225	1.213	1.203	1.188	1.131	1.080	1.034	0.991	0.952	0.916
$\alpha_P \times 10^3$/K^{-1}	1.427	1.416	1.404	1.392	1.382	1.369	1.315	1.266	1.221	1.180	1.142	1.106
γ_V/MPa·K^{-1}	1.142	1.143	1.146	1.148	1.149	1.152	1.162	1.172	1.181	1.190	1.199	1.207
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.6	−0.8	−1.0	−1.9	−2.6	−3.3	−3.8	−4.3	−4.8
						$T = 318.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.315	1.302	1.288	1.274	1.263	1.247	1.184	1.128	1.078	1.032	0.990	0.951
$\alpha_P \times 10^3$/K^{-1}	1.452	1.440	1.427	1.414	1.404	1.390	1.332	1.280	1.233	1.190	1.150	1.113
γ_V/MPa·K^{-1}	1.104	1.106	1.108	1.111	1.112	1.115	1.125	1.135	1.144	1.153	1.162	1.170
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.6	−0.8	−1.1	−2.0	−2.8	−3.4	−4.0	−4.5	−4.9
						$T = 323.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.385	1.370	1.354	1.339	1.327	1.309	1.241	1.179	1.124	1.074	1.029	0.987
$\alpha_P \times 10^3$/K^{-1}	1.478	1.466	1.452	1.438	1.427	1.412	1.350	1.295	1.245	1.200	1.158	1.119
γ_V/MPa·K^{-1}	1.068	1.070	1.072	1.074	1.076	1.078	1.088	1.098	1.108	1.117	1.125	1.133
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.5	−0.7	−0.9	−1.1	−2.1	−2.9	−3.6	−4.2	−4.7	−5.1
						$T = 328.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.460	1.443	1.426	1.409	1.395	1.376	1.301	1.233	1.173	1.119	1.070	1.025
$\alpha_P \times 10^3$/K^{-1}	1.506	1.492	1.477	1.462	1.451	1.434	1.369	1.310	1.257	1.209	1.165	1.125
γ_V/MPa·K^{-1}	1.032	1.034	1.036	1.038	1.040	1.042	1.052	1.062	1.071	1.080	1.089	1.097
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.5	−0.7	−0.9	−1.2	−2.2	−3.1	−3.8	−4.4	−4.9	−5.3
						$T = 333.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.540	1.522	1.503	1.484	1.469	1.448	1.364	1.291	1.225	1.166	1.113	1.065
$\alpha_P \times 10^3$/K^{-1}	1.535	1.520	1.504	1.488	1.475	1.457	1.387	1.325	1.269	1.218	1.172	1.129
γ_V/MPa·K^{-1}	0.996	0.998	1.000	1.003	1.004	1.007	1.017	1.026	1.036	1.044	1.053	1.060
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.5	−0.8	−1.0	−1.3	−2.3	−3.2	−3.9	−4.5	−5.0	−5.4
						$T = 338.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.628	1.608	1.586	1.565	1.549	1.525	1.433	1.352	1.280	1.216	1.158	1.106
$\alpha_P \times 10^3$/K^{-1}	1.565	1.549	1.531	1.514	1.501	1.481	1.406	1.340	1.280	1.226	1.177	1.133
γ_V/MPa·K^{-1}	0.961	0.963	0.965	0.968	0.969	0.972	0.982	0.991	1.000	1.008	1.016	1.024
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.6	−0.8	−1.0	−1.4	−2.5	−3.4	−4.1	−4.7	−5.2	−5.5
						$T = 343.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.723	1.700	1.676	1.653	1.634	1.608	1.506	1.417	1.338	1.269	1.206	1.150
$\alpha_P \times 10^3$/K^{-1}	1.597	1.579	1.560	1.542	1.527	1.506	1.425	1.354	1.291	1.234	1.182	1.135
γ_V/MPa·K^{-1}	0.927	0.929	0.931	0.933	0.935	0.937	0.947	0.956	0.964	0.972	0.980	0.987
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.6	−0.9	−1.1	−1.4	−2.6	−3.5	−4.3	−4.9	−5.3	−5.6
						$T = 348.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.826	1.801	1.774	1.748	1.727	1.697	1.584	1.486	1.400	1.324	1.257	1.196
$\alpha_P \times 10^3$/K^{-1}	1.631	1.611	1.591	1.570	1.555	1.532	1.445	1.368	1.301	1.240	1.186	1.136
γ_V/MPa·K^{-1}	0.893	0.895	0.897	0.899	0.900	0.903	0.912	0.921	0.929	0.936	0.944	0.950
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.6	−1.0	−1.2	−1.5	−2.8	−3.7	−4.5	−5.0	−5.4	−5.7
						$T = 353.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.940	1.911	1.881	1.851	1.828	1.795	1.669	1.561	1.466	1.383	1.310	
$\alpha_P \times 10^3$/K^{-1}	1.666	1.645	1.622	1.600	1.583	1.559	1.464	1.382	1.309	1.245	1.187	
γ_V/MPa·K^{-1}	0.859	0.861	0.863	0.865	0.866	0.868	0.877	0.885	0.893	0.900	0.907	
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.7	−1.0	−1.3	−1.6	−2.9	−3.9	−4.6	−5.1	−5.5	
						$T = 358.15$ K						
$k_T \times 10^3$/MPa^{-1}	2.064	2.032	1.997	1.964	1.938	1.901	1.760	1.640	1.537	1.446		
$\alpha_P \times 10^3$/K^{-1}	1.704	1.681	1.656	1.632	1.613	1.586	1.483	1.395	1.317	1.249		
γ_V/MPa·K^{-1}	0.825	0.827	0.829	0.831	0.832	0.834	0.843	0.850	0.857	0.863		
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.4	−0.7	−1.1	−1.4	−1.8	−3.1	−4.1	−4.8	−5.2		
						$T = 363.15$ K						
$k_T \times 10^3$/MPa^{-1}	2.201	2.165	2.126	2.088	2.059	2.017	1.860	1.726	1.612	1.513		
$\alpha_P \times 10^3$/K^{-1}	1.744	1.718	1.691	1.664	1.644	1.614	1.502	1.406	1.323	1.250		
γ_V/MPa·K^{-1}	0.792	0.794	0.795	0.797	0.798	0.800	0.808	0.815	0.821	0.826		
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.4	−0.8	−1.2	−1.5	−1.9	−3.3	−4.2	−4.9	−5.3		

Table 10. (Continued)

	P/MPa											
	0.10	1.00	2.00	3.00	3.80	5.00	10.00	15.00	20.00	25.00	30.00	35.00
						$T = 368.15$ K						
$k_T \times 10^3$/MPa^{-1}	2.353	2.312	2.267	2.224	2.191	2.144	1.967	1.819	1.693			
$\alpha_P \times 10^3$/K^{-1}	1.786	1.758	1.728	1.698	1.676	1.643	1.521	1.417	1.327			
γ_V/MPa·K^{-1}	0.759	0.760	0.762	0.764	0.765	0.766	0.773	0.779	0.784			
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.4	−0.9	−1.3	−1.6	−2.0	−3.4	−4.4	−5.0			
						$T = 373.15$ K						
$k_T \times 10^3$/MPa^{-1}	2.523	2.475	2.424	2.376	2.338	2.284	2.085	1.919	1.780			
$\alpha_P \times 10^3$/K^{-1}	1.832	1.800	1.766	1.734	1.709	1.673	1.538	1.425	1.328			
γ_V/MPa·K^{-1}	0.726	0.727	0.729	0.730	0.731	0.732	0.738	0.742	0.746			
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.5	−0.9	−1.4	−1.7	−2.2	−3.6	−4.5	−5.0			
						$T = 378.15$ K						
$k_T \times 10^3$/MPa^{-1}	2.714	2.659	2.600	2.544	2.501	2.439	2.214	2.028				
$\alpha_P \times 10^3$/K^{-1}	1.881	1.845	1.807	1.771	1.743	1.703	1.554	1.431				
γ_V/MPa·K^{-1}	0.693	0.694	0.695	0.696	0.697	0.698	0.702	0.705				
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.5	−1.0	−1.5	−1.8	−2.3	−3.8	−4.6				
						$T = 383.15$ K						
$k_T \times 10^3$/MPa^{-1}	2.929	2.865	2.797	2.732	2.683	2.612	2.355	2.147				
$\alpha_P \times 10^3$/K^{-1}	1.934	1.893	1.851	1.810	1.778	1.733	1.568	1.433				
γ_V/MPa·K^{-1}	0.660	0.661	0.662	0.662	0.663	0.664	0.666	0.667				
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.5	−1.1	−1.6	−2.0	−2.5	−3.9	−4.7				
						$T = 388.15$ K						
$k_T \times 10^3$/MPa^{-1}	3.175	3.100	3.020	2.945	2.887	2.806	2.512					
$\alpha_P \times 10^3$/K^{-1}	1.991	1.945	1.896	1.850	1.814	1.764	1.580					
γ_V/MPa·K^{-1}	0.627	0.627	0.628	0.628	0.628	0.629	0.629					
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.6	−1.2	−1.7	−2.1	−2.6	−4.1					
						$T = 393.15$ K						
$k_T \times 10^3$/MPa^{-1}	3.457	3.368	3.274	3.186	3.119	3.024	2.686					
$\alpha_P \times 10^3$/K^{-1}	2.054	2.000	1.944	1.891	1.851	1.793	1.587					
γ_V/MPa·K^{-1}	0.594	0.594	0.594	0.594	0.593	0.593	0.591					
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.7	−1.3	−1.9	−2.3	−2.8	−4.2					

