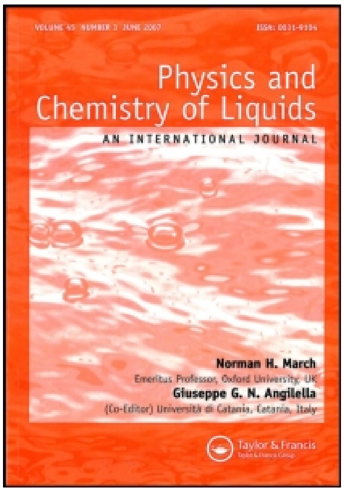

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Temperature dependence of the derived properties of mixtures containing chlorobenzene and aliphatic linear alkanes (C_6–C_{12})

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This article reports experimental densities, refractive indices and speeds of sound of the binary mixtures chlorobenzene + (*n*-hexane, *n*-heptane, *n*-octane, *n*-nonane, *n*-decane, *n*-undecane or *n*-dodecane) and speeds of sound of the ternary mixtures chlorobenzene + *n*-hexane + (*n*-undecane or *n*-dodecane) at 298.15 K and atmospheric pressure, over the whole concentration range. The corresponding derived properties were computed from the experimental data. The results were fitted by means of the Redlich–Kister equation for binary mixtures and the Nagata equation for ternary mixtures. A set of estimation methods were applied, and an interpretation in terms of structure and length of molecular chain of the *n*-alkane molecules was made.

Keywords: derived properties; chlorobenzene; *n*-alkane; density; speed of sound; refractive index; estimation

1. Introduction

A regulated chemical waste is defined as a waste which, due to its quantity, concentration or physical and chemical characteristics, may cause an increase in mortality, serious or incapacitating illness or pose a substantial or potential threat to human health or the environment when improperly treated, stored, transported, disposed of, or otherwise managed. The disposal of regulated waste and other unwanted chemicals has become increasingly complicated. Many US and European environmental protection agencies regulate the treatment and disposal of chemical wastes. The main aim of these agencies is to determine exactly what is and is not a regulated chemical waste. In doing so, the chemical industry may be able to design processes with waste minimisation, and dispose chemical waste generated in a manner consistent with legal requirements in use.

Nowadays, it is necessary to design efficient and clean industrial procedures for environmental protection, which need the knowledge of different thermodynamic properties on mixing. Indeed, the contamination of air, surface water or ground with halogenated aromatic and hydrocarbons of different nature is perhaps one of the most serious problems that mankind faces today. The purpose of this study is to

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continue our research in the field of physical properties of mixtures for a better understanding of the mixing trend of chemicals related to environment cleaning, food or pharmacologic industries [1–4]. In this way, the first step is the thermodynamic characterisation of the mixtures (physical properties, vapour–liquid equilibria, liquid–liquid equilibria, etc.) involved in the separation problem, and then an engineering study to evaluate, optimise and design. We present new measurements of different thermodynamic properties (speeds of sound, densities and refractive indices) of the binary mixtures chlorobenzene + (*n*-hexane, *n*-heptane, *n*-octane, *n*-nonane, *n*-decane, *n*-undecane or *n*-dodecane) and speeds of sound of the ternary mixtures chlorobenzene + *n*-hexane + (*n*-undecane or *n*-dodecane) at 298.15 K, as well as the corresponding derived magnitudes (change in isentropic compressibilities on mixing excess molar volumes and change in refractive indices on mixing). These estimations were attempted using different procedures (equations of state for density, mixing rules for refractive indices, the collision factor theory (CFT) and free length theory (FLT) for isentropic compressibilities). The corresponding derived magnitudes were correlated by application of the Redlich–Kister or the Nagata equation, such fitting parameters being gathered. An interpretation in terms of structure and length of molecular chain of aliphatic alkanes was made from the obtained results. A survey of the literature has shown that only a few measurements on excess molar volumes of binary mixtures are available in the open literature.

