Article

(ρ, T, p) Measurements of the Methyl Nonafluorobutyl Ether (HFE-7100) + 1-Propanol Mixture at Pressures up to 70 MPa and Temperatures from 298.15 to 393.15 K

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ABSTRACT: The characterization of the thermophysical properties of new environmentally friendly fluids, such as hydrofluoroether fluids (HFEs) and their mixtures with other compounds, is necessary nowadays in order to properly design the machinery and piping networks involved in their utilization. However, scarce data concerning these kinds of fluids are actually available. In this work, new experimental high pressure density data (742 points) for the binary system x HFE-7100 + $(1 − x)$ 1-propanol are presented. This property was measured by using an Anton Paar vibrating tube densitometer in the temperature range of 298.15−393.15 K and in the pressure interval of 0.1−70 MPa. A comparison between our experimental high pressure density data and those found in the literature was carried out only for the pure compounds, since no density data for the binary mixture were found. To perform this comparison, we used a Tait-like equation in order to correlate our results to those of the literature. Concerning the experimental density data, the derivative properties of isothermal compressibility, κ_T, and isobaric expansion, α_P, were determined over the same pressure and temperature ranges. Excess molar volumes of the binary system were also determined and compared with those of the mixture x HFE-7100 + $(1 − x)$ 2-propanol published in one of our previous works.
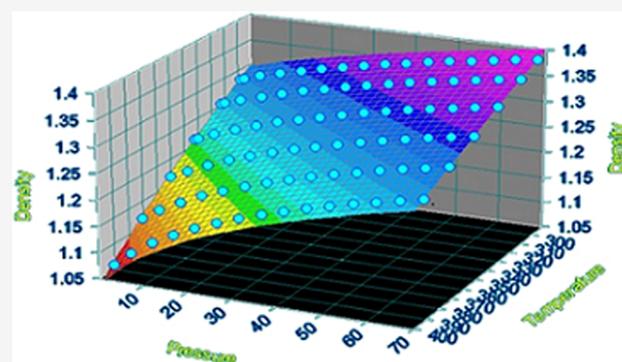
1. INTRODUCTION

HCFCs and HFCs are being widely used for common purposes as refrigerant fluids, heat transfer media, precision cleaning fluids, or aerosol applications among others. Although HFCs emerged as an alternative to the CFCs and HCFCs phase out proposal at the expense of the Montreal Protocol, in 1987, some of these fluorocarbons show high ozone depletion potentials (ODP), high global warming potentials (GWP), and large atmospheric lifetimes (ALT). Due to this, many researchers led efforts to search for new fluids with the same properties as CFCs, HCFCs and HFCs but with zero or near zero ODP, low GWP, and short atmospheric lifetimes.

Hydrofluoroether fluids (HFEs) were found as an alternative to these fluids, since they have similar properties and are capable of substituting CFCs, HCFCs, and HFCs in a wide array of applications.[1] HFEs have low GWP and short atmospheric lifetimes, properties that are provided by the oxygen atom of the ether in the molecule. HFEs also showed zero ODP. HFEs are nonflammable fluids and are compatible with most metals and hard polymers.[2] With respect to toxicity, HFEs briefly exhibit relatively low toxicity from the results of acute toxicity tests.[3]

Methyl nonafluorobutyl ether, known as HFE-7100, possesses some desirable properties, such as high latent heat of vaporization, high liquid density, and low viscosity. These properties make it ideal to be used as CFC, HCFC, and HFC replacement, both as pure components or in a mixture with other compounds such as ethers or alkanols.

Low-molecular-weight alcohols are acceptable rinsing and cleaning agents, but they are flammable, so the addition of fluorinated compounds to the mixture will reduce or eliminate the flammability.[4]

The binary mixture HFE-7100 + 1-propanol is a viable option for the replacement of some fluorocarbons. This binary mixture forms an azeotrope at a weight concentration of HFE-7100 of 97.90% that can be considered as a good replacement
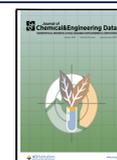
Table 1. Description of the Chemicals

compound	source	formula	molar mass/g·mol^{-1}	stated purity[a]	CAS number
HFE-7100[b]	3 M Company	$C_5H_3F_9O$	250.06	>99.5[c]	163702−08−7/163702−07−6[d]
1-propanol	Sigma-Aldrich	C_3H_8O	60.096	>99.8[e,f]	71−23−8

[a]Determined by gas chromatography (GC) by the supplier. [b]HFE-7100 = 1-methoxy-nonafluorobutane. [c]Mass fraction purity, wt % [d]Binary mixture of two isomers with a mass ratio of 0.5. [e]The water content was checked to be less than 0.01% by the titration method. [f]Mole fraction purity, mol %.

for HCFC-225ca/cb,[5] a mixture of isomers primarily used in vapor degreasing and aerosol applications.

Density is the most important physical property, and its determination as a function of temperature and pressure allows the obtaining of other valuable properties such as isothermal compressibility and isobaric expansion. With the molar mass, excess volumes can also be determined. In this work, densities for six mole fractions, x = (0.1502, 0.3258, 0.5010, 0.6754, 0.8495 and 0.9184) of the binary mixture x HFE-7100 + (1 − x) 1-propanol have been measured within the temperature range from 298.15 to 393.15 K and in the pressure range from 0.1 to 70 MPa by using an Anton Paar U-tube densitometer with an uncertainty of +0.7 kg·m^{-3} for the density. The derivative properties, that is, the isothermal compressibility and the isobaric expansion, are also reported in the same pressure and temperature ranges.

2. EXPERIMENTAL SECTION

2.1. Materials. Methyl nonafluorobutyl ether or 1-methoxy-nonafluorobutane was obtained from 3 M Company. This fluid, also known as HFE-7100 ($C_5H_3F_9O$, molar mass 250.06 g·mol^{-1}), consists of two inseparable isomers with essentially identical properties (CAS 163702−08−7/163702−07−6). The compositions of the binary isomers of HFE-7100 were determined with F NMR using a Varian Unity Inova 400 MHz apparatus. The results of F NMR show that the mole fraction of the isomer with CAS number 163702−08−7 is 51.9%, whereas the mole composition of the isomer with CAS 163702−07−6 is 48.1%, with an expanded uncertainty $U(x)$ = 0.05, for k = 2. These results and the peaks obtained have been provided in ref 6.[6]

The supplier certifies a mass purity for HFE-7100 greater than 0.995. 1-Propanol (C_3H_8O, molar mass 60.096 g·mol^{-1}, CAS 71−23−8) was obtained from Sigma-Aldrich with a mole fraction purity of 0.998 and stored over molecular sieves type 0.4 to avoid any moisture. The two fluids were subject to no further purification method except careful degassing before the use. The specifications of both fluids are reflected in Table 1.

2.2. Measurement Technique and Experimental Procedure. To determine high pressure density values of the binary system x HFE-7100 + (1 − x) 1-propanol, an Anton Paar DMA HPM high-pressure vibrating tube densitometer was employed. This technique belongs to the direct methods to determine the density of a fluid and is based on the determination of the vibration period of the U-tube located inside the apparatus containing the sample. Thus, the vibration period depends on the mass of the fluid that is contained inside the U-tube; with this datum, the calibration constants A and B, the sample mass, and the inner U-tube volume and density can be easily obtained.

By using this apparatus, densities were determined in the pressure range of 0.1−70 MPa at every 5 MPa step and along six isotherms (298.15, 313.15, 333.15, 353.15, 373.15, and 393.15) K. The experimental setup was described in one of our previous papers.[7] Concerning the calibration of the densitometer, the followed procedure was that described by Comuñas et al.,[8] which is a modification of the procedure previously proposed by Lagourette et al.[9] The calibration was performed by using two reference fluids: vacuum and water, and taking the density values of water from the equation of state (EoS) reported by Wagner and Pruss.[10] Due to the fact that no measurements were done at temperatures over the boiling point of water (373.15 K) at 0.1 MPa, it was not necessary to consider other fluids to perform the calibrations at temperatures higher than 373.15 K and at 0.1 MPa.