that only for the first two substances the liquid density could be measured in all the temperature range at $P = 0.1$ MPa. Therefore the saturated liquid state was selected here as the reference state. Once the reference state is chosen, the values

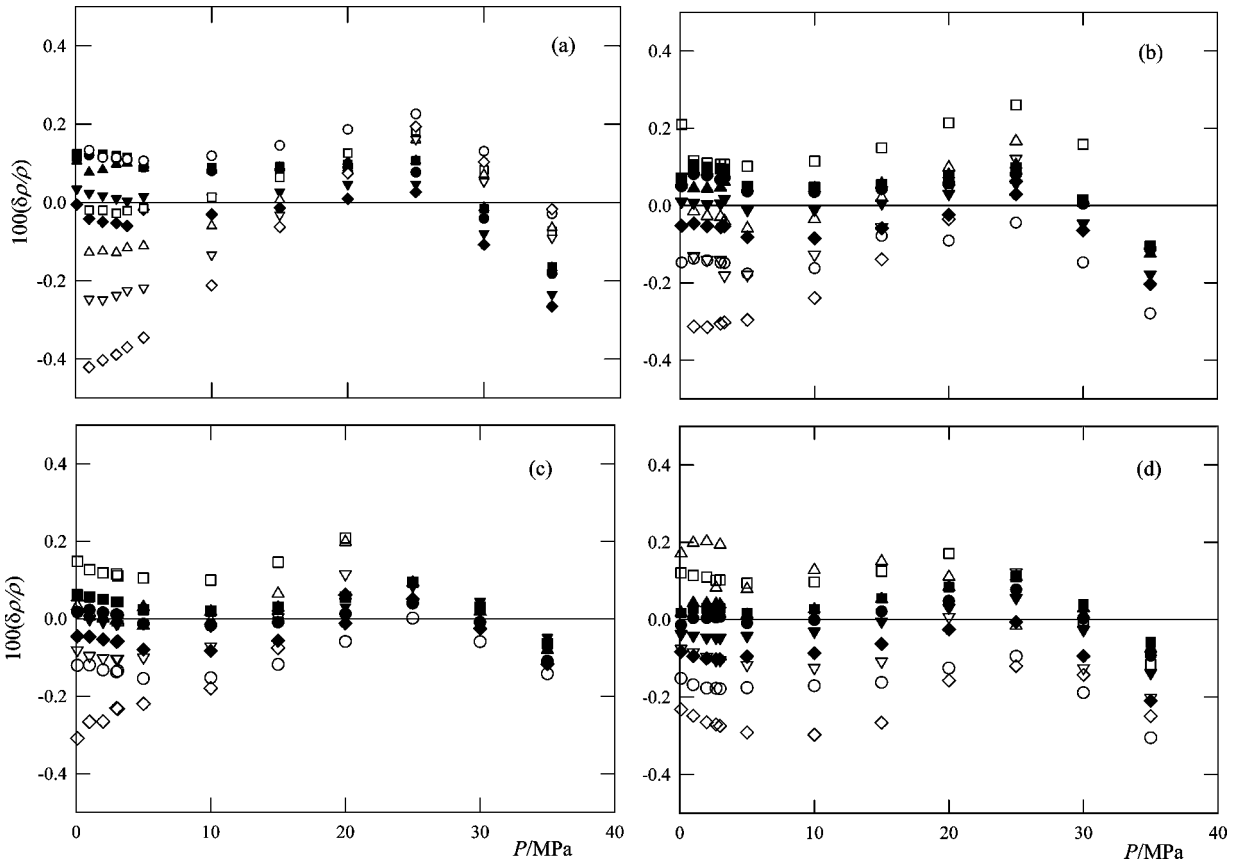

Figure 5. Percentage density deviations between the values obtained with eq 6 and experimental data: (a) ethyl acetate, (b) propyl acetate, (c) *n*-butyl acetate, (d) *n*-pentyl acetate. The temperatures are ●, 303.15 K; ■, 313.15 K; ▲, 323.15 K; ▼, 333.15 K; ◆, 343.15 K; ○, 353.15 K; □, 363.15 K; △, 373.15 K; ▽, 383.15 K; ◇, 393.15 K. The quantity $100(\delta\rho/\rho)$ means $100(\rho_{eq\,6} - \rho_{exp})/\rho_{exp}$.

Table 11. Isothermal Compressibility (κ_T), Isobaric Expansivity (α_P), Thermal Pressure (γ_V), and Change in Molar Heat Capacity ($\Delta C_{P,m}$) for Propyl Acetate

