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Experimental Liquid Densities of *n*-Pentane, *n*-Octane, and *n*-Nonane and Their Binary Mixtures from (273.15 to 363.15) K at 0.1 MPa

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ABSTRACT: This paper presents experimental liquid densities for *n*-pentane, *n*-octane, and *n*-nonane and their binary mixtures from (273.15 to 363.15) K over the entire composition range (for the mixtures) at atmospheric pressure. The experimental apparatus is a vibrating-tube densimeter. It is possible to compare the results to a generalized correlation for liquid densities of *n*-alkanes and to molecular dynamics simulations. The average absolute percentage deviation is (0.06 and 0.8) % using the equation and the simulation results.

INTRODUCTION

This work is part of an investigation[1] to determine liquid densities of hydrocarbon mixtures. Density measurements of *n*-alkanes and their mixtures are important in the development of new theories using molecular simulations. Also, they are important in the development of new technologies and equipment design of the fuel industry. Experimental liquid densities for *n*-alkane mixtures are scarce, and few densities exist for the binary systems formed by *n*-pentane, *n*-octane, and *n*-nonane. Chevalier et al.[2] have measured the density of *n*-octane + *n*-nonane at 298.15 K and atmospheric pressure. They use an Anton Paar densimeter with an overall accuracy of ± 0.5 $\text{kg}\cdot\text{m}^{-3}$. Aucejo et al.[3] also have measured the densities of *n*-pentane + *n*-octane, *n*-pentane + *n*-nonane, and *n*-octane + *n*-nonane at 298.15 K and 0.101 MPa. Ben'kovskii et al.[4] measure the atmospheric liquid density of *n*-octane + *n*-nonane at (258.15, 274.15, 285.15, and 298.15) K. To the best of our knowledge, these are the only data reported for mixtures of *n*-pentane, *n*-octane, and *n*-nonane. Several researchers have developed correlations to predict molar volume or density. Recently, Ramos-Estrada et al.[1] have improved the characteristic parameters of the Tait equation using density data from methane through *n*-hexadecane. They used for the reference state the atmospheric pressure and a new general correlation for the atmospheric density.

This work presents measurements of the atmospheric liquid densities for *n*-pentane, *n*-octane, and *n*-nonane along with those of their binary mixtures from (273.15 to 363.15) K over the entire composition range. Also, the results are compared to a correlation based upon the principle of congruence for the atmospheric mass densities and to the predictions from a molecular dynamics simulation.

EXPERIMENTAL SECTION

Apparatus and Procedures. A vibrating densimeter (model DMA 5000 from Anton Paar) measures the density of the three binary systems and their pure components. The cell contains a platinum resistance thermometer that has an uncertainty of ± 0.01 K on ITS-90. Standard deviations of the repeatability in density and temperature measurements provided by the manufacturers are ± $1.6\cdot10^{-5}$ $\text{g}\cdot\text{cm}^{-3}$ and ± 0.002 K, respectively. The overall uncertainty in density measurements is ± $3\cdot10^{-5}$ $\text{g}\cdot\text{cm}^{-3}$.

Samples. *n*-Pentane came from J.T. Baker with a mole fraction purity greater than 0.99, while Merck and Aldrich supplied *n*-octane and *n*-nonane with mole fraction purities of 0.99 for both *n*-octane and *n*-nonane. The water grade was high-performance liquid chromatography (HPLC). The reagents were used as received. The mixtures were prepared gravimetrically using an analytical balance (Ohaus model AS120S) with a precision of ± 0.1 mg. The hydrocarbons remained at 273.15 K during the preparations to avoid evaporation. The overall uncertainty in the mole fractions is ± 0.002.