Prior to making any measurement, it was necessary to ensure that all of the circuit was completely clean in order to avoid contamination of the sample, so vacuum was generated for almost 1 h. All of the samples were degassed before their introduction in the densitometer by using an ultrasonic bath PSelecta, model Ultrasons-H. The mixtures were prepared immediately before being measured by weighing them in glass vials sealed to prevent evaporation. For the weighing process, a Mettler Toledo balance model MS 204S was used, with a resolution of 10^{-4} g and an uncertainty equal to 0.0001 g. The estimated expanded uncertainty in the composition of the mixture was 4 × 10^{-5} in mole fraction. Therefore, the excess molar volume should be accurate to within 0.004 cm^3·mol^{-1}.

After the mixtures were prepared and degassed, the densitometer was filled with the sample and brought to the desired temperature by means of the thermostatic bath and to the desired pressure by using the step-by-step engine. Considering the thermostatic bath, the estimated expanded uncertainty of the measured temperature was 0.03 K (Pt 100 calibrated probe). For the pressure, the estimated expanded uncertainty of the measured pressure was 0.04 MPa (pressure transducer, WIKA CPH 6000). Both temperature and pressure sensors were periodically calibrated before and after the measurement campaign. As mentioned above, the technique leads to the determination of the vibrational period of the U-tube. Thus, in order to bring this datum, the DMA HPM measuring cell is connected to the Anton Paar mPDS 2000 V3 evaluation unit, which evaluates the oscillation period from the measuring cell filled with the sample. The estimated expanded uncertainty (k = 2) is 0.0007 g·cm^{-3}, which was calculated by using the recommended document EA-4/02,[11] taking into account the accuracy of the temperature, the pressure, the period of oscillation measurement for water, vacuum, and the studied systems, and the water density accuracy.

3. RESULTS AND DISCUSSION

3.1. Density. High pressure densities were measured along six isotherms from 298.15 to 393.15 K and in the pressure range from 0.1 to 70 MPa at every 5 MPa. To obtain a good representation of the density behavior in the whole composition range, eight mole compositions of the mixture x HFE-7100 + (1 − x) 1-propanol were measured (x = 0.0000, 0.1502, 0.3258, 0.4963, 0.6754, 0.8495, 0.9184, and 1.0000),

Table 2. Experimental Values of Density ρ at Temperatures T and Pressures p for the Binary Mixture x HFE-7100 + $(1 − x)$ 1-Propanol[a]

		T/K					
x	p/MPa	298.15	313.15	333.15	353.15	373.15	393.15
		ρ/g·cm^{-3}					
0.0000	0.10	0.7996	0.7873	0.7703	0.7522		
	1.00	0.8003	0.7880	0.7712	0.7532	0.7335	0.7117
	5.00	0.8035	0.7915	0.7751	0.7577	0.7386	0.7177
	10.00	0.8073	0.7955	0.7796	0.7628	0.7445	0.7245
	15.00	0.8108	0.7994	0.7839	0.7675	0.7500	0.7308
	20.00	0.8142	0.8031	0.7880	0.7720	0.7550	0.7366
	25.00	0.8176	0.8067	0.7918	0.7764	0.7598	0.7421
	30.00	0.8207	0.8099	0.7955	0.7804	0.7644	0.7471
	35.00	0.8237	0.8133	0.7991	0.7844	0.7686	0.7518
	40.00	0.8267	0.8164	0.8024	0.7881	0.7727	0.7564
	45.00	0.8297	0.8194	0.8057	0.7915	0.7766	0.7606
	50.00	0.8324	0.8224	0.8089	0.7950	0.7803	0.7647
	55.00	0.8351	0.8252	0.8119	0.7983	0.7839	0.7686
	60.00	0.8378	0.8279	0.8149	0.8014	0.7873	0.7724
	65.00	0.8404	0.8307	0.8178	0.8046	0.7907	0.7761
	70.00	0.8429	0.8333	0.8207	0.8076	0.7939	0.7796
0.1502	0.10	0.9994	0.9804	0.9523	0.9242		
	1.00	1.0005	0.9816	0.9541	0.9261	0.8961	0.8632
	5.00	1.0058	0.9876	0.9609	0.9340	0.9055	0.8748
	10.00	1.0119	0.9944	0.9687	0.9430	0.9160	0.8874
	15.00	1.0175	1.0007	0.9760	0.9511	0.9255	0.8985
	20.00	1.0226	1.0066	0.9827	0.9587	0.9340	0.9083
	25.00	1.0276	1.0122	0.9889	0.9657	0.9420	0.9174
	30.00	1.0323	1.0173	0.9949	0.9722	0.9495	0.9257
	35.00	1.0367	1.0224	1.0005	0.9786	0.9562	0.9334
	40.00	1.0410	1.0269	1.0057	0.9843	0.9628	0.9405
	45.00	1.0451	1.0315	1.0109	0.9898	0.9688	0.9472
	50.00	1.0490	1.0359	1.0157	0.9952	0.9746	0.9536
	55.00	1.0529	1.0400	1.0203	1.0003	0.9802	0.9596
	60.00	1.0566	1.0440	1.0248	1.0051	0.9854	0.9655
	65.00	1.0602	1.0480	1.0292	1.0098	0.9905	0.9710
	70.00	1.0636	1.0517	1.0334	1.0144	0.9953	0.9763
0.3267	0.10	1.1572	1.1324	1.0978			
	1.00	1.1589	1.1344	1.1002	1.0637	1.0237	0.9789
	5.00	1.1662	1.1427	1.1100	1.0756	1.0383	0.9977
	10.00	1.1748	1.1521	1.1210	1.0886	1.0539	1.0168
	15.00	1.1827	1.1608	1.1311	1.1002	1.0676	1.0331
	20.00	1.1900	1.1689	1.1402	1.1106	1.0797	1.0472
	25.00	1.1970	1.1765	1.1488	1.1204	1.0907	1.0598
	30.00	1.2035	1.1836	1.1567	1.1293	1.1009	1.0713
	35.00	1.2098	1.1904	1.1643	1.1377	1.1101	1.0817
	40.00	1.2158	1.1967	1.1712	1.1455	1.1189	1.0914
	45.00	1.2216	1.2029	1.1780	1.1528	1.1270	1.1003
	50.00	1.2270	1.2088	1.1844	1.1599	1.1347	1.1087
	55.00	1.2324	1.2144	1.1905	1.1665	1.1419	1.1167
	60.00	1.2375	1.2198	1.1964	1.1729	1.1488	1.1243
	65.00	1.2425	1.2251	1.2020	1.1790	1.1555	1.1315
	70.00	1.2472	1.2301	1.2075	1.1848	1.1618	1.1383
0.5004	0.10	1.2817	1.2530	1.2118			
	1.00	1.2838	1.2556	1.2150	1.1706	1.1223	1.0663
	5.00	1.2931	1.2663	1.2282	1.1868	1.1430	1.0936
	10.00	1.3037	1.2785	1.2429	1.2043	1.1644	1.1202
	15.00	1.3136	1.2896	1.2561	1.2197	1.1826	1.1419
	20.00	1.3226	1.2998	1.2679	1.2335	1.1983	1.1605
	25.00	1.3312	1.3093	1.2789	1.2460	1.2127	1.1768
	30.00	1.3392	1.3182	1.2890	1.2574	1.2257	1.1914
	35.00	1.3469	1.3267	1.2985	1.2680	1.2377	1.2048