	P/MPa											
	0.10	1.00	2.00	3.00	3.30	5.00	10.00	15.00	20.00	25.00	30.00	35.00
						$T = 298.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.017	1.010	1.003	0.996	0.993	0.981	0.947	0.915	0.886	0.858	0.833	0.809
$\alpha_P \times 10^3$/K^{-1}	1.244	1.236	1.227	1.219	1.216	1.202	1.162	1.125	1.090	1.057	1.027	0.998
γ_V/MPa·K^{-1}	1.223	1.223	1.224	1.224	1.224	1.225	1.227	1.229	1.231	1.232	1.232	1.234
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.3	−0.5	−0.5	−0.8	−1.5	−2.2	−2.8	−3.3	−3.8	−4.2
						$T = 303.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.063	1.055	1.047	1.039	1.037	1.023	0.986	0.952	0.920	0.891	0.863	0.837
$\alpha_P \times 10^3$/K^{-1}	1.262	1.254	1.245	1.235	1.233	1.218	1.176	1.137	1.101	1.066	1.034	1.004
γ_V/MPa·K^{-1}	1.187	1.188	1.188	1.189	1.189	1.190	1.192	1.194	1.196	1.197	1.198	1.199
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.3	−0.5	−0.6	−0.9	−1.6	−2.3	−2.9	−3.5	−3.9	−4.4
						$T = 308.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.111	1.103	1.094	1.085	1.083	1.068	1.028	0.991	0.956	0.924	0.895	0.867
$\alpha_P \times 10^3$/K^{-1}	1.281	1.272	1.262	1.253	1.250	1.234	1.190	1.149	1.111	1.075	1.042	1.011
γ_V/MPa·K^{-1}	1.153	1.153	1.154	1.154	1.154	1.155	1.158	1.160	1.162	1.163	1.164	1.166
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.5	−0.6	−0.9	−1.7	−2.4	−3.1	−3.6	−4.1	−4.5
						$T = 313.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.162	1.153	1.143	1.134	1.131	1.115	1.071	1.031	0.994	0.960	0.928	0.898
$\alpha_P \times 10^3$/K^{-1}	1.300	1.291	1.281	1.270	1.267	1.251	1.204	1.161	1.121	1.084	1.049	1.017
γ_V/MPa·K^{-1}	1.119	1.119	1.120	1.120	1.121	1.122	1.124	1.126	1.128	1.130	1.131	1.132
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.6	−0.6	−1.0	−1.8	−2.6	−3.2	−3.8	−4.3	−4.7
						$T = 318.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.216	1.206	1.196	1.185	1.182	1.165	1.117	1.074	1.033	0.996	0.962	0.930
$\alpha_P \times 10^3$/K^{-1}	1.320	1.310	1.299	1.289	1.286	1.268	1.219	1.174	1.132	1.093	1.057	1.023
γ_V/MPa·K^{-1}	1.086	1.086	1.087	1.087	1.088	1.088	1.091	1.093	1.095	1.097	1.098	1.100
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.6	−0.7	−1.0	−1.9	−2.7	−3.3	−3.9	−4.4	−4.9
						$T = 323.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.274	1.263	1.251	1.240	1.236	1.218	1.166	1.118	1.075	1.035	0.998	0.964
$\alpha_P \times 10^3$/K^{-1}	1.341	1.331	1.319	1.308	1.304	1.286	1.234	1.186	1.142	1.102	1.064	1.028
γ_V/MPa·K^{-1}	1.053	1.054	1.054	1.055	1.055	1.056	1.059	1.061	1.063	1.065	1.066	1.067
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.7	−0.7	−1.1	−2.0	−2.8	−3.5	−4.1	−4.6	−5.0
						$T = 328.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.335	1.323	1.310	1.298	1.294	1.273	1.217	1.165	1.118	1.075	1.035	0.999
$\alpha_P \times 10^3$/K^{-1}	1.363	1.352	1.339	1.327	1.324	1.304	1.249	1.199	1.153	1.110	1.070	1.034
γ_V/MPa·K^{-1}	1.021	1.022	1.022	1.023	1.023	1.024	1.027	1.029	1.031	1.033	1.034	1.035
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.5	−0.7	−0.8	−1.1	−2.1	−2.9	−3.7	−4.3	−4.8	−5.2
						$T = 333.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.400	1.387	1.373	1.359	1.355	1.333	1.271	1.214	1.164	1.117	1.074	1.035
$\alpha_P \times 10^3$/K^{-1}	1.386	1.374	1.361	1.348	1.344	1.323	1.265	1.212	1.163	1.118	1.077	1.038
γ_V/MPa·K^{-1}	0.990	0.990	0.991	0.992	0.992	0.993	0.995	0.998	1.000	1.001	1.002	1.003
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.5	−0.7	−0.8	−1.2	−2.2	−3.1	−3.8	−4.4	−4.9	−5.4
						$T = 338.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.470	1.455	1.440	1.425	1.420	1.395	1.328	1.267	1.211	1.161	1.115	1.073
$\alpha_P \times 10^3$/K^{-1}	1.409	1.397	1.383	1.369	1.365	1.342	1.281	1.224	1.173	1.126	1.083	1.042
γ_V/MPa·K^{-1}	0.959	0.960	0.960	0.961	0.961	0.962	0.964	0.967	0.968	0.970	0.971	0.972
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.5	−0.8	−0.9	−1.3	−2.3	−3.2	−4.0	−4.6	−5.1	−5.5
						$T = 343.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.544	1.528	1.511	1.495	1.490	1.463	1.388	1.322	1.262	1.207	1.158	1.112
$\alpha_P \times 10^3$/K^{-1}	1.434	1.420	1.405	1.391	1.386	1.362	1.297	1.237	1.183	1.133	1.088	1.046
γ_V/MPa·K^{-1}	0.929	0.929	0.930	0.930	0.931	0.932	0.934	0.936	0.938	0.939	0.940	0.940
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.5	−0.8	−0.9	−1.3	−2.5	−3.4	−4.2	−4.8	−5.3	−5.7
						$T = 348.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.624	1.607	1.588	1.570	1.564	1.534	1.453	1.380	1.315	1.256	1.202	1.154
$\alpha_P \times 10^3$/K^{-1}	1.460	1.445	1.429	1.413	1.409	1.383	1.313	1.250	1.193	1.140	1.093	1.049
γ_V/MPa·K^{-1}	0.899	0.899	0.900	0.901	0.901	0.902	0.904	0.906	0.907	0.908	0.909	0.909
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.6	−0.9	−1.0	−1.4	−2.6	−3.6	−4.3	−4.9	−5.4	−5.8
						$T = 353.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.710	1.691	1.670	1.650	1.644	1.611	1.521	1.442	1.371	1.307	1.249	1.197
$\alpha_P \times 10^3$/K^{-1}	1.487	1.471	1.454	1.437	1.432	1.404	1.329	1.262	1.202	1.147	1.096	1.050
γ_V/MPa·K^{-1}	0.869	0.870	0.870	0.871	0.871	0.872	0.874	0.875	0.877	0.877	0.877	0.877
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.6	−0.9	−1.0	−1.5	−2.7	−3.7	−4.5	−5.1	−5.6	−5.9
						$T = 358.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.803	1.782	1.759	1.736	1.730	1.693	1.595	1.508	1.430	1.361	1.299	1.242
$\alpha_P \times 10^3$/K^{-1}	1.515	1.498	1.480	1.461	1.456	1.426	1.346	1.275	1.210	1.152	1.099	1.051
γ_V/MPa·K^{-1}	0.840	0.841	0.841	0.842	0.842	0.843	0.844	0.845	0.846	0.846	0.846	0.846
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.7	−1.0	−1.1	−1.6	−2.9	−3.9	−4.7	−5.3	−5.7	−6.0
						$T = 363.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.904	1.880	1.854	1.829	1.822	1.781	1.673	1.578	1.493	1.418	1.351	
$\alpha_P \times 10^3$/K^{-1}	1.545	1.527	1.506	1.487	1.481	1.449	1.363	1.286	1.218	1.157	1.101	
γ_V/MPa·K^{-1}	0.812	0.812	0.812	0.813	0.813	0.813	0.815	0.815	0.816	0.816	0.815	
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.7	−1.1	−1.2	−1.7	−3.0	−4.1	−4.8	−5.4	−5.8	

Table 11. (Continued)

	P/MPa											
	0.10	1.00	2.00	3.00	3.30	5.00	10.00	15.00	20.00	25.00	30.00	35.00
						$T = 368.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	2.013	1.987	1.958	1.930	1.922	1.877	1.757	1.652	1.560	1.478		
$\alpha_P \times 10^3$/K^{-1}	1.577	1.556	1.534	1.513	1.507	1.472	1.380	1.298	1.225	1.160		
γ_V/MPa·K^{-1}	0.783	0.783	0.784	0.784	0.784	0.785	0.785	0.786	0.785	0.784		
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.4	−0.8	−1.1	−1.2	−1.8	−3.2	−4.2	−5.0	−5.5		
						$T = 373.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	2.132	2.102	2.070	2.039	2.030	1.980	1.847	1.732	1.631	1.542		
$\alpha_P \times 10^3$/K^{-1}	1.610	1.588	1.564	1.541	1.534	1.496	1.396	1.308	1.231	1.161		
γ_V/MPa·K^{-1}	0.755	0.755	0.755	0.755	0.756	0.756	0.756	0.756	0.755	0.753		
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.4	−0.8	−1.2	−1.3	−1.9	−3.4	−4.4	−5.1	−5.6		
						$T = 378.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	2.263	2.229	2.193	2.158	2.148	2.092	1.944	1.817	1.707			
$\alpha_P \times 10^3$/K^{-1}	1.645	1.620	1.594	1.569	1.562	1.521	1.413	1.318	1.235			
γ_V/MPa·K^{-1}	0.727	0.727	0.727	0.727	0.727	0.727	0.727	0.725	0.724			
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.4	−0.9	−1.3	−1.4	−2.0	−3.5	−4.6	−5.3			
						$T = 383.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	2.406	2.368	2.327	2.288	2.277	2.214	2.049	1.909	1.787			
$\alpha_P \times 10^3$/K^{-1}	1.682	1.655	1.626	1.599	1.591	1.546	1.428	1.327	1.237			
γ_V/MPa·K^{-1}	0.699	0.699	0.699	0.699	0.699	0.698	0.697	0.695	0.692			
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.5	−0.9	−1.4	−1.5	−2.2	−3.7	−4.7	−5.3			
						$T = 388.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	2.564	2.521	2.475	2.431	2.418	2.347	2.163	2.007				
$\alpha_P \times 10^3$/K^{-1}	1.721	1.692	1.660	1.630	1.621	1.572	1.443	1.333				
γ_V/MPa·K^{-1}	0.671	0.671	0.671	0.670	0.670	0.670	0.667	0.664				
$\Delta C_{P,m}$/Jmol^{-1}·K^{-1}	0.0	−0.5	−1.0	−1.5	−1.6	−2.3	−3.9	−4.9				
						$T = 393.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	2.739	2.690	2.638	2.588	2.573	2.493	2.287	2.114				
$\alpha_P \times 10^3$/K^{-1}	1.763	1.730	1.695	1.662	1.652	1.598	1.457	1.338				
γ_V/MPa·K^{-1}	0.644	0.643	0.643	0.642	0.642	0.641	0.637	0.633				
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.5	−1.1	−1.6	−1.7	−2.5	−4.1	−5.0				