2. Experimental

All chemicals used were of Merck chromatographic grade and were treated as usual in previous works [4]. Ultrasonic treatment was used for degassing, and molecular sieves (type 4a or 3a, 1/16 inch, Aldrich cat. no 20.860-4 or 20.858-2, respectively) were introduced into the bottles to reduce possible water contents in solvents. The gas chromatographic analysis of pure components showed that the major peak area exceeds 99.0% for any solvent. The composition of the solution was determined gravimetrically, special care being taken during solution preparation to avoid losses due to evaporation. Further details of experimental procedure and mode of operation in our laboratory were provided in our earlier articles. The refractive indices of the pure liquids and mixtures were measured with the automatic refractometer ABBEMAT-HP Dr Kernchen with a precision of $\pm 10^{-5}$, and thermostated with a PolyScience controller bath model 9010 with a temperature stability of $\pm 10^{-2}$ K. The densities and speeds of sound were measured with an Anton Paar DSA-48 digital densimeter and sound analyzer with a precision of $\pm 10^{-4}\,\mathrm{g\,cm^{-3}}$ and $1\,\mathrm{m\,s^{-1}}$, respectively. Calibration of these apparatuses was performed periodically, in accordance to technical specifications, using millipore quality water (resistivity, $18.2\,\mathrm{M\Omega\,cm}$) and ambient air. A PolyScience controller bath model 9010 with a temperature stability of $\pm 10^{-2}$ K was used to thermostat the samples at least for 30 min. Samples were prepared by mass using a Mettler AT-261 Delta Range balance with an accuracy of $\pm 10^{-4}$ g, covering the whole composition range of the mixtures. The accuracy of the mole fractions, densities, refractive indices and speeds of sound were estimated better than 10^{-4}, $2 \times 10^{-4}\,\mathrm{g\,cm^{-3}}$, 5×10^{-5} and $1\,\mathrm{m\,s^{-1}}$, respectively. Maximum deviation in the calculation of excess molar volumes, changes of refractive indices on mixing and changes of isentropic compressibilities for these mixtures have been estimated better than $10^{-3}\,\mathrm{cm^3\,mol^{-1}}$, 10^{-4}, and $1\,\mathrm{TPa^{-1}}$, respectively. The values of the pure components, as well as the open literature data, are given in Table 1.

3. Data procedure

3.1. *Correlation of derived magnitudes*

The excess molar volumes, changes in refractive indices and changes in isentropic compressibilities on mixing (based on Newton–Laplace equation) values are presented in Tables 2 and 3 and were computed using following equations:

$$V^{\mathrm{E}} = \sum_{i=1}^{n} x_i M_i \left(\rho^{-1} - \rho_i^{-1}\right), \tag{1}$$

$$\delta n_{\mathrm{D}} = n_{\mathrm{D}} - \sum_{i=1}^{n} x_i n_{\mathrm{D}i}, \tag{2}$$

$$\delta \kappa_{\mathrm{S}} = \frac{1}{\rho u^2} - \sum_{i=1}^{n} \frac{x_i}{\rho_i u_i^2}, \tag{3}$$

where ρ is the density, n_{D} the refractive index on mixing and κ_{S} the isentropic compressibility on mixing. The symbols ρ_i, $n_{\mathrm{D}i}$ and $\kappa_{\mathrm{S}i}$ represent the properties of pure chemicals and n is the number of components in the mixture. A Redlich–Kister [12] type equation was used to correlate the derived properties of the binary mixtures, by using the unweighted least squares method, with all experimental points weighting equally. The Redlich–Kister equation can be expressed as follows:

$$\delta Q_{ij} = x_i x_j \sum_{p=0}^{m} A_p (x_i - x_j)^p, \tag{4}$$

where δQ is V^{E} ($\mathrm{cm^3\,mol^{-1}}$), δn_{D} or $\delta \kappa_{\mathrm{S}}$ ($\mathrm{TPa^{-1}}$), respectively. The degree of this equation (m parameter) was optimised by applying F-test [13]. We have not found any data in the open literature for the changes in refractive indices or the changes in isentropic compressibilities of the mixtures at the studied conditions. The fitting parameters A_p are given in Table 4, with the corresponding root mean square deviations. These parameters were computed using a non-linear optimisation algorithm.

The ternary-derived magnitudes were fitted to the following equation

$$\Delta Q_{123} = \Delta Q_{12} + \Delta Q_{13} + \Delta Q_{23} + \Delta Q_{\mathrm{ter}}, \tag{5}$$

where the binary magnitudes ΔQ_{ij} have been correlated with Equation (4), and ΔQ_{ter} is the ternary contribution fitted by means of the equation of Nagata [14]

$$\begin{aligned}\Delta Q_{\mathrm{ter}} = x_1 x_2 x_3 RT(B_0 - B_1 x_1 - B_2 x_2 - B_3 x_1^2 - B_4 x_2^2 - B_5 x_1 x_2 - B_6 x_1^3 \\ - B_7 x_2^3 - B_8 x_1^2 x_2).\end{aligned} \tag{6}$$

Table 1. Molar weight, gas–liquid chromatography (GLC) purity and comparison of data with the open literature for pure liquids at 298.15 K.