Table 2. continued

x	p/MPa	T/K					
		298.15	313.15	333.15	353.15	373.15	393.15
	40.00	1.3542	1.3345	1.3075	1.2777	1.2483	1.2170
	45.00	1.3611	1.3421	1.3160	1.2871	1.2586	1.2282
	50.00	1.3676	1.3493	1.3239	1.2958	1.2683	1.2388
	55.00	1.3740	1.3562	1.3315	1.3041	1.2773	1.2487
	60.00	1.3802	1.3627	1.3387	1.3120	1.2859	1.2581
	65.00	1.3861	1.3691	1.3457	1.3195	1.2940	1.2669
	70.00	1.3917	1.3752	1.3524	1.3268	1.3017	1.2754
0.6757	0.10	1.3772	1.3427	1.2942			
	1.00	1.3797	1.3456	1.2980	1.2469	1.1905	1.1267
	5.00	1.3906	1.3582	1.3133	1.2661	1.2153	1.1602
	10.00	1.4031	1.3722	1.3301	1.2865	1.2404	1.1919
	15.00	1.4144	1.3850	1.3451	1.3041	1.2615	1.2173
	20.00	1.4249	1.3967	1.3586	1.3197	1.2796	1.2386
	25.00	1.4348	1.4076	1.3709	1.3339	1.2959	1.2573
	30.00	1.4440	1.4176	1.3823	1.3467	1.3105	1.2738
	35.00	1.4526	1.4271	1.3929	1.3586	1.3237	1.2887
	40.00	1.4609	1.4359	1.4027	1.3696	1.3361	1.3023
	45.00	1.4688	1.4444	1.4121	1.3799	1.3475	1.3148
	50.00	1.4763	1.4525	1.4210	1.3896	1.3582	1.3266
	55.00	1.4835	1.4601	1.4293	1.3989	1.3681	1.3375
	60.00	1.4904	1.4675	1.4374	1.4075	1.3776	1.3479
	65.00	1.4970	1.4746	1.4450	1.4159	1.3867	1.3576
	70.00	1.5033	1.4814	1.4524	1.4239	1.3952	1.3668
0.8495	0.10	1.4558	1.4178				
	1.00	1.4586	1.4211	1.3687	1.3128	1.2515	1.1822
	5.00	1.4708	1.4353	1.3863	1.3350	1.2806	1.2218
	10.00	1.4848	1.4512	1.4054	1.3584	1.3093	1.2583
	15.00	1.4975	1.4655	1.4223	1.3782	1.3332	1.2870
	20.00	1.5091	1.4786	1.4373	1.3958	1.3536	1.3108
	25.00	1.5200	1.4906	1.4511	1.4116	1.3717	1.3315
	30.00	1.5302	1.5017	1.4638	1.4259	1.3879	1.3499
	35.00	1.5397	1.5122	1.4755	1.4391	1.4026	1.3662
	40.00	1.5489	1.5220	1.4859	1.4513	1.4162	1.3813
	45.00	1.5575	1.5313	1.4963	1.4626	1.4287	1.3951
	50.00	1.5656	1.5402	1.5061	1.4733	1.4405	1.4078
	55.00	1.5736	1.5486	1.5154	1.4834	1.4515	1.4198
	60.00	1.5811	1.5566	1.5243	1.4930	1.4618	1.4311
	65.00	1.5883	1.5643	1.5328	1.5021	1.4717	1.4417
	70.00	1.5952	1.5718	1.5409	1.5109	1.4810	1.4518
0.9184	0.10	1.4835	1.4445				
	1.00	1.4865	1.4481	1.3944	1.3372	1.2751	1.2049
	5.00	1.4992	1.4629	1.4128	1.3605	1.3054	1.2462
	10.00	1.5137	1.4794	1.4326	1.3848	1.3353	1.2840
	15.00	1.5268	1.4941	1.4502	1.4054	1.3600	1.3136
	20.00	1.5389	1.5077	1.4657	1.4235	1.3811	1.3382
	25.00	1.5502	1.5201	1.4799	1.4399	1.3998	1.3596
	30.00	1.5606	1.5316	1.4930	1.4546	1.4165	1.3784
	35.00	1.5705	1.5425	1.5052	1.4683	1.4316	1.3953
	40.00	1.5799	1.5526	1.5163	1.4808	1.4457	1.4107
	45.00	1.5888	1.5622	1.5271	1.4925	1.4585	1.4249
	50.00	1.5972	1.5713	1.5371	1.5035	1.4706	1.4380
	55.00	1.6053	1.5800	1.5465	1.5139	1.4819	1.4502
	60.00	1.6131	1.5882	1.5556	1.5237	1.4925	1.4618
	65.00	1.6206	1.5962	1.5642	1.5331	1.5026	1.4727
	70.00	1.6276	1.6038	1.5726	1.5421	1.5122	1.4831
1.0000	0.10	1.5155	1.4759				
	1.00	1.5186	1.4796	1.4253	1.3677	1.3048	1.2339
	5.00	1.5318	1.4950	1.4444	1.3918	1.3361	1.2766
	10.00	1.5468	1.5120	1.4649	1.4169	1.3670	1.3153

Table 2. continued

x	p/MPa	T/K					
		298.15	313.15	333.15	353.15	373.15	393.15
	15.00	1.5603	1.5273	1.4830	1.4381	1.3924	1.3457
	20.00	1.5728	1.5413	1.4991	1.4568	1.4141	1.3710
	25.00	1.5844	1.5542	1.5138	1.4736	1.4333	1.3929
	30.00	1.5952	1.5660	1.5273	1.4888	1.4505	1.4122
	35.00	1.6054	1.5772	1.5397	1.5029	1.4660	1.4295
	40.00	1.6151	1.5876	1.5513	1.5157	1.4804	1.4453
	45.00	1.6243	1.5975	1.5623	1.5277	1.4936	1.4598
	50.00	1.6329	1.6068	1.5725	1.5390	1.5060	1.4732
	55.00	1.6413	1.6158	1.5822	1.5497	1.5175	1.4858
	60.00	1.6492	1.6242	1.5916	1.5597	1.5284	1.4977
	65.00	1.6569	1.6324	1.6005	1.5693	1.5388	1.5088
	70.00	1.6642	1.6403	1.6090	1.5786	1.5486	1.5194

[a]Estimated expanded uncertainties ($k = 2$) are temperature, $U(T) = 0.03$ K; pressure, $U(p) = 0.04$ MPa; mole fraction, $U(x) = 0.00004$; density, $U(\rho) = 0.0007$ g·cm^{-3}. Data at the mole composition $x = 1.000$ come from ref 6.

Table 3. Parameters and Deviations for the Density Correlation by Using Equations 1−3 for the Mixture x HFE-7100 + $(1 − x)$ 1-Propanol[a,b,c,d,e,f]

parameters	x			
	0.0000	0.1502	0.3267	0.5004
A_0/g cm^{-3}	1.3311	0.92037	2.2516	1.8395
A_1/g cm^{-3} K^{-1}	-3.7889×10^{-3}	2.2955×10^{-3}	-7.9219×10^{-3}	-3.2115×10^{-3}
A_2/g cm^{-3} K^{-2}	1.0206×10^{-5}	-8.6342×10^{-6}	2.1709×10^{-5}	8.7935×10^{-6}
A_3/g cm^{-3} K^{-3}	-1.1660×10^{-8}	6.1268×10^{-9}	-2.4982×10^{-8}	-1.4419×10^{-8}
B_0/MPa	300.66	403.44	285.95	325.61
B_1/MPa K^{-1}	-0.85493	-1.6493	-1.0919	-1.3773
B_2/MPa K^{-2}	4.9307×10^{-4}	1.7312×10^{-3}	1.0272×10^{-3}	1.4691×10^{-3}
C	0.088972	0.083944	0.084335	0.08547
AAD/(%)	0.01	0.03	0.01	0.02
MD/(%)	0.03	0.10	0.03	0.08
bias/(%)	-2.10×10^{-5}	9.91×10^{-4}	-1.09×10^{-5}	1.44×10^{-5}
σ/(g·cm^{-3})	9.61×10^{-5}	3.43×10^{-4}	1.27×10^{-4}	3.65×10^{-4}
RMSD /(g·cm^{-3})	9.32×10^{-5}	3.29×10^{-4}	1.22×10^{-4}	3.50×10^{-4}
parameters	x			
	0.6757	0.8495	0.9184	1.0000
A_0/g cm^{-3}	2.9673	3.1167	3.0445	2.9319
A_1/g cm^{-3} K^{-1}	-1.1779×10^{-2}	-1.2115×10^{-2}	-1.1106×10^{-2}	-9.7459×10^{-3}
A_2/g cm^{-3} K^{-2}	3.2992×10^{-5}	3.3621×10^{-5}	3.0401×10^{-5}	2.6218×10^{-5}
A_3/g cm^{-3} K^{-3}	-3.8143×10^{-8}	-3.9136×10^{-8}	-3.5922×10^{-8}	-3.1740×10^{-8}
B_0/MPa	289.07	291.19	289.05	290.35
B_1/MPa K^{-1}	-1.2083	-1.2489	-1.2471	-1.2565
B_2/MPa K^{-2}	1.2619×10^{-3}	1.3432×10^{-3}	1.3509×10^{-3}	1.3679×10^{-3}
C	0.084411	0.084191	0.08404	0.084905
AAD/(%)	0.01	0.01	0.01	0.01
MD/(%)	0.03	0.05	0.06	0.12
bias/(%)	4.86×10^{-5}	-4.74×10^{-5}	-4.31×10^{-5}	4.13×10^{-5}
σ/(g·cm^{-3})	1.68×10^{-4}	2.19×10^{-4}	1.99×10^{-4}	3.00×10^{-4}
RMSD/(g·cm^{-3})	1.60×10^{-4}	2.10×10^{-4}	1.89×10^{-4}	2.90×10^{-4}

[a]N is the number of experimental data points and m is the number of parameters. [b]Absolute average deviation: $\text{AAD} = \frac{100}{N} \sum_{i=1}^{N} \left| \frac{\rho_i^{\text{exp}} - \rho_i^{\text{calc}}}{\rho_i^{\text{exp}}} \right|$.