$\rho^{ref} = \rho^{\prime\sigma}$ were obtained by fitting eq 6 to isothermal density data using values of pressure lower than the critical pressure value. The value of vapor pressure needed in eq 6 was obtained from Wagner equation. We have used subcritical pressures to avoid bad extrapolations, which can result from the use of density at higher pressures far from the equilibrium pressure (P^σ). The density data of the saturated liquid ($\rho^{\prime\sigma}$) calculated as stated before are reported in Table 7 and are compared with literature values in Figure 4. Our results are in good agreement with values from the literature. The Rackett equation

$$\frac{1}{\rho^{\prime\sigma}} = \left\{\frac{RT_c}{MP_c}\right\} Z_{RA}^{[1+(1-T_r)^{2/7}]} \tag{8}$$

was fitted to the density data of the saturated liquid obtained as referred before in the range (298.15 to 393.15) K. The values of the fitted parameter Z_{RA} and the associated standard deviation of the fit are listed in Table 8. In the same table values of density at the critical point (ρ_c) obtained from eq 8 are compared with literature ones. The accordance is very good. The calculated values of the saturated liquid density from eq 8 are also represented in Figure 4. It is remarkable that all the saturation curves can be well-predicted in all the liquid + gas equilibrium range using the eq 8 fitted density data in very narrow ranges of temperature.

Equation 6 was fitted to the experimental *PVT* data in the temperature range of (298.15 to 393.15) K and up to pressures of 35 MPa. The vapor pressure (P^σ) and the saturated liquid density ($\rho^{\prime\sigma}$) used in eq 6 were calculated from eqs 7 and 8, respectively. The coefficient *C* was treated as constant for each substance, while the parameter *B* was considered temperature-dependent following a function proposed by Kumagai and Iwasaki.[5] They have found that *B* is proportional to the reciprocal of temperature. This dependence is given by

$$B = b_1 + \frac{b_2}{T} \tag{9}$$

where b_1 and b_2 are parameters obtained from the fitting of eq 6 to *PVT* data. As we have concluded including more terms in powers of T^{-1} does not improve the fittings. In Table 9, we list the parameters of the Tait equation, the average absolute deviation (AAD), and the standard deviation of the fittings (σ) for the esters studied.

In Figure 5, the percentage density deviations plots between the calculated values with eq 6 and experimental data are depicted. The absolute percentage deviations are less than 0.2 % in the majority part of the temperature and pressure domains. The AAD is of the order of 0.1 % for all the substances (see Table 9).

From eq 6 some mechanical coefficients were calculated as functions of pressure and temperature. For the isothermal compressibility (κ_T) defined as

$$\kappa_T = -\frac{1}{V_m}\left(\frac{\partial V_m}{\partial P}\right)_T = \frac{1}{\rho}\left(\frac{\partial \rho}{\partial P}\right)_T = \left(\frac{\partial \ln \rho}{\partial P}\right)_T \tag{10}$$

the final expression is

$$\kappa_T = \left(\frac{C}{B+P}\right)\left(\frac{\rho}{\rho^{\prime\sigma}}\right) \tag{11}$$

The isothermal compressibilities of the esters are listed in Tables 10 to 13, and the values for ethyl acetate are shown in Figure 6. For the other alkyl esters the representations will be similar.

Table 12. Isothermal Compressibility (κ_T), Isobaric Expansivity (α_P), Thermal Pressure (γ_V), and Change in Molar Heat Capacity ($\Delta C_{P,m}$) for *N*-Butyl Acetate

	P/MPa											
	0.10	1.00	2.00	3.00	3.10	5.00	10.00	15.00	20.00	25.00	30.00	35.00
						$T = 298.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	0.923	0.920	0.916	0.912	0.911	0.904	0.886	0.868	0.851	0.835	0.819	0.804
$\alpha_P \times 10^3$/K^{-1}	1.138	1.131	1.124	1.116	1.116	1.102	1.067	1.033	1.000	0.969	0.939	0.910
γ_V/MPa·K^{-1}	1.233	1.230	1.227	1.224	1.224	1.219	1.204	1.190	1.176	1.161	1.146	1.131
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.1	−0.3	−0.5	−0.5	−0.8	−1.5	−2.1	−2.7	−3.2	−3.6	−4.0
						$T = 303.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	0.962	0.958	0.954	0.949	0.949	0.941	0.921	0.902	0.883	0.866	0.849	0.833
$\alpha_P \times 10^3$/K^{-1}	1.153	1.146	1.138	1.130	1.129	1.115	1.078	1.043	1.009	0.976	0.945	0.914
γ_V/MPa·K^{-1}	1.199	1.196	1.193	1.191	1.190	1.185	1.171	1.156	1.142	1.127	1.112	1.098
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.3	−0.5	−0.5	−0.8	−1.6	−2.2	−2.8	−3.3	−3.7	−4.1
						$T = 308.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.002	0.998	0.993	0.989	0.988	0.980	0.958	0.937	0.917	0.899	0.881	0.863
$\alpha_P \times 10^3$/K^{-1}	1.168	1.161	1.153	1.144	1.144	1.128	1.090	1.053	1.017	0.983	0.951	0.919
γ_V/MPa·K^{-1}	1.166	1.163	1.160	1.158	1.157	1.152	1.138	1.123	1.109	1.094	1.079	1.064
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.3	−0.5	−0.5	−0.9	−1.6	−2.3	−2.9	−3.4	−3.9	−4.3
						$T = 313.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.045	1.040	1.035	1.030	1.030	1.020	0.997	0.974	0.953	0.933	0.913	0.895
$\alpha_P \times 10^3$/K^{-1}	1.184	1.176	1.168	1.159	1.158	1.142	1.102	1.063	1.026	0.990	0.956	0.923
γ_V/MPa·K^{-1}	1.133	1.131	1.128	1.125	1.125	1.120	1.105	1.091	1.076	1.062	1.047	1.032
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.5	−0.6	−0.9	−1.7	−2.4	−3.0	−3.6	−4.0	−4.4
						$T = 318.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.089	1.084	1.079	1.073	1.073	1.063	1.037	1.013	0.990	0.968	0.947	0.928
$\alpha_P \times 10^3$/K^{-1}	1.200	1.192	1.183	1.174	1.173	1.156	1.114	1.073	1.034	0.997	0.962	0.928
γ_V/MPa·K^{-1}	1.102	1.099	1.097	1.094	1.093	1.088	1.074	1.059	1.045	1.030	1.015	1.000
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.6	−0.6	−0.9	−1.8	−2.5	−3.2	−3.7	−4.2	−4.5
						$T = 323.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.137	1.131	1.125	1.119	1.119	1.108	1.080	1.054	1.029	1.005	0.983	0.962
$\alpha_P \times 10^3$/K^{-1}	1.217	1.209	1.199	1.190	1.189	1.171	1.126	1.084	1.043	1.004	0.967	0.931
γ_V/MPa·K^{-1}	1.071	1.069	1.066	1.063	1.063	1.057	1.043	1.028	1.014	0.999	0.984	0.968
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.6	−0.6	−1.0	−1.9	−2.6	−3.3	−3.9	−4.3	−4.7
						$T = 328.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.186	1.180	1.174	1.168	1.167	1.155	1.125	1.096	1.070	1.044	1.020	0.997
$a_P \times 10^3$/K^{-1}	1.235	1.226	1.216	1.206	1.205	1.186	1.139	1.094	1.051	1.011	0.972	0.935
γ_V/MPa·K^{-1}	1.041	1.038	1.036	1.033	1.032	1.027	1.012	0.998	0.983	0.968	0.953	0.937
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.6	−0.7	−1.1	−2.0	−2.8	−3.4	−4.0	−4.5	−4.8
						$T = 333.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.239	1.233	1.225	1.218	1.218	1.205	1.172	1.141	1.112	1.085	1.059	1.034
$\alpha_P \times 10^3$/K^{-1}	1.253	1.243	1.233	1.222	1.221	1.201	1.152	1.104	1.060	1.017	0.976	0.937
γ_V/MPa·K^{-1}	1.011	1.009	1.006	1.003	1.003	0.997	0.983	0.968	0.953	0.937	0.922	0.906
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.7	−0.7	−1.1	−2.1	−2.9	−3.6	−4.1	−4.6	−5.0
						$T = 338.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.295	1.288	1.280	1.272	1.272	1.257	1.222	1.188	1.157	1.128	1.100	1.073
$\alpha_P \times 10^3$/K^{-1}	1.272	1.262	1.250	1.239	1.238	1.217	1.165	1.115	1.068	1.023	0.980	0.940
γ_V/MPa·K^{-1}	0.982	0.980	0.977	0.974	0.974	0.968	0.953	0.938	0.923	0.907	0.892	0.876
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.5	−0.7	−0.7	−1.2	−2.2	−3.0	−3.7	−4.3	−4.8	−5.1
						$T = 343.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.354	1.346	1.338	1.329	1.329	1.313	1.274	1.238	1.204	1.172	1.142	1.114
$\alpha_P \times 10^3$/K^{-1}	1.292	1.281	1.269	1.257	1.256	1.234	1.178	1.125	1.076	1.029	0.984	0.942
γ_V/MPa·K^{-1}	0.954	0.951	0.948	0.945	0.945	0.939	0.924	0.909	0.893	0.878	0.862	0.845
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.5	−0.8	−0.8	−1.2	−2.3	−3.2	−3.9	−4.4	−4.9	−5.2
						$T = 348.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.417	1.408	1.399	1.390	1.389	1.372	1.330	1.291	1.254	1.219	1.187	1.156
$\alpha_P \times 10^3$/K^{-1}	1.312	1.300	1.288	1.275	1.274	1.250	1.191	1.136	1.084	1.034	0.987	0.943
γ_V/MPa·K^{-1}	0.926	0.923	0.920	0.917	0.917	0.911	0.896	0.880	0.864	0.848	0.832	0.815
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.5	−0.8	−0.8	−1.3	−2.4	−3.3	−4.0	−4.6	−5.0	−5.3
						$T = 353.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.484	1.474	1.464	1.454	1.453	1.435	1.389	1.346	1.306	1.269	1.234	
$\alpha_P \times 10^3$/K^{-1}	1.333	1.321	1.307	1.294	1.292	1.268	1.205	1.146	1.091	1.039	0.989	
γ_V/MPa·K^{-1}	0.899	0.896	0.893	0.890	0.889	0.883	0.868	0.852	0.835	0.819	0.802	
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.6	−0.8	−0.9	−1.4	−2.5	−3.4	−4.2	−4.7	−5.1	
						$T = 358.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.555	1.545	1.534	1.523	1.522	1.502	1.451	1.405	1.361	1.321	1.283	
$\alpha_P \times 10^3$/K^{-1}	1.355	1.342	1.327	1.313	1.312	1.285	1.219	1.156	1.098	1.043	0.991	
γ_V/MPa·K^{-1}	0.871	0.869	0.865	0.862	0.862	0.856	0.840	0.823	0.807	0.790	0.773	
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.6	−0.9	−0.9	−1.4	−2.6	−3.6	−4.3	−4.9	−5.3	
						$T = 363.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.631	1.620	1.608	1.596	1.595	1.573	1.518	1.467	1.419	1.376	1.335	
$\alpha_P \times 10^3$/K^{-1}	1.378	1.364	1.349	1.333	1.332	1.303	1.233	1.166	1.105	1.046	0.992	
γ_V/MPa·K^{-1}	0.845	0.842	0.839	0.835	0.835	0.829	0.812	0.795	0.778	0.761	0.743	
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.6	−0.9	−1.0	−1.5	−2.8	−3.7	−4.5	−5.0	−5.3	