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■ EXPERIMENTAL RESULTS

Density measurements for pure water before and after the experiments check the calibration of the densimeter. Current measurements agree with density values from the equation of state for water adopted by the International Association for the Properties of Water and Steam (IAPWS) and developed by Wagner and Pruss[5] within ± 0.005 %. Measured experimental densities (ρ) range from (273.15 to 363.15) K at atmospheric pressure. Table 1 shows the experimental results for *n*-octane and *n*-nonane. Previously, this laboratory has reported the experimental densities of pure *n*-pentane.[1] The experimental values agree with experimental data in the TRC Database[6] within an average absolute deviation of 0.03 % with a maximum value of 0.1 % as shown in Table 1. Experimental density measurements for the binary mixtures appear in Tables 2 to 4. Current densities agree with the experimental values of Chevalier et al.[2] and Aucejo et al.[3] within an average absolute percentage deviation of (0.085 and 0.02) %, respectively. A comparison of current density measurements to those of Ben'kovskii et al.[4] at 298.15 K reveal agreement within an average absolute percentage error of 0.04 %. Also, comparison of the experimental results with an equation previously developed by Ramos-Estrada et al.[1]

$$\rho_0 = (1 - 4.8203 \cdot 10^{-4} T - 2.72932 \cdot 10^{-12} T^{3.5}) - (0.55240422 + 7.775 \cdot 10^{-5} T^{1.5}) n^{-0.87} \qquad (1)$$

where T is in kelvin and n is the carbon number is within an average absolute percentage deviation of 0.06 %. For the mixture, the equivalent carbon number is

$$n = \sum_{i=1} n_i x_i \qquad (2)$$

where x_i is the mole fraction and n_i is the number of carbons of pure component i in the mixture. Figure 1 shows the deviation of eq 1 from the experimental measurements. Hollow symbols represent literature percentage deviations. Also, the experimental densities of *n*-pentane + *n*-octane are compared to molecular simulations. For the simulation,

Table 1. Experimental Densities of *n*-Octane and *n*-Nonane

	ρ/g·cm^{-3}			ρ/g·cm^{-3}	
T/K	this work	lit.	T/K	this work	lit.
	n-Octane			*n*-Nonane	
273.15	0.71825		273.15	0.73283	
278.15	0.71431		278.15	0.72901	
283.15	0.71034	0.71064[12]	283.15	0.72516	0.72539[12]
288.15	0.70635	0.7064[13]	288.15	0.72132	0.72135[13]
293.15	0.70235	0.70252[3]	293.15	0.71745	0.71758[3]
298.15	0.69834	0.69818[14]	298.15	0.71358	0.7138[12]
303.15	0.69430	0.6939[15]	303.15	0.70969	0.70998[20]
308.15	0.69024	0.6904[15]	308.15	0.70578	0.70610[20]
313.15	0.68617	0.68628[16]	313.15	0.70186	0.70166[22]
318.15	0.68206	0.68221[17]	318.15	0.69791	0.69807[22]
323.15	0.67794	0.6785[18]	323.15	0.69395	0.6939[22]
328.15	0.67379		328.15	0.68997	0.69024[22]
333.15	0.66961	0.66956[19]	333.15	0.68597	0.68589[22]
338.15	0.66540	0.66607[20]	338.15	0.68194	0.68202[22]
343.15	0.66116		343.15	0.67788	0.67754[22]
348.15	0.65688	0.6574[21]	348.15	0.67391	0.67357[22]
353.15	0.65257		353.15	0.66971	0.66966[22]
358.15	0.64823		358.15	0.66558	0.66561[22]
363.15	0.64383		363.15	0.66114	0.66142[22]

Table 2. Experimental Densities for the Binary Mixture of *n*-Pentane + *n*-Octane