[c]Maximum deviation: $\text{MD} = \max\left(100 \left| \frac{\rho_i^{\text{exp}} - \rho_i^{\text{calc}}}{\rho_i^{\text{exp}}} \right| \right)$. [d]Average deviation: $\text{bias} = \frac{100}{N} \sum_{i=1}^{N} \frac{\rho_i^{\text{exp}} - \rho_i^{\text{calc}}}{\rho_i^{\text{exp}}}$. [e]Standard deviation: $\sigma = \sqrt{\frac{\sum_{i=1}^{N}(\rho_i^{\text{exp}} - \rho_i^{\text{calc}})^2}{N \cdot m}}$.

[f]Root mean square deviation: $\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{N}(\rho_i^{\text{exp}} - \rho_i^{\text{calc}})^2}{N}}$.

where the mole fraction $x = 0.9184$ corresponds to the azeotropic composition of the binary mixture.[6] For the mole composition $x = 1.000$, the density data are referred to in our previous work.[12] Table 2 gathers the data of the experimental measurements obtained by using the vibrating tube densitometer. The boiling points at 0.1 MPa for the pure
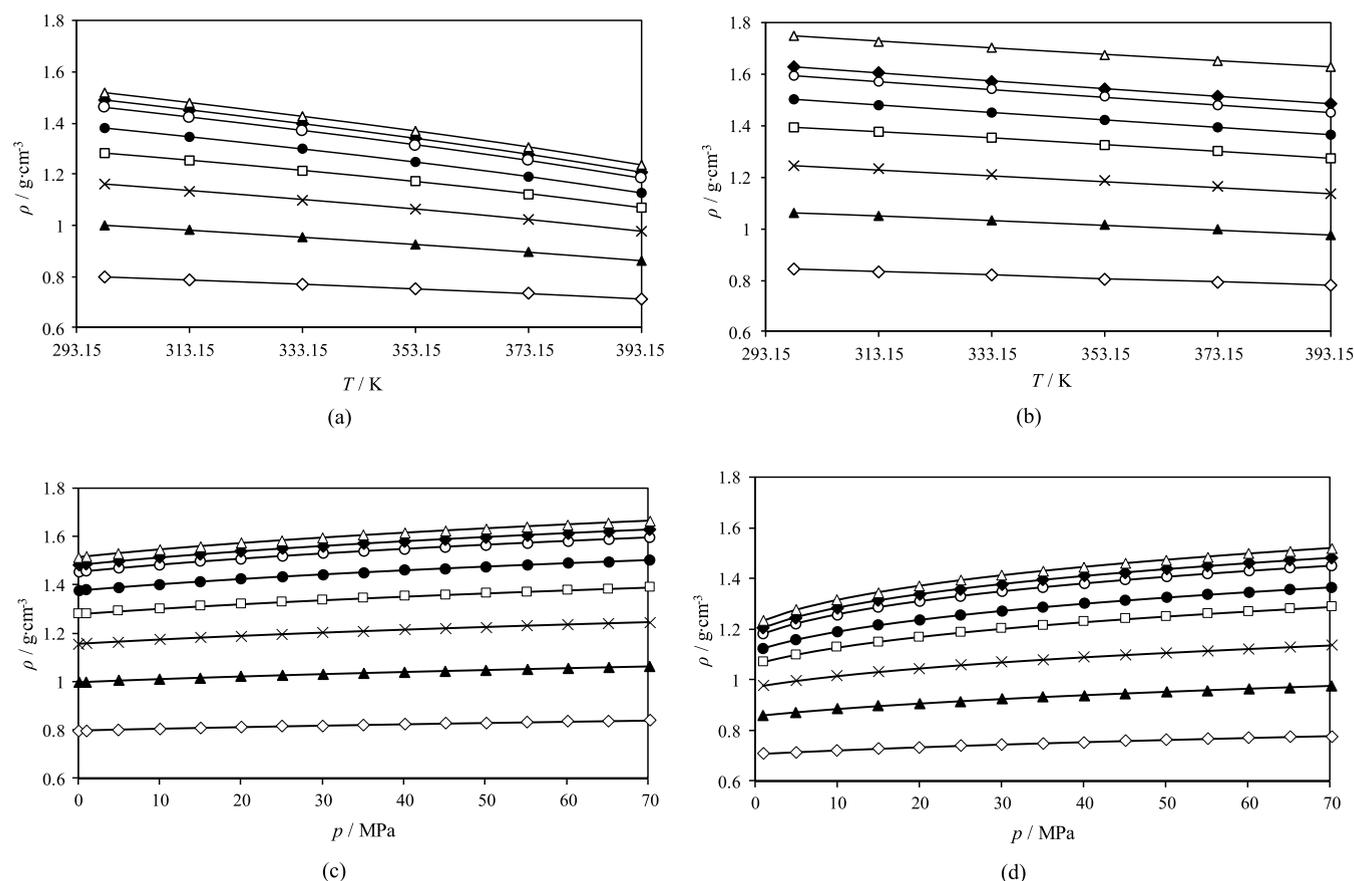
Figure 1. Experimental values of densities, ρ, for different mole fractions of x HFE-7100 + $(1 - x)$ 1-propanol versus (a) the temperature, T at 1 MPa, (b) the temperature, T at 70 MPa, (c) the pressure, p at 298.15 K, and (d) the pressure, p at 393.15 K. $\Diamond$: $x = 0.0000$, $\blacktriangle$: $x = 0.1502$, $\times$: $x = 0.3258$, $\square$: $x = 0.4963$, $\bullet$: $x = 0.6754$, $\bigcirc$: $x = 0.8495$, $\blacklozenge$: $x = 0.9184$, $\triangle$: $x = 1.0000$, (—): eqs 1−3
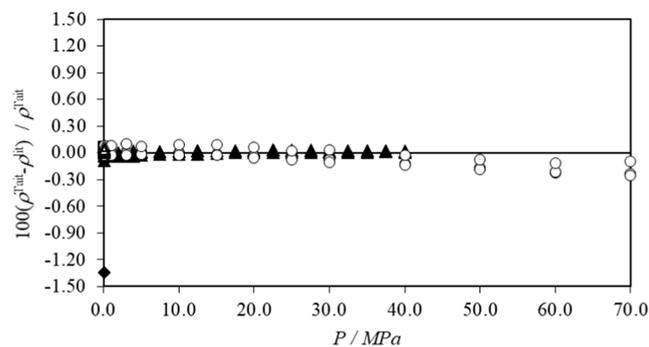
Figure 2. Deviations between the experimental values of densities and those obtained in the literature for pure HFE-7100. $\blacktriangle$: ref 16, $\bigcirc$: ref 17, $\blacksquare$: ref 18, $\blacklozenge$: ref 19, $\triangle$: ref 20, $\square$: ref 21.[21]

components determine the boiling point for the different mole compositions of the mixture at 0.1 MPa. Taking this into account, we found that the boiling temperature for HFE-7100 was $T_b = 332.85$ K[1] and that for pure 1-propanol was $T_b = 370.26$ K,[13] and then it was estimated that for the mole compositions $x = 0.0000$ and 0.1502, no measurements should be done at 0.1 MPa and at 373.15 and 393.15 K, since the mixture would be in the vapor phase. The same occurs for the mole compositions $x = 0.3258$, 0.4963, and 0.6754 at 0.1 MPa and at 353.15, 373.15, and 393.15 K and for the mole compositions $x = 0.8495$, 0.9184, and 1.0000, for which measurements at 0.1 MPa and at temperatures of 333.15,

353.15, 373.15, and 393.15 K should not be done. Following these estimations, no measurements were done at the aforementioned pressures and temperatures for the different mole compositions, which finally resulted in a total amount of 742 density points.