Table 12. (Continued)

	P/MPa											
	0.10	1.00	2.00	3.00	3.10	5.00	10.00	15.00	20.00	25.00	30.00	35.00
					T = 368.15 K							
$\kappa_T \times 10^3$/MPa^{-1}	1.713	1.701	1.688	1.674	1.673	1.649	1.588	1.533	1.481	1.434		
$\alpha_P \times 10^3$/K^{-1}	1.402	1.387	1.370	1.354	1.352	1.322	1.247	1.176	1.110	1.049		
γ_V/MPa·K^{-1}	0.818	0.815	0.812	0.809	0.808	0.802	0.785	0.767	0.750	0.732		
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.7	−1.0	−1.0	−1.6	−2.9	−3.9	−4.6	−5.1		
					T = 373.15 K							
$\kappa_T \times 10^3$/MPa^{-1}	1.801	1.788	1.773	1.758	1.757	1.730	1.664	1.603	1.547	1.495		
$\alpha_P \times 10^3$/K^{-1}	1.427	1.411	1.393	1.376	1.374	1.341	1.260	1.185	1.115	1.050		
γ_V/MPa·K^{-1}	0.792	0.789	0.786	0.782	0.782	0.775	0.758	0.740	0.721	0.703		
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.7	−1.1	−1.1	−1.7	−3.1	−4.1	−4.8	−5.2		
					T = 378.15 K							
$\kappa_T \times 10^3$/MPa^{-1}	1.896	1.881	1.865	1.848	1.847	1.817	1.744	1.678	1.616			
$\alpha_P \times 10^3$/K^{-1}	1.454	1.436	1.417	1.398	1.396	1.361	1.274	1.194	1.120			
γ_V/MPa·K^{-1}	0.767	0.763	0.760	0.756	0.756	0.749	0.731	0.712	0.693			
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.4	−0.8	−1.1	−1.2	−1.8	−3.2	−4.2	−4.9			
					T = 383.15 K							
$\kappa_T \times 10^3$/MPa^{-1}	1.998	1.982	1.963	1.946	1.944	1.911	1.831	1.757	1.690			
$\alpha_P \times 10^3$/K^{-1}	1.481	1.462	1.441	1.421	1.419	1.381	1.288	1.202	1.123			
γ_V/MPa·K^{-1}	0.741	0.738	0.734	0.730	0.730	0.723	0.704	0.684	0.664			
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.4	−0.8	−1.2	−1.2	−1.9	−3.4	−4.4	−5.0			
					T = 388.15 K							
$\kappa_T \times 10^3$/MPa^{-1}	2.109	2.091	2.070	2.051	2.049	2.012	1.923	1.843	1.769			
$\alpha_P \times 10^3$/K^{-1}	1.510	1.489	1.467	1.445	1.443	1.402	1.301	1.209	1.124			
γ_V/MPa·K^{-1}	0.716	0.712	0.708	0.705	0.704	0.697	0.677	0.656	0.635			
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.4	−0.9	−1.3	−1.3	−2.0	−3.5	−4.5	−5.1			
					T = 393.15 K							
$\kappa_T \times 10^3$/MPa^{-1}	2.230	2.209	2.187	2.165	2.162	2.122	2.023	1.934				
$\alpha_P \times 10^3$/K^{-1}	1.541	1.518	1.494	1.470	1.467	1.423	1.314	1.215				
γ_V/MPa·K^{-1}	0.691	0.687	0.683	0.679	0.679	0.671	0.650	0.628				
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.4	−0.9	−1.3	−1.4	−2.1	−3.7	−4.6				

For the isobaric expansivity (α_P) defined as

$$\alpha_P = \frac{1}{V_m}\left(\frac{\partial V_m}{\partial T}\right)_P = -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_P = -\left(\frac{\partial \ln \rho}{\partial T}\right)_P \qquad (12)$$

the following expression is derived from the Tait and the Rackett equations:

$$\alpha_P = -\frac{2}{7}\frac{\ln(Z_{RA})}{T_c(1-T_r)^{5/7}} - C\left\{\frac{\frac{dB}{dT}(P^\sigma - P) - \gamma^\sigma(B+P)}{\left[1 - C\ln\left(\frac{B+P}{B+P^\sigma}\right)\right](B+P^\sigma)(B+P)}\right\} \qquad (13)$$

where $dB/dT = -b_2/T^2$ and $\gamma^\sigma = dP^\sigma/dT$ is the slope of the vapor pressure curve at the given temperature *T*. The values of α_P are presented in Tables 10 to 13 and are plotted in Figure 7 for ethyl acetate.