	ρ								
x_1	g·cm^{-3}								
	T = 278.15 K	T = 283.15 K	T = 288.15 K	T = 293.15 K	T = 298.15 K	T = 303.15 K	T = 308.15 K	T = 313.15 K	T = 318.16 K
0.1002	0.70935	0.70534	0.70131	0.69726	0.69319	0.68909	0.68497	0.68083	0.67664
0.2008	0.70452	0.70046	0.69638	0.69229	0.68816	0.68401	0.67984	0.67563	0.67138
0.3023	0.69824	0.69411	0.68994	0.68574	0.68152	0.67728	0.67300	0.66870	0.66436
0.4019	0.69187	0.68766	0.68343	0.67916	0.67487	0.67054	0.66619	0.66180	0.65738
0.5001	0.68519	0.68091	0.67660	0.67226	0.66788	0.66347	0.65903	0.65459	0.65006
0.5982	0.67800	0.67365	0.66926	0.66483	0.66037	0.65587	0.65133	0.64675	0.64212
0.7022	0.66963	0.66518	0.66068	0.65615	0.65158	0.64696	0.64231	0.63761	0.63285
0.8003	0.66099	0.65645	0.65185	0.64721	0.64252	0.63779	0.63300	0.62816	0.62327
0.8991	0.65139	0.64673	0.64204	0.63729	0.63249	0.62764	0.62272	0.61796	
	T = 323.16	T = 328.16	T = 333.15 K	T = 338.15 K	T = 343.15 K	T = 348.15 K	T = 353.15 K	T = 358.15 K	T = 363.15 K
0.1002	0.67243	0.66820	0.66394	0.65963	0.65528	0.65090	0.64647	0.64200	0.63748
0.2008	0.66711	0.66281	0.65848	0.65410	0.64968	0.64521	0.64070	0.63615	0.63154
0.3023	0.65999	0.65559	0.65116	0.64668	0.64213	0.63757	0.63294	0.62827	0.62354
0.4019	0.65292	0.64842							
0.5001	0.64550	0.64090							
0.5982	0.63745	0.63273							
0.7022	0.62804								
0.8003									
0.8991									

Table 3. Experimental Densities for the Binary Mixture of *n*-Pentane + *n*-Nonane

x_1	ρ / $g \cdot cm^{-3}$																		
	$T = 273.15$ K	$T = 278.15$ K	$T = 283.15$ K	$T = 288.15$ K	$T = 293.15$ K	$T = 298.15$ K	$T = 303.15$ K	$T = 308.15$ K	$T = 313.15$ K	$T = 318.15$ K	$T = 323.15$ K	$T = 328.15$ K	$T = 333.15$ K	$T = 338.15$ K	$T = 343.15$ K	$T = 348.15$ K	$T = 353.15$ K	$T = 358.15$ K	$T = 363.15$ K
0.1034	0.72717	0.72331	0.71943	0.71553	0.71162	0.70769	0.70375	0.69978	0.69579	0.69178	0.68774	0.68368	0.67960	0.67548	0.67134	0.66716	0.66295	0.65870	0.65442
0.2050	0.72115	0.71724	0.71331	0.70935	0.70538	0.70139	0.69738	0.69335	0.68930	0.68521	0.68110	0.67697	0.67280	0.66860	0.66437	0.66010	0.65579	0.65145	0.64707
0.3028	0.71481	0.71084	0.70684	0.70282	0.69879	0.69473	0.69065	0.68654	0.68241	0.67825	0.67406	0.66983	0.66558	0.66128	0.65696	0.65259	0.64819	0.64374	0.63925
0.4006	0.70786	0.70382	0.69975	0.69566	0.69154	0.68741	0.68324	0.67905	0.67483	0.67058	0.66629	0.66197	0.65761	0.65321	0.64878	0.64430	0.63979		
0.5016	0.70000	0.69588	0.69173	0.68756	0.68336	0.67913	0.67487	0.67058	0.66626	0.66190	0.65751	0.65307	0.64860	0.64408					
0.5988	0.69184	0.68764	0.68340	0.67914	0.67484	0.67052	0.66616	0.66176	0.65733	0.65286	0.64834	0.64378	0.63917	0.63451					
0.6992	0.68227	0.67796	0.67362	0.66925	0.66484	0.66039	0.65591	0.65139	0.64682	0.64221	0.63754	0.63282	0.62805						
0.7993	0.67239	0.66797	0.66351	0.65901	0.65447	0.64988	0.64526	0.64058	0.63585	0.63107	0.62624	0.62134	0.61638						
0.8993	0.65926	0.65469	0.65007	0.64541	0.64071	0.63596	0.63115	0.62628	0.62136	0.61637									