3.2. Tait Representation. As experimental measurements give density points at a fixed pressure p and temperature T, it is necessary to establish a correlation to better determine the behavior of density over the whole pressure and temperature ranges. Here, a Tait-like equation was used for this purpose, as well as to obtain the derivative properties. This equation was used in some of our previous works.[12,14,15] The equation is as follows

$$\rho(T, p) = \frac{\rho_0(T)}{1 - C \ln\left(\frac{B(T) + p}{B(T) + 0.1 \text{ MPa}}\right)} \tag{1}$$

where

$$\rho_0(T) = A_0 + A_1 T + A_2 T^2 + A_3 T^3 \tag{2}$$

$$B(T) = B_0 + B_1 T + B_2 T^2 \tag{3}$$

To obtain the A_i, B_i, and C parameter values, it is necessary to correlate simultaneously all of the experimental density values versus pressure and temperature. The obtained parameters for the mixture x HFE-7100 + $(1 - x)$ 1-propanol are listed in Table 3 along with its deviations (average absolute deviation AAD%, maximum deviation MD%, average deviation

Table 4. Comparison between the Values Generated Using the Tait-Like Equation at Exactly the Same Experimental p, T Sets Given for 1-Propanol for Several Literature References[a]

reference	year	N_P	T_{min}/K	T_{max}/K	p_{min}/MPa	p_{max}/MPa	AAD/%	MD/%	bias/%	density uncertainty
Kubota et al.[22]	1987	27	298.15	348.15	0.1	139.0	0.06	0.13	−0.05	0.8 kg·m^{-3}
Ormanoudis et al.[23]	1991	11	298.15	308.15	0.1	33.8	0.04	0.06	−0.04	10^{-4} g·cm^{-3}
Papaioannou et al.[24]	1993	10	298.15	298.15	0.1	33.9	0.05	0.07	−0.05	10^{-4} g·cm^{-3}
Papaioannou and Panayiotou[25]	1995	10	298.15	298.15	0.1	33.9	0.06	0.09	−0.06	10^{-4} g·cm^{-3}
Yaginuma et al.[26]	1998	12	313.15	313.15	0.1	9.8	0.07	0.10	0.04	0.1 kg·m^{-3}
Zúñiga-Moreno and Galicia-Luna[27]	2002	164	298.07	362.77	0.1	25.090	0.08	0.12	0.08	<0.05%
Kitajima et al.[28]	2003	16	315.15	390.15	5.12	27.0	0.03	0.04	−0.03	0.16%
Gil-Hernández et al.[29]	2005	20	298.15	308.15	0.1	19.7	0.05	0.14	−0.04	0.1 kg·m^{-3}
Zéberg-Mikkelsen and Andersen[30]	2005	28	303.15	333.15	0.1	30.0	0.01	0.03	0.01	0.05%
Watson et al.[31,32]	2006	84	303.15	353.15	0.1	65.0	0.04	0.09	3.41 × 10^{-3}	0.5 kg·m^{-3}
Abdulagatov et al.[33]	2008	36	298.15	373.15	0.11	39.95	0.04	0.11	0.04	0.02%
Torcal et al.[34]	2010	15	298.15	328.15	0.1	20.0	0.03	0.09	−0.02	0.5 kg·m^{-3}
Torcal et al.[35]	2010	15	298.15	328.15	20.0	60.0	0.04	0.09	0.04	0.5 kg·m^{-3}
Dávila et al.[36]	2012	98	298.15	358.15	0.1	60.0	0.12	0.21	0.12	0.0012 g·cm^{-3}
Kariznovi et al.[37]	2013	22	303.2	323.2	0.1	10.0	0.07	0.12	−0.02	0.1 kg·m^{-3}
Alaoui et al.[38]	2014	60	293.15	353.15	0.1	140.0	0.02	0.08	−1.54 × 10^{-3}	0.05% g·cm^{-3}

[a]N_P: number of data points that are in our p, T ranges.
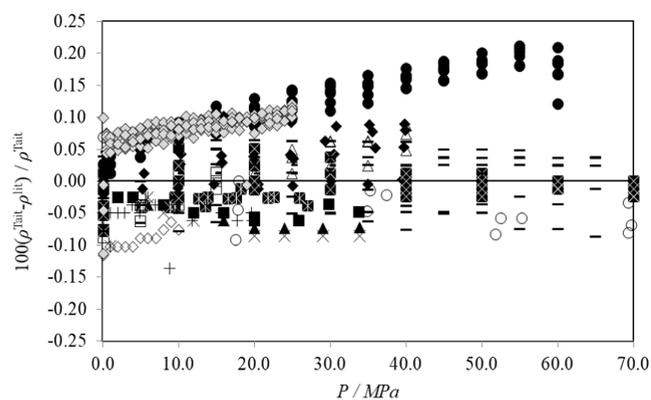
Figure 3. Deviations between the calculated values of densities obtained using eqs 1–3 and those obtained in the literature for pure 1-propanol. ○: ref 22, ■: ref 23, ▲: ref 24, x: ref 25, *: ref 26, ♦: ref 27, Že: ref 28, +: ref 29, -: ref 30, —: refs 31,32, ♦: ref 33, □: ref 34, △: ref 35, ●: ref 36, ◇: ref 37, x: ref 38.

AD%, standard deviation σ, and root mean square deviation RMSD). Different plots for density versus temperature/pressure representations for the eight mole compositions can be observed in Figure 1. Graph (a) presents high pressure density data versus temperature at 1 MPa, while graph (b) shows density versus temperature at the maximum pressure measured, 70 MPa. For all of the compositions, density decreases when increasing temperature, following the principle that an increase in temperature promotes molecular agitation and its separation, resulting in a decrease in density values. Comparing graphs (a) and (b), it can be seen that the highest density values are found at 70 MPa, as a result of the approximation of the molecules due to the increase of pressure.

When density values versus pressure are compared, graphs (c) and (d) prove the influence of temperature on density. At lower temperatures, which is the case of graph (c) (298.15 K), the values of density are quite higher than those of graph (d), at 393.15 K when considering the same mole composition. As mentioned above, an increase in temperature implies a decrease in density. The representation given by the Tait-like

equation is also shown in Figure 1, demonstrating the good capability of this equation to correlate the density values.

3.3. Comparison with Literature Data. Since the density of both pure fluids was previously measured by some authors, a comparison between our values and those found in the literature was carried out. When making the comparison, the experimental high pressure density data were correlated by using eqs 1–3, as some of the published data were not in the same P, T sets as ours. For pure HFE-7100, scarce density data were available. Only two references report data at high pressure,[16,17] while four references give density data at 0.1 MPa.[18−21] At atmospheric pressure, the four references give density values at 298.15 K, with refs 20,21 being the ones that bring more than one point. Ref 20 provides density data at atmospheric pressure in the temperature interval of 298.15−363.15 K, whereas ref 21 brings a total set of six points within the temperature interval of 298.15−323.12 K. The highest deviation is found for ref 19, with AAD% = MD% = Bias% = 1.35. For the two references at high pressure, ref 17 is the one that provides data at pressures higher than that measured by us (100 MPa), with a total of 116 points in our P, T ranges and with MD% = 0.25. For ref 16, a total of 60 points provide better deviations, with MD% = 0.08. These results are shown in Figure 2.