The thermal pressure coefficient (γ_V) was calculated according

$$\gamma_V = \left(\frac{\partial P}{\partial T}\right)_\rho = \frac{\alpha_P}{\kappa_T} \qquad (14)$$

and the values for this property are listed in Tables 10 to 13 and plotted in Figure 8 for ethyl acetate. The values of α_P are similar in magnitude for all the esters in the tested ranges of temperature and pressure. The same is true for κ_T and γ_V. The dependence on *P* and *T* of these mechanical coefficients follows the expected behavior. The coefficients α_P and κ_T show an increase with the temperature, which is more significant at lower pressures. At high pressures the value of α_P is practically constant, independent of temperature. At fixed pressure the value of the thermal pressure coefficient decreases markedly with the increasing temperature. From Tables 10 to 13, it is observed that the isothermal compressibility decreases as -CH_2- units are added to the alkyl group of the ester molecule. A similar behavior is observed for α_P. This behavior is a consequence of the global decreasing in the density with the increase of the alkyl chain length as explained before.

The α_P and k_T data from this work are compared with the values reported by Malhotra and Woolf[4] for propyl and *n*-butyl acetates in Table 14. The absolute percentage deviation for both the coefficients are between 1 % and 3 %.

Taking into account the influence of pressure into the isobaric molar heat capacity ($C_{P,m}$) at constant temperature

$$\left(\frac{\partial C_{P,m}}{\partial P}\right)_T = -T\left(\frac{\partial^2 V_m}{\partial T^2}\right)_P \qquad (15)$$

the following equation is obtained for the change in the isobaric molar heat capacity due to the increase on the pressure from 0.1 MPa to *P*:

$$\Delta C_{P,m}(T,P) - C_{P,m}(T,P) - C_{P,m}(T, P = 0.1\ \text{MPa}) = -T\int_{0.1}^{P}\left\{\frac{M}{\rho}\left[\left(\frac{\partial \alpha_P}{\partial T}\right)_P + (\alpha_P)^2\right]\right\} dP \qquad (16)$$

where *M* is the molar mass. The quantities in the integrand of eq 16 were calculated from the Tait equation. The values of $\Delta C_{P,m}$ are given in Tables 10 to 13. The most appreciable changes in $C_{P,m}$ occur at high pressure and high temperature. However in the range of pressure covered by this work, the $\Delta C_{P,m}$ is small as compared with the value of $C_{P,m}(T, P = 0.1$ MPa). To stress this aspect, we can compare the recommended

Table 13. Isothermal Compressibility (κ_T), Isobaric Expansivity (α_P), Thermal Pressure (γ_V), and Change in Molar Heat Capacity ($\Delta C_{P,m}$) for *N*-Pentyl Acetate

	P/MPa											
	0.10	1.00	2.00	2.70	3.00	5.00	10.00	15.00	20.00	25.00	30.00	35.00
						$T = 298.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	0.926	0.920	0.915	0.911	0.909	0.898	0.872	0.847	0.823	0.801	0.781	0.761
$\alpha_P \times 10^3$/K^{-1}	1.075	1.069	1.063	1.058	1.056	1.043	1.012	0.983	0.956	0.930	0.905	0.882
γ_V/MPa·K^{-1}	1.162	1.162	1.162	1.162	1.162	1.162	1.162	1.161	1.161	1.160	1.160	1.159
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.1	−0.3	−0.4	−0.5	−0.8	−1.5	−2.1	−2.7	−3.3	−3.8	−4.3
						$T = 303.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	0.960	0.955	0.948	0.944	0.942	0.930	0.902	0.875	0.851	0.827	0.805	0.784
$\alpha_P \times 10^3$/K^{-1}	1.088	1.082	1.075	1.070	1.068	1.055	1.023	0.993	0.964	0.938	0.912	0.888
γ_V/MPa·K^{-1}	1.133	1.134	1.134	1.134	1.134	1.134	1.134	1.134	1.134	1.134	1.133	1.132
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.3	−0.4	−0.5	−0.8	−1.6	−2.2	−2.9	−3.4	−4.0	−4.4
						$T = 308.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	0.996	0.990	0.983	0.979	0.977	0.964	0.934	0.905	0.879	0.854	0.830	0.808
$\alpha_P \times 10^3$/K^{-1}	1.102	1.095	1.088	1.083	1.081	1.067	1.034	1.002	0.973	0.945	0.919	0.894
γ_V/MPa·K^{-1}	1.106	1.106	1.106	1.106	1.106	1.107	1.107	1.108	1.108	1.108	1.107	1.107
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.3	−0.5	−0.5	−0.8	−1.6	−2.3	−3.0	−3.6	−4.1	−4.6
						$T = 313.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.033	1.027	1.020	1.015	1.013	0.999	0.966	0.936	0.908	0.881	0.856	0.833
$\alpha_P \times 10^3$/K^{-1}	1.115	1.108	1.101	1.096	1.094	1.079	1.045	1.012	0.982	0.953	0.926	0.901
γ_V/MPa·K^{-1}	1.079	1.079	1.080	1.080	1.080	1.080	1.081	1.082	1.082	1.082	1.082	1.082
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.5	−0.5	−0.9	−1.7	−2.5	−3.1	−3.7	−4.3	−4.8
						$T = 318.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.072	1.065	1.058	1.052	1.050	1.035	1.000	0.968	0.938	0.909	0.883	0.858
$\alpha_P \times 10^3$/K^{-1}	1.129	1.122	1.114	1.109	1.107	1.092	1.056	1.022	0.991	0.961	0.934	0.907
γ_V/MPa·K^{-1}	1.053	1.054	1.054	1.054	1.054	1.055	1.056	1.056	1.057	1.057	1.058	1.058
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.5	−0.6	−0.9	−1.8	−2.6	−3.3	−3.9	−4.5	−5.0
						$T = 323.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.113	1.105	1.097	1.091	1.089	1.073	1.036	1.001	0.968	0.938	0.910	0.884
$\alpha_P \times 10^3$/K^{-1}	1.144	1.136	1.128	1.123	1.120	1.105	1.067	1.033	1.000	0.970	0.941	0.914
γ_V/MPa·K^{-1}	1.028	1.028	1.028	1.029	1.029	1.029	1.031	1.032	1.033	1.033	1.034	1.034
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.5	−0.6	−1.0	−1.9	−2.7	−3.4	−4.1	−4.7	−5.2
						$T = 328.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.155	1.147	1.138	1.132	1.130	1.113	1.072	1.035	1.001	0.968	0.938	0.910
$\alpha_P \times 10^3$/K^{-1}	1.159	1.151	1.143	1.137	1.134	1.118	1.079	1.043	1.009	0.978	0.948	0.920
γ_V/MPa·K^{-1}	1.003	1.003	1.004	1.004	1.004	1.005	1.006	1.008	1.009	1.010	1.010	1.011
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.6	−0.6	−1.0	−2.0	−2.8	−3.6	−4.2	−4.9	−5.4
						$T = 333.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.200	1.191	1.181	1.175	1.172	1.154	1.110	1.071	1.034	1.000	0.968	0.938
$\alpha_P \times 10^3$/K^{-1}	1.174	1.166	1.157	1.151	1.149	1.132	1.091	1.054	1.019	0.986	0.955	0.927
γ_V/MPa·K^{-1}	0.979	0.979	0.980	0.980	0.980	0.981	0.983	0.984	0.985	0.986	0.987	0.988
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.4	−0.6	−0.7	−1.1	−2.1	−2.9	−3.7	−4.4	−5.1	−5.6
						$T = 338.15$ K						
$\kappa_T \times 10^3$/MPa^{-1}	1.246	1.237	1.226	1.219	1.216	1.197	1.150	1.108	1.068	1.032	0.998	0.966
$\alpha_P \times 10^3$/K^{-1}	1.190	1.182	1.173	1.166	1.163	1.146	1.103	1.064	1.028	0.994	0.963	0.933
γ_V/MPa·K^{-1}	0.955	0.956	0.956	0.956	0.957	0.957	0.959	0.961	0.963	0.964	0.965	0.966
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.5	−0.6	−0.7	−1.1	−2.2	−3.1	−3.9	−4.6	−5.3	−5.9
						$T = 343.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.295	1.285	1.274	1.266	1.263	1.241	1.192	1.146	1.104	1.065	1.029	0.995
$\alpha_P \times 10^3$/K^{-1}	1.207	1.198	1.188	1.182	1.179	1.160	1.116	1.075	1.038	1.003	0.970	0.939
γ_V/MPa·K^{-1}	0.932	0.933	0.933	0.933	0.934	0.935	0.937	0.939	0.940	0.942	0.943	0.944
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.5	−0.7	−0.7	−1.2	−2.3	−3.2	−4.1	−4.8	−5.5	−6.1
						$T = 348.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.346	1.335	1.323	1.315	1.311	1.288	1.235	1.186	1.141	1.099	1.061	1.026
$\alpha_P \times 10^3$/K^{-1}	1.224	1.215	1.205	1.198	1.195	1.175	1.129	1.087	1.048	1.011	0.977	0.946
γ_V/MPa·K^{-1}	0.909	0.910	0.910	0.911	0.911	0.912	0.914	0.916	0.918	0.920	0.921	0.922
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.2	−0.5	−0.7	−0.8	−1.3	−2.4	−3.4	−4.3	−5.0	−5.7	−6.3
						$T = 353.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.400	1.388	1.375	1.366	1.362	1.337	1.280	1.227	1.179	1.135	1.094	1.057
$\alpha_P \times 10^3$/K^{-1}	1.242	1.232	1.221	1.214	1.211	1.190	1.142	1.098	1.057	1.020	0.985	0.952
γ_V/MPa·K^{-1}	0.887	0.888	0.888	0.889	0.889	0.890	0.893	0.895	0.897	0.898	0.900	0.901
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.5	−0.7	−0.8	−1.3	−2.5	−3.5	−4.5	−5.3	−6.0	−6.6
						$T = 358.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.456	1.443	1.429	1.420	1.415	1.389	1.327	1.270	1.219	1.172	1.129	1.089
$\alpha_P \times 10^3$/K^{-1}	1.260	1.250	1.239	1.231	1.228	1.206	1.156	1.110	1.067	1.028	0.992	0.958
γ_V/MPa·K^{-1}	0.866	0.866	0.867	0.867	0.867	0.868	0.871	0.874	0.876	0.877	0.879	0.880
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.6	−0.8	−0.9	−1.4	−2.6	−3.7	−4.7	−5.5	−6.2	−6.8
						$T = 363.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.515	1.502	1.486	1.476	1.471	1.443	1.376	1.316	1.261	1.210	1.164	1.122
$\alpha_P \times 10^3$/K^{-1}	1.279	1.268	1.257	1.248	1.245	1.222	1.170	1.122	1.077	1.037	0.999	0.964
γ_V/MPa·K^{-1}	0.844	0.845	0.845	0.846	0.846	0.847	0.850	0.853	0.855	0.857	0.858	0.859
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.6	−0.8	−0.9	−1.5	−2.8	−3.9	−4.9	−5.7	−6.5	−7.1