Table 4. Experimental Densities for the Binary Mixture of *n*-Octane + *n*-Nonane

x_1	ρ / $g \cdot cm^{-3}$																		
	$T = 273.15$ K	$T = 278.15$ K	$T = 283.15$ K	$T = 288.15$ K	$T = 293.15$ K	$T = 298.15$ K	$T = 303.15$ K	$T = 308.15$ K	$T = 313.15$ K	$T = 318.15$ K	$T = 323.15$	$T = 328.15$	$T = 333.15$ K	$T = 338.15$ K	$T = 343.15$ K	$T = 348.15$ K	$T = 353.15$ K	$T = 358.15$ K	$T = 363.15$ K
0.1017	0.73151	0.72769	0.72384	0.71999	0.71612	0.71224	0.70834	0.70441	0.70048	0.69652	0.69253	0.68853	0.68450	0.68044	0.67636	0.67225	0.66811	0.66393	0.65972
0.2023	0.73003	0.72620	0.72235	0.71848	0.71460	0.71070	0.70679	0.70286	0.69890	0.69493	0.69093	0.68691	0.68286	0.67878	0.67468	0.67055	0.66639	0.66218	0.65795
0.3016	0.72878	0.72494	0.72107	0.71719	0.71329	0.70938	0.70546	0.70151	0.69754	0.69355	0.68953	0.68549	0.68143	0.67734	0.67322	0.66907	0.66488	0.66067	0.65641
0.4000	0.72743	0.72357	0.71970	0.71580	0.71190	0.70797	0.70403	0.70007	0.69608	0.69208	0.68805	0.68399	0.67991	0.67580	0.67166	0.66750	0.66329	0.65905	0.65478
0.4987	0.72578	0.72191	0.71801	0.71411	0.71018	0.70624	0.70228	0.69830	0.69430	0.69027	0.68622	0.68215	0.67805	0.67391	0.66975	0.66556	0.66133	0.65707	0.65277
0.6006	0.72452	0.72065	0.71675	0.71283	0.70890	0.70495	0.70097	0.69698	0.69297	0.68892	0.68487	0.68078	0.67666	0.67250	0.66833	0.66412	0.65987	0.65560	0.65127
0.7002	0.72297	0.71908	0.71516	0.71122	0.70727	0.70331	0.69932	0.69531	0.69128	0.68722	0.68314	0.67903	0.67489	0.67073	0.66653	0.66230	0.65802	0.65372	0.64936
0.7986	0.72150	0.71759	0.71366	0.70971	0.70575	0.70176	0.69775	0.69373	0.68968	0.68560	0.68150	0.67737	0.67322	0.66903	0.66481	0.66056	0.65627	0.65194	0.64756
0.8989	0.71999	0.71607	0.71212	0.70816	0.70418	0.70018	0.69615	0.69211	0.68804	0.68395	0.67983	0.67569	0.67151	0.66730	0.66306	0.65878	0.65447	0.65010	0.64572

the alkyl groups and functional groups are semiflexible with fixed bond lengths and bending and torsional degrees of freedom. A united atom (UA) model represents alkyl segments CH_2 and CH_3. A truncated Lennard−Jones (LJ) potential describes the nonbonded interactions among different molecules and within sites:

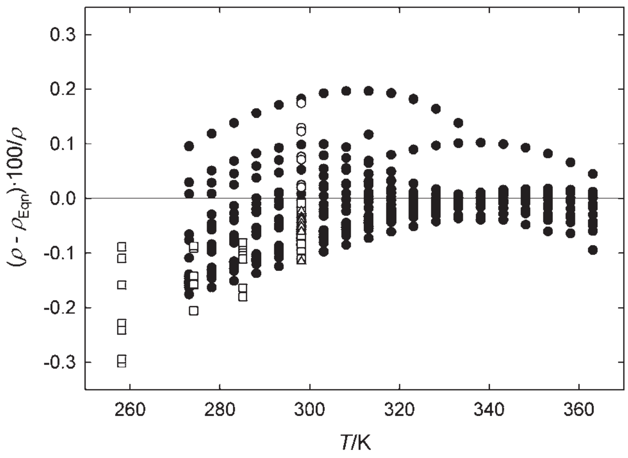

Figure 1. Percentage deviation of eq 1 from experimental density measurements: ●, this work; △, Chevalier et al.;[2] ○, Aucejo et al.;[3] □, Ben'kovskii et al.[4].