High pressure density data for pure 1-propanol are reported by several authors. A set of 16 references[22−38] were found in the literature over different pressure and temperature ranges. Most of them report data at pressures lower than those measured by us, with refs 22,38 being the ones that bring a set of data at higher pressures, with values of 139.0 and 140.0 MPa, respectively. With respect to the temperatures, only ref 33 provides density values at higher temperatures, although we have considered only those that fit our temperature range. Concerning the deviations, the results are quite satisfactory. The best results were found for ref 30, with AAD% = 0.01, Bias % = 0.01, and MD% = 0.03, while the worst values are those of ref 36, with AAD% = Bias% = 0.12, and MD% = 0.21. Very few references have values of average deviations (AD%) higher than the expanded uncertainty (0.07%), with only two of them 27 and 36 being above that value with AD% = 0.08 and 0.12, respectively. Table 4 presents the summary of the references,
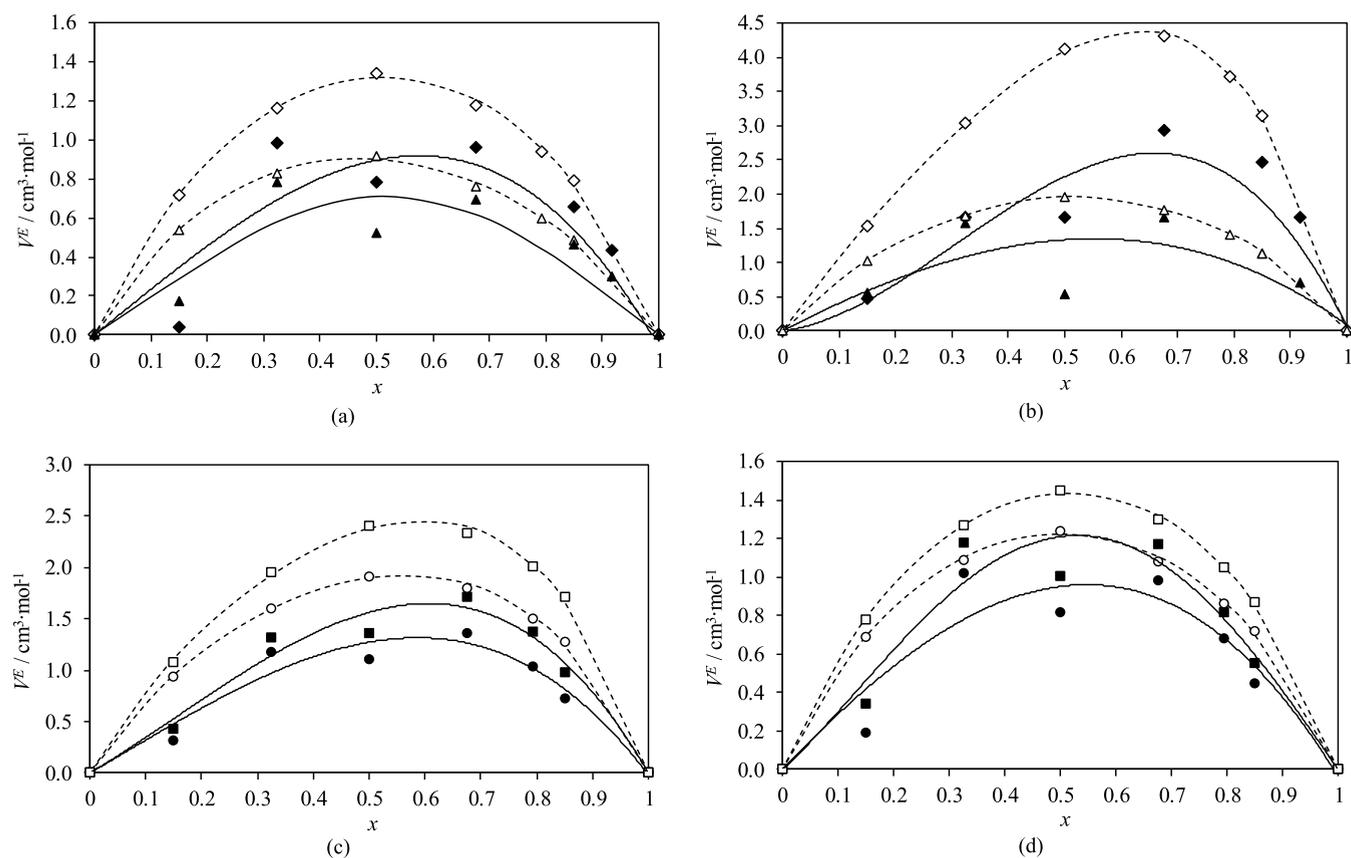
Figure 4. Comparison between the experimental values for excess volumes obtained for the binary mixture x HFE-7100 + $(1 - x)$ 1-propanol and the values of excess volumes for the system x HFE-7100 + $(1 - x)$ 2-propanol, ref 12 as a function of the mole fraction and at different pressures, (a) at 298.15 K and (b) at 393.15 K, where ◆: 1 MPa, ▲: 70 MPa (for the mixture x HFE-7100 + $(1 - x)$ 1-propanol), ◇: 1 MPa, △: 70 MPa (for the mixture x HFE-7100 + $(1 - x)$ 2-propanol) and (c) at p = 1 MPa and (d) at p = 70 MPa at various temperatures, where ●: 333.15 K, ■: 353.15 K (for the mixture x HFE-7100 + $(1 - x)$ 1-propanol), ○: 333.15 K, □: 353.15 K (for the mixture x HFE-7100 + $(1 - x)$ 2-propanol). (—): Redlich−Kister's equation (x HFE-7100 + $(1 - x)$ 1-propanol) and (- -): Redlich−Kister's equation (x HFE-7100 + $(1 - x)$ 2-propanol).

along with their deviations and the number of points that are in our p, T ranges, whereas Figure 3 gathers a representation of the deviations versus the pressure for all of the references found in the literature. No data were found in the literature for the mixture x HFE-7100 + $(1 - x)$ 1-propanol to compare with.

3.4. Excess Molar Volumes. To determine the difference in volume of the mixture between the theoretical results of mixing the two pure compounds and the experimental ones, the excess molar volumes, V^E, were determined. These data were calculated by using eq 4.

$$V^E = \sum_{i=1}^{n} x_i M_i [(1/\rho) - (1/\rho_i)] \tag{4}$$

In this equation, n is the number of components, x_i is the mole fraction of component i in the mixture, M_i is the molar mass of component i, and ρ and ρ_i are the measured densities of the mixture and pure component i, respectively.

Figure 4 shows different representations of excess volumes V^E versus the composition x, both considering a fixed temperature and evaluating the influence of pressure changes, as is the case of plots (a) at 298.15 K and (b) at 393.15 K, or considering a fixed value in pressure evaluating temperature changes, as can be seen in plots (c) at p = 1 MPa and (d) at p = 70 MPa. For the four graphs, (a), (b), (c), and (d), the solid

figures represent the excess volumes for the binary mixture x HFE-7100 + $(1 - x)$ 1-propanol.

In all of the cases, the excess volumes show a positive trend at the different temperatures and pressures measured. The size of the HFE-7100 molecules is much larger than the size of the 1-propanol molecules, so the approximation of both types of molecules generates an expansion that takes place in the mixture, resulting in positive values of V^E. The low polarity of HFE compared to that of alkanol leads to a low packing effect, contributing to the relatively high values of excess volumes.

In plots (a) and (b), it can be seen that the differences in the V^E values become higher when the temperature increases; this behavior is shown in both plots at different pressures, 1 and 70 MPa, considering a fixed temperature, 298.15 K for (a) and 393.15 K for (b). If we evaluate the pressure at 1 MPa, the excess volumes are higher in both cases (a) and (b) than those for 70 MPa.