Table 13. (Continued)

	P/MPa											
	0.10	1.00	2.00	2.70	3.00	5.00	10.00	15.00	20.00	25.00	30.00	35.00
						$T = 368.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.578	1.563	1.547	1.535	1.530	1.499	1.427	1.363	1.304	1.250	1.201	1.156
$\alpha_P \times 10^3$/K^{-1}	1.299	1.288	1.275	1.267	1.263	1.239	1.184	1.134	1.088	1.045	1.006	0.970
γ_V/MPa·K^{-1}	0.823	0.824	0.825	0.825	0.825	0.826	0.829	0.832	0.834	0.836	0.838	0.839
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.6	−0.9	−0.9	−1.6	−2.9	−4.1	−5.1	−6.0	−6.7	−7.4
						$T = 373.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.644	1.628	1.610	1.598	1.593	1.559	1.481	1.412	1.349	1.292	1.239	1.192
$\alpha_P \times 10^3$/K^{-1}	1.320	1.308	1.294	1.285	1.282	1.257	1.199	1.146	1.098	1.054	1.013	0.976
γ_V/MPa·K^{-1}	0.803	0.803	0.804	0.805	0.805	0.806	0.809	0.812	0.814	0.816	0.818	0.819
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.3	−0.7	−0.9	−1.0	−1.6	−3.1	−4.3	−5.3	−6.2	−7.0	−7.6
						$T = 378.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.714	1.696	1.677	1.664	1.658	1.622	1.538	1.463	1.396	1.335	1.279	1.228
$\alpha_P \times 10^3$/K^{-1}	1.341	1.328	1.314	1.305	1.301	1.275	1.213	1.158	1.108	1.062	1.020	0.981
γ_V/MPa·K^{-1}	0.782	0.783	0.784	0.784	0.785	0.786	0.789	0.792	0.794	0.796	0.798	0.799
$\Delta C_{P,m}$/J×mol^{-1}·K^{-1}	0.0	−0.3	−0.7	−1.0	−1.1	−1.7	−3.2	−4.5	−5.6	−6.5	−7.3	−7.9
						$T = 383.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.788	1.769	1.748	1.733	1.727	1.688	1.597	1.517	1.445	1.379	1.320	1.266
$\alpha_P \times 10^3$/K^{-1}	1.364	1.350	1.335	1.325	1.321	1.293	1.229	1.171	1.118	1.071	1.027	0.987
γ_V/MPa·K^{-1}	0.763	0.763	0.764	0.764	0.765	0.766	0.769	0.772	0.774	0.776	0.778	0.779
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.4	−0.7	−1.0	−1.1	−1.8	−3.4	−4.7	−5.8	−6.8	−7.5	−8.2
						$T = 388.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.867	1.846	1.823	1.807	1.801	1.758	1.660	1.573	1.496	1.426	1.363	1.306
$\alpha_P \times 10^3$/K^{-1}	1.387	1.372	1.357	1.346	1.342	1.312	1.244	1.184	1.129	1.079	1.033	0.992
γ_V/MPa·K^{-1}	0.743	0.744	0.744	0.745	0.745	0.746	0.750	0.752	0.755	0.757	0.758	0.759
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0.0	−0.4	−0.8	−1.1	−1.2	−1.9	−3.6	−4.9	−6.1	−7.0	−7.8	−8.5
						$T = 393.15$ K						
$k_T \times 10^3$/MPa^{-1}	1.950	1.927	1.902	1.885	1.878	1.832	1.726	1.632	1.549	1.475	1.407	1.347
$\alpha_P \times 10^3$/K^{-1}	1.411	1.396	1.379	1.368	1.363	1.332	1.260	1.196	1.139	1.087	1.039	0.996
γ_V/MPa·K^{-1}	0.724	0.724	0.725	0.726	0.726	0.727	0.730	0.733	0.735	0.737	0.739	0.740
$\Delta C_{P,m}$/J×mol^{-1}·K^{-1}	0.0	−0.4	−0.8	−1.1	−1.3	−2.0	−3.8	−5.2	−6.4	−7.3	−8.1	−8.8

values of $C_{P,m}$(T = 340 K, P = 0.1 MPa) from Zábranský et al.[23] and $\Delta C_{P,m}$ data at T = 340 K and 35 MPa. For ethyl, propyl, and *n*-butyl acetates, the $C_{P,m}$(T = 340 K, P = 0.1 MPa) values are respectively 182.2, 213.0, and 238.8 J·mol^{-1}·K^{-1}. The corresponding changes in the isobaric heat capacity are −5.6, −5.6, and −5.1 J·mol^{-1}·K^{-1}. For *n*-pentyl acetate, the highest temperature available for comparison is 300 K. At this temperature and atmospheric pressure $C_{P,m}$ = 270 J·mol^{-1}·K^{-1} and $\Delta C_{P,m}$(300 K, 35 MPa) = −4.3 J·mol^{-1}·K^{-1}.

In Table 14, we compare our values of $\Delta C_{P,m}$ for propyl and *n*-butyl acetates with those obtained by Malhotra and Woolf.[4] The two sets of results are in close agreement.