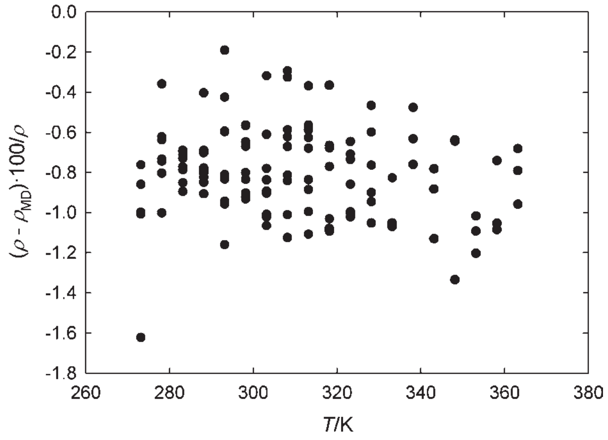

Figure 2. Percentage deviations of the density from molecular dynamics simulation with respect to the new density measurements for the *n*-pentane + *n*-octane mixture.

$$u(r_{ij}) = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] \tag{3}$$

where r_{ij}, σ_{ij}, and ε_{ij} are the site—site separation, the LJ diameter, and the LJ well-depth. Parameter values correspond to those provided by Martin and Siepmann[7] in the Transferable Potentials for Phase Equilibria (TraPPE) model ($\sigma_{\mathrm{CH_3}}$ = 3.75 Å, $\sigma_{\mathrm{CH_2}}$ = 3.95 Å, $\varepsilon_{\mathrm{CH_3}}/k$ = 98 K, and $\varepsilon_{\mathrm{CH_2}}/k$ = 46 K). Lorentz—Berthelot combination rules represent unlike LJ interactions. The energy caused by bending effects of beads separated by two bonds is calculated by a harmonic potential

$$u(\theta) = \frac{k_\theta}{2}(\cos\theta - \cos\theta_{\mathrm{o}})^2 \tag{4}$$

where θ_{o} is the equilibrium bond angle of 114°, θ is the current bond angle, and k_θ is the force constant equal to 62 500k K·rad^{-2} where k is the Boltzmann constant. The sites are connected by bond lengths equal to 1.54 Å as in the TraPPE model. The energy for dihedral interactions excluding improper torsions is a cosine series proposed by Ryckaert and Bellemans[8]

$$u(\phi) = \sum_{i=0}^{5} c_i \cos^i(\phi) \tag{5}$$

where c_{k} are constants with c_0/k = 1116 K, c_1/k = 1462 K, c_2/k = −1578 K, c_3/k = −368 K, c_4/k = 3156 K, and c_5/k = −3788 K.

The simulation box is replicated periodically and contains different numbers of molecules according to the experimental mole fraction. The total number of molecules in the box ranges from 64 to 216. Initially, the molecules form a diamond-type arrangement, so the chains are well-distributed avoiding overlaps. An NPT ensemble is used, and the pressure and temperature are maintained constant using the method developed by Berendsen et al.[9] About 400 000 integration steps are required for equilibration where the velocity distribution, the translational order parameter, and fluctuations in density, pressure, temperature, and energy are monitored to ensure equilibrium before using 600 000 production steps. These steps were subdivided into 400 steps to calculate the standard deviation of the average of the properties. The time integration step is of 0.9 fs. For the integration of Newton's equations of motion, the velocity-Velvet method[10] is used, and the bond length constraints are solved using the RATTLE algorithm.[11] Figure 2 illustrates that the prediction of density is within 0.8 % for the mixture *n*-pentane + *n*-octane. The molecular dynamics simulation overestimates the value of the density. This provides an opportunity for improvement of the force field model.

■ CONCLUSIONS

This paper has presented liquid densities of *n*-pentane, *n*-octane, and *n*-nonane and their corresponding binary mixtures from (273.15 to 363.15) K at atmospheric pressure using a vibrating-tube densimeter. The experimental densities agree with previously published densities within a maximum absolute percentage error of 0.08 %. The new values agree within an average absolute percentage deviation of 0.06 and 0.8 from predicted densities from a generalized correlation and densities obtained from a molecular dynamics simulation.

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