By studying graphs (c) and (d), where a value of pressure is fixed and the changes in temperature are shown, it can be seen that for (c), at p = 1 MPa, the values of V^E are higher than those for (d) at p = 70 MPa for the two temperatures studied, 333.15 and 353.15 K. Considering the temperature, lower values are found when the temperature is lower; then, for both graphs, values at 333.15 K are lower than values at 353.15 K, which is a consequence of the approximation of the molecules promoted by the decrease in temperature. In this case, the maximum value of V^E is found for the mole composition x =

Table 5. Values of Parameters z_i of Eq 5 and the Corresponding Standard Deviation, σ, for the Binary System x HFE-7100 + $(1 − x)$ 1-propanol at 298.15 and 393.15 K for Different Pressures and at 1.0 MPa, 35.0, and 70.0 MPa for All of the Temperatures Measured

	z_1	z_2	z_3	σ (V^E)/cm^3·mol^{-1}
p/MPa	(T = 298.15 K)			
0.10	4.0445	1.3620	−3.0917	0.14
1.00	4.0492	1.3356	−3.0521	0.14
35.00	3.4601	0.6956	−2.2125	0.13
50.00	3.1758	0.4345	−1.5798	0.12
70.00	2.8412	0.2379	−0.8906	0.11
p/MPa	(T = 393.15 K)			
1.00	8.5461	7.8258	3.0543	0.27
35.00	6.6186	1.3842	3.4652	0.33
50.00	5.6358	1.0185	3.8922	0.34
70.00	4.6790	0.9201	4.2242	0.35
T/K	(p = 1.00 MPa)			
298.15	4.0492	1.3356	−3.0521	0.14
313.15	4.5102	1.7289	−2.6695	0.14
333.15	5.2403	1.9771	−0.9525	0.12
353.15	6.2577	3.0492	0.0167	0.11
373.15	6.4842	4.8158	3.7563	0.25
393.15	8.5461	7.8258	3.0543	0.27
T/K	(p = 35.00 MPa)			
298.15	3.4601	0.6956	−2.2125	0.13
313.15	4.0224	1.0967	−2.7305	0.14
333.15	4.7810	0.9683	−1.8112	0.12
353.15	5.7896	1.0307	−1.1828	0.12
373.15	5.0855	1.1341	4.3957	0.32
393.15	6.6186	1.3842	3.4652	0.33
T/K	(p = 70.00 MPa)			
298.15	2.8412	0.2379	−0.8906	0.11
313.15	3.3671	0.7735	−1.9915	0.13
333.15	4.0912	0.8366	−1.8719	0.13
353.15	4.8389	0.7572	−1.4379	0.12
373.15	3.6801	0.7984	4.6316	0.32
393.15	4.6790	0.9201	4.2242	0.35

0.6757 at p = 1 MPa and at T = 353.15 K with V^E = 1.71 cm^3·mol^{-1}.

A comparison has been carried out between the obtained excess molar volumes for the mixture x HFE-7100 + $(1 − x)$ 1-propanol and the previously studied mixture x HFE-7100 + $(1 − x)$ 2-propanol,[12] considering the same temperatures and pressures at practically the same mole compositions (x = 0.000, 0.1490, 0.3255, 0.4996, 0.6758, 0.7940, 0.8497 and 1.0000). The representation of the excess molar volumes of the mixture x HFE-7100 + $(1 − x)$ 2-propanol can be seen in Figure 4 together with the ones of the mixture x HFE-7100 + $(1 − x)$ 1-propanol, being represented in the graphs with the hollow symbols.

In the same way that happens for the mixture x HFE-7100 + $(1 − x)$ 1-propanol, a positive tendency is observed for the mixture x HFE-7100 + $(1 − x)$ 2-propanol, the values of excess volumes being higher in the case of this mixture when compared with the system x HFE-7100 + $(1 − x)$ 1-propanol. This fact is noticed in the four graphs in Figure 4. The different sizes between the two alkanol molecules promote the difference in excess volumes. The maximum value of V^E is found at the same mole composition, pressure, and temperature as for the mixture x HFE-7100 + $(1 − x)$ 1-propanol; x =

0.6757, p = 1 MPa, and at T = 393.15 K, with a value of V^E = 4.30 cm^3·mol^{-1}.

Comparing what happens with the two mixtures in graphs (c) and (d), it can be stated that for the binary system x HFE-7100 + $(1 − x)$ 2-propanol, the tendency remains the same as for the mixture x HFE-7100 + $(1 − x)$ 1-propanol, but its V^E values are higher than those of the mixture x HFE-7100 + $(1 − x)$ 1-propanol for all of the pressures and temperatures. For this mixture, the highest value of V^E is found at the same pressure and temperature as for the mixture x HFE-7100 + $(1 − x)$ 1-propanol (p = 1 MPa and T = 353.15 K) but for a different mole composition, x = 0.4996, with V^E = 2.40 cm^3·mol^{-1}.

In addition, Figure 4 shows the fitting curves obtained for both binary systems using a Redlich−Kister polynomial of the following type.

$$V^E = x(1 − x) \sum_i z_i (2x − 1)^{i−1} \tag{5}$$

In eq 5, z_i are the adjustable parameters, and x is the mole fraction of HFE-7100. Then, for the mixture studied in this work, x HFE-7100 + $(1 − x)$ 1-propanol, the solid line represents the fitting curve to the experimental data, while for the previously studied system, x HFE-7100 + $(1 − x)$ 2-propanol, the dashed line corresponds to the fitting to the Redlich−Kister polynomial.

Table 5 reports the values of the adjustable parameters, z_i, and the standard deviations obtained by using eq 5 for different pressures at T = 298.15 and 393.15 K, as well as for all of the temperatures measured at 1.0, 35.0, and 70.0 MPa.

3.5. Derived Thermodynamic Properties. It is possible to obtain, from experimental density data, other properties of importance that will give valuable information concerning the dependence of the volumetric properties on the temperature and pressure. These are the so-called derivative properties, which are the isothermal compressibility κ_T and the isobaric expansion α_P. The isothermal compressibility gives information about the effect of pressure on the density when the temperature remains constant, and it can be expressed as follows.

$$\kappa_T = \left(\frac{1}{\rho}\right)\left(\frac{\partial \rho}{\partial p}\right)_T = \frac{C}{\left(1 − C \ln\left(\frac{B(T) + p}{B(T) + 0.1 \, \text{MPa}}\right)\right)(B(T) + p)} \tag{6}$$

Figure 5 shows a representation of κ_T versus the mole composition at (a) 298.15 K and (b) 393.15 K. In both plots, the studied pressures are p = 1, 20, 40, and 70 MPa. It can be seen for both plots (a) and (b) that for this property, the higher the content of HFE-7100 in the mixture, the higher the value of κ_T, with the exception of the case at 393.15 K and at 1 MPa, for which the value of κ_T at x = 1.0000 is slightly lower than for the precedent mole composition (x = 0.9184). Moreover, an increase in temperature promotes an increase in the values of isothermal compressibility. Therefore, when pressure increases, κ_T decreases, with the mole composition x = 0.0000 at 298.15 and at 70.0 MPa being the one with the lowest κ_T value of 5.9 MPa^{-1}.

Similarly, the isobaric expansion, α_P, could also be obtained by differentiating eq 1 and taking into account the temperature dependence of $\rho_0(T)$ and B(T).
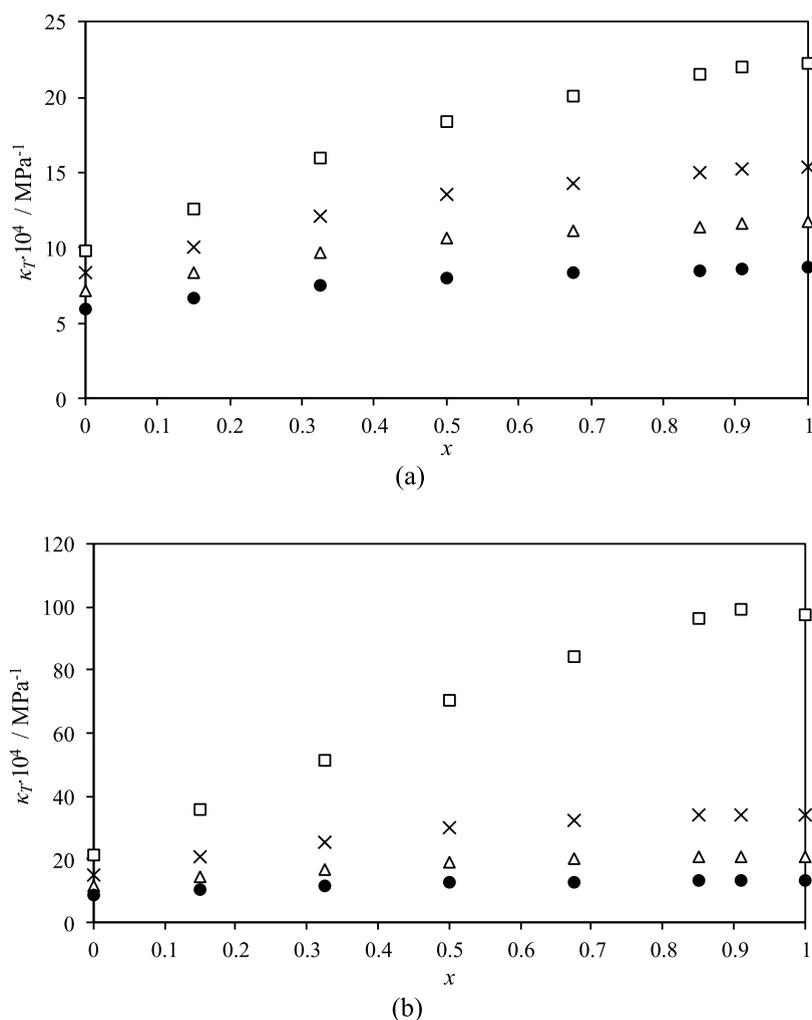
Figure 5. Isothermal compressibility κ_T values for the binary mixture x HFE-7100 + $(1 - x)$ 1-propanol versus the mole composition at different pressures p and at (a) 298.15 K and (b) 393.15 K. □: p = 1 MPa, ×: p = 20 MPa, Δ: p = 40 MPa, ●: p = 70 MPa.