The Tait equation was also used to predict density of the alkyl esters. For this purpose, the method of Thomson et al.[6] was applied. In this method, the parameters B and C of eq 6 are predicted by the following equations:[6]

$$B/P_c = -1.0 + a(1 - T_r)^{1/3} + b(1 - T_r)^{2/3} + d(1 - T_r) + e(1 - T_r)^{4/3} \quad (17)$$

$$C = j + k\omega \quad (18)$$

$$e = \exp(f + g\omega + h\omega^2) \quad (19)$$

where ω is the Pitzer acentric factor and a = −9.070217, b = 62.45326, d = −135.1102, f = 4.79594, g = 0.250047, h = 1.14188, j = 0.0861488, and k = 0.0344483. The necessary vapor pressure and saturated liquid densities to be used in eq 6 were provided by eqs 7 and 8, respectively. The AAD between

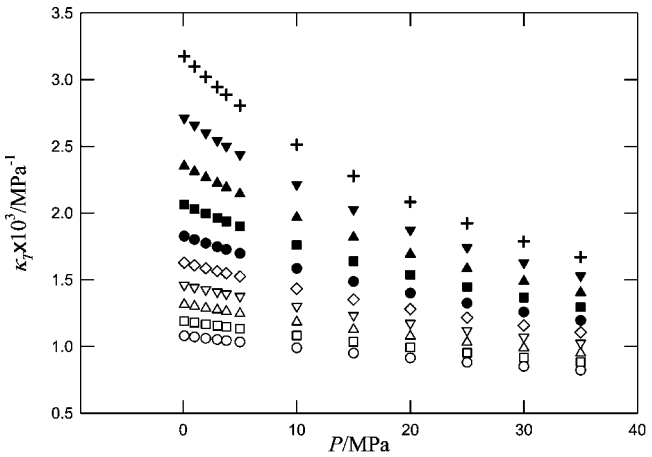

Figure 6. Isothermal compressibility of ethyl acetate at the temperatures: ○, 298.15 K; □, 308.15 K; △, 318.15 K; ▽, 328.15 K; ◇, 338.15 K; ●, 348.15 K; ■, 358.15 K; ▲, 368.15 K; ▼, 378.15 K; +, 388.15 K.

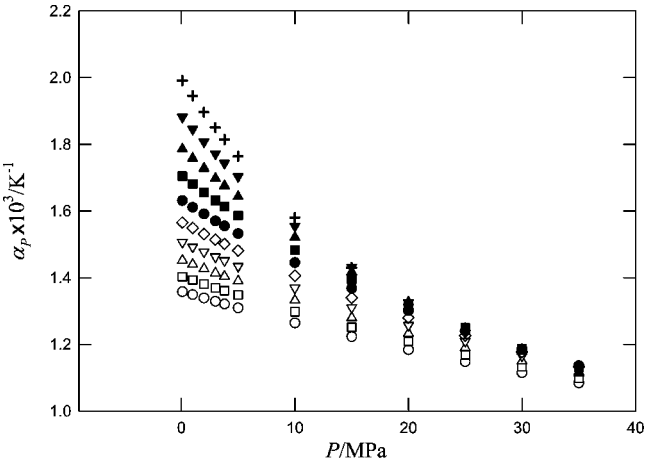

Figure 7. Isobaric expansivity of ethyl acetate at the temperatures: ○, 298.15 K; □, 308.15 K; △, 318.15 K; ▽, 328.15 K; ◇, 338.15 K; ●, 348.15 K; ■, 358.15 K; ▲, 368.15 K; ▼, 378.15 K; +, 388.15 K.

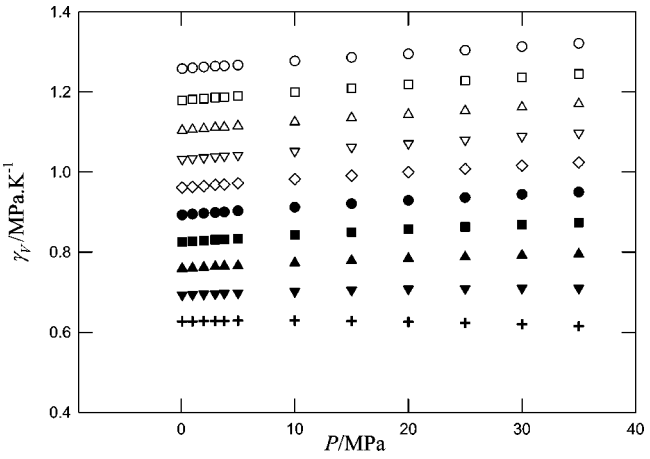

Figure 8. Thermal pressure of ethyl acetate at the temperatures: ○, 298.15 K; □, 308.15 K; △, 318.15 K; ▽, 328.15 K; ◇, 338.15 K; ●, 348.15 K; ■, 358.15 K; ▲, 368.15 K; ▼, 378.15 K; +, 388.15 K.

Table 14. Comparison of α_P and κ_T Data from This Work with the Data from Malhotra and Woolf[4] for Propyl Acetate and *N*-Butyl Acetate

	$P = 0.1$ MPa		$P = 200$ MPa	
	ref 4	this work	ref 4	this work
		Propyl Acetate		
		$T = 298.14$ K		
$\alpha_P \times 10^3$/K^{-1}	1.094	1.017	0.906	0.890
$\kappa_T \times 10^3$/MPa^{-1}	1.27	1.24	1.12	1.09
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0	0	−3	−2.8
		$T = 313.14$ K		
$\alpha_P \times 10^3$/K^{-1}	1.245	1.112	1.006	0.994
$\kappa_T \times 10^3$/MPa^{-1}	1.31	1.30	1.15	1.12
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0	0	−3	−3.2
		$T = 323.14$ K		
$\alpha_P \times 10^3$/K^{-1}	1.304	1.274	1.064	1.075
$\kappa_T \times 10^3$/MPa^{-1}	1.35	1.34	1.17	1.14
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0	0	−4	−3.5
		$T = 338.13$ K		
$\alpha_P \times 10^3$/K^{-1}	1.513	1.470	1.190	1.211
$\kappa_T \times 10^3$/MPa^{-1}	1.39	1.41	1.20	1.17
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0	0	−4	−4.0
		N-Butyl Acetate		
		$T = 298.14$ K		
$\alpha_P \times 10^3$/K^{-1}	1.029	0.923	0.858	0.851
$\kappa_T \times 10^3$/MPa^{-1}	1.17	1.14	1.04	1.00
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0	0	−3	−2.7
		$T = 313.14$ K		
$\alpha_P \times 10^3$/K^{-1}	1.151	1.045	0.945	0.953
$\kappa_T \times 10^3$/MPa^{-1}	1.21	1.18	1.06	1.03
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0	0	−3	−3.0
		$T = 323.14$ K		
$\alpha_P \times 10^3$/K^{-1}	1.272	1.137	1.012	1.029
$\kappa_T \times 10^3$/MPa^{-1}	1.24	1.22	1.07	1.04
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0	0	−3	−3.3
		$T = 338.13$ K		
$\alpha_P \times 10^3$/K^{-1}	1.426	1.295	1.118	1.157
$\kappa_T \times 10^3$/MPa^{-1}	1.28	1.27	1.09	1.07
$\Delta C_{P,m}$/J·mol^{-1}·K^{-1}	0	0	−3	−3.7

experimental and predicted values of density is 0.2 % or less. The predicted value of parameter C ($C \approx 0.10$) is of the same magnitude as that presented in Table 9.

Conclusions

In this work experimental density data of alkyl acetates (ethyl, propyl, *n*-butyl, and *n*-pentyl) over the pressure range of (0.1 to 35) MPa and the temperature range of (298.15 to 393.15) K are presented. We have extended the temperature domains of the experimental measurements for ethyl, propyl, and butyl acetates considering the available literature data. Our measurements are in close agreement in the (P, T) domain covered by other authors. As much as we know, density data for the pentyl acetate at wide ranges of temperature and pressure are original. We have found that the density of the alkyl esters decreases with the increasing of the alkyl chain length.

In this work, the Tait equation was fitted to the density data using simultaneously the pressure and the temperature, which is a more direct and fast methodology than to fit the equation to isothermal (ρ, P) data, as some authors do. With this procedure the mechanical coefficients α_P, κ_T, and γ_V and the change in the isobaric molar heat capacity ($\Delta C_{P,m}$), from $P =$ 0.1 MPa to P at fixed T were accessed in wide (P, T) ranges. All the values of these *PVT* properties agree closely with those from other authors. The calculated values of the change in the isobaric heat capacity ($\Delta C_{P,m}$) are always small and negative and represent (2 to 3) % of the values of $C_{P,m}(T, P = 0.1$ MPa). The method of Thomson et al.[6] can be applied to the prediction of density of the esters with excellent results.

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