$$\alpha_p = -\left(\frac{1}{\rho}\right)\left(\frac{\partial \rho}{\partial T}\right)_p \tag{7}$$

As some authors have reported previously,[39,40] the estimated isobaric expansion depends on the form of functions $B(T)$ and $\rho_0(T)$. Also, Jaquemin et al.[41] noticed that the differences that were sometimes found for α_P in the literature were due to the difference in density values and also to the fitting equations. Thus, as an alternative, it was proposed to derive the isobaric expansion from the isobaric densities, and then at each pressure, we suppose that $\rho_p(T) = a_0 + a_1 T + a_2 T^2$ and consequently $(\partial \rho / \partial T)_p = a_1 + 2a_2 T$. By doing so, a set (a_0, a_1, a_2) is obtained for each pressure.

By inserting the differentiated density and the calculated densities $\rho_p(T)$ into $\alpha_p = -(1/\rho(\partial \rho/\partial T)_p)$, the isobaric expansion at different T, p conditions has been derived as follows.

$$\alpha_p = -\frac{a_1 + 2a_2 T}{a_0 + a_1 T + a_2 T^2} \tag{8}$$

The estimated uncertainty following ref[11] is 1% for the isothermal compressibility and around 3% for the isobaric expansion, as recently indicated in similar high-pressure density studies[7,8] and[31] with the same methods.

Figure 6a,b shows the values of isobaric expansion at 298.15 and 393.15 K, respectively, at different pressures. At 298.15 K (a), it can be observed that the values of α_p follow a tendency to decrease with increasing pressure in all cases. When taking a look at the mole composition at a fixed pressure, α_p decreases when the content of HFE-7100 is higher, except for the case of pure HFE-7100, whose value increases rapidly. Similarly, as observed at 298.15 K, at 393.15 K (b), the values of α_p are lower at high pressures when considering a fixed mole composition. Evaluating the mole compositions, the values of α_p are lower for the mixtures with less content of HFE-7100 up to a mole composition of x = 0.8495; then, the α_p values tend to decrease rapidly when increasing the HFE-7100 content. If we compare graphs (a) and (b), the values of isobaric expansion at 393.15 K are higher than those for 298.15 K.

4. CONCLUSIONS

Experimental determination of (ρ, T, p) values for the binary system x HFE-7100 + $(1 - x)$ 1-propanol was carried out by employing a vibrating tube densitometer in the pressure range from 0.1 to 70 MPa and along six isotherms ranging from 298.15 to 393.15 K. The experimental high pressure density data were fitted to a Tait-like equation to properly correlate the density values over the entire p, T ranges, showing the low
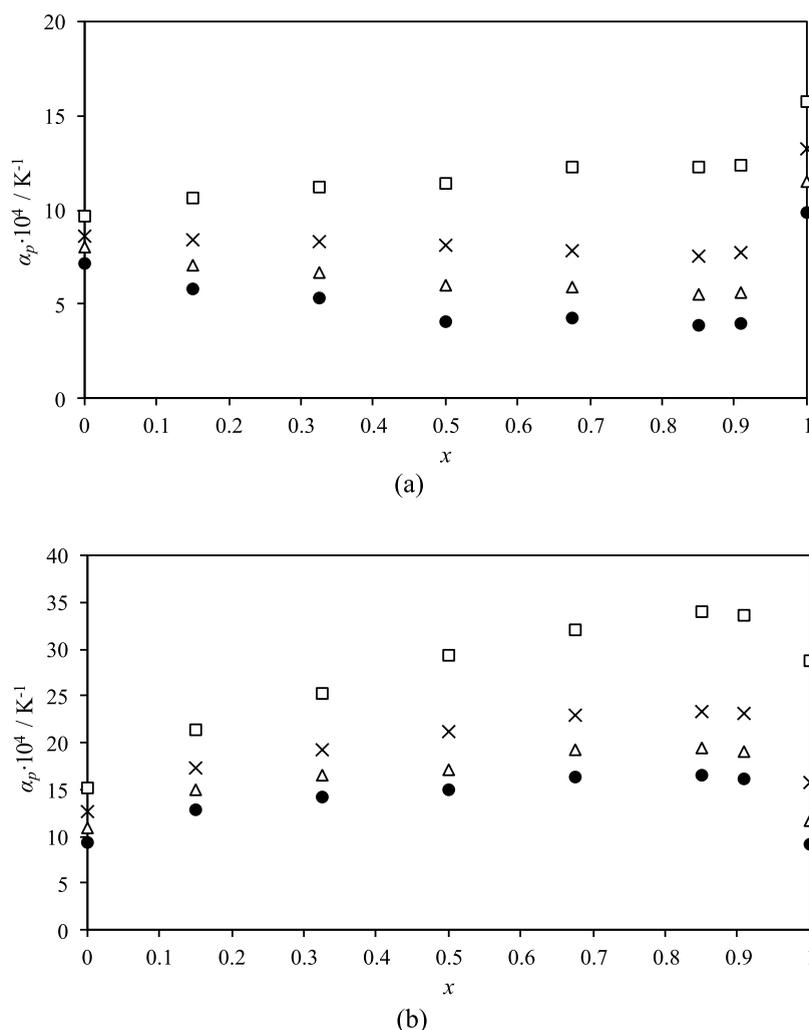
Figure 6. Isobaric expansion α_P values for the binary mixture x HFE-7100 + $(1 - x)$ 1-propanol versus the mole composition at different pressures p and at (a) 298.15 K and (b) 393.15 K. □: $p = 1$ MPa, ×: $p = 20$ MPa, Δ: $p = 40$ MPa, ●: $p = 70$ MPa.

deviations obtained between the calculated and the experimental data. A comparison between the experimental density data and the values obtained in the literature was carried out for both pure HFE-7100 and 1-propanol. No data were found in the literature for the binary mixture. Based on the experimental density measurements, excess volumes V^E were obtained, and a comparison between these values and those measured previously concerning the binary mixture x HFE-7100 + $(1 - x)$ 2-propanol was conducted. Finally, by differentiating the Tait-like equation, isobaric expansion α_P and isothermal compressibilities κ_T were determined.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.jced.3c00563.

> Values of isothermal compressibility $\kappa_T \cdot 10^4$ for x HFE-7100 + $(1 - x)$ 1-propanol as a function of pressure p and at different temperatures T, and values of isobaric expansion $\alpha_P \cdot 10^4$ for x HFE-7100 + $(1 - x)$ 1-propanol as a function of pressure p and at different temperatures T (PDF)

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Notes

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◼ LIST OF SYMBOLS

AAD	absolute average deviation
a_i	coefficients of isobaric thermal expansivity correlation
A_i, B_i, C	coefficients of density correlation
Bias	average deviation
exp	experimental
i	constituent identification
lit	literature
MD	maximum deviation
N_P	number of experimental data points that are in our p, T ranges
p	pressure
p_0	reference pressure
RMSD	root mean square deviation
T	temperature
V^E	excess molar volume

◼ GREEK LETTERS

σ	standard deviation
α_p	isobaric expansion
ρ	density
ρ_0	density at a reference pressure P_0
κ_T	isothermal compressibility

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