		Purity	ρ (g cm^{-3})		n_D		u (m s^{-1})	
Component	Molar weight (g mol^{-1})	Mass %	Experimental	Literature [5]	Experimental	Literature [5]	Experimental	Literature
Chlorobenzene	112.558	>99.5	1.1008	1.1011	1.52378	1.52138	1267.60	1094.69 [5]
n-hexane	86.177	>99.2	0.6551	0.65484 0.65490 [6]	1.37234	1.37226	1077.00	1076.37 [7]
n-heptane	100.204	>99.9	0.6794	0.67940	1.38512	1.3850	1130.50	1131.00 [8]
n-octane	114.231	>99.3	0.6985	0.69862	1.39514	1.39505	1172.00	1180.00 [9]
n-nonane	128.258	>99.2	0.7142	0.71375	1.40336	1.40311	1207.35	1212.00 [10]
n-decane	142.285	>99.6	0.7261	0.72614	1.40937	1.40967	1234.75	1234.00 [9]
n-undecane	156.312	>99.0	0.7365	0.73650	1.41473	1.41507	1258.16	1257.95 [11]
n-dodecane	170.338	>99.6	0.7451	0.74518	1.41953	1.41949	1279.61	1277.97 [11]

Note: Numbers in square brackets denote the corresponding reference.

Table 2. Densities ρ, refractive indices n_D, speeds of sound u, isentropic compressibilities κ_S, excess molar volumes V^E, changes of refractive indices δn_D and changes of isentropic compressibilities $\delta \kappa_S$ for the binary mixtures chlorobenzene + (*n*-hexane, *n*-heptane, *n*-octane, *n*-nonane, *n*-decane, *n*-undecane, or *n*-dodecane) at 298.15 K.

x	ρ (g cm^{-3})	n_D	u (m s^{-1})	κ_S (TPa^{-1})	(cm^3 M^{-1})	δn_D	$\delta\kappa_S$ (TPa^{-1})
Chlorobenzene + *n*-hexane							
0.0609	0.6770	1.37986	1084.4	1256.1	−0.09633	−0.00170	−14.3
0.1099	0.6952	1.38608	1090.4	1210.0	−0.18532	−0.00290	−23.6
0.1971	0.7283	1.39719	1101.9	1130.9	−0.30205	−0.00500	−37.2
0.3077	0.7722	1.41160	1118.1	1035.9	−0.40511	−0.00734	−49.2
0.4047	0.8126	1.42531	1133.9	957.2	−0.48308	−0.00832	−55.0
0.5087	0.8578	1.44073	1153.6	876.0	−0.52266	−0.00865	−58.1
0.6098	0.9039	1.45608	1173.8	803.0	−0.52264	−0.00861	−55.2
0.7098	0.9515	1.47178	1195.8	735.1	−0.47791	−0.00805	−48.1
0.8063	0.9994	1.48743	1217.5	675.1	−0.38537	−0.00702	−35.7
0.9055	1.0504	1.50504	1242.2	617.0	−0.21044	−0.00443	−19.3
0.9522	1.0754	1.51412	1254.6	590.8	−0.13133	−0.00242	−10.4
Chlorobenzene + *n*-heptane							
0.0625	0.6982	1.39118	1133.7	1114.3	−0.01591	−0.00277	−0.7
0.1063	0.7118	1.39561	1136.5	1087.7	−0.03721	−0.00441	−1.6
0.2013	0.7427	1.40530	1143.2	1030.3	−0.09241	−0.00788	−3.3
0.3164	0.7828	1.41842	1153.1	960.7	−0.15116	−0.01070	−5.4
0.4125	0.8188	1.43004	1163.3	902.5	−0.20083	−0.01238	−7.3
0.5051	0.8559	1.44232	1174.8	846.6	−0.24908	−0.01293	−8.9
0.6054	0.8988	1.45591	1188.8	787.2	−0.26849	−0.01323	−9.4
0.7066	0.9452	1.47049	1205.4	728.2	−0.24851	−0.01266	−9.1
0.8059	0.9942	1.48625	1224.4	670.9	−0.20210	−0.01065	−8.2
0.8993	1.0437	1.50289	1243.7	619.4	−0.12596	−0.00695	−4.9
0.9512	1.0728	1.51318	1255.6	591.2	−0.07320	−0.00384	−2.7
Chlorobenzene + *n*-octane							
0.0784	0.7188	1.40134	1173.9	1009.6	0.00613	−0.00389	4.9
0.1119	0.7279	1.40433	1174.6	995.8	0.00949	−0.00520	7.0
0.2070	0.7550	1.41260	1177.5	955.3	0.00538	−0.00917	11.8
0.3114	0.7873	1.42244	1182.2	908.8	−0.01359	−0.01276	15.1
0.4101	0.8207	1.43306	1187.9	863.4	−0.04090	−0.01484	16.8
0.5055	0.8559	1.44418	1195.1	818.1	−0.06785	−0.01599	17.0
0.6083	0.8975	1.45710	1205.0	767.3	−0.09672	−0.01629	15.2
0.6994	0.9379	1.46950	1215.6	721.5	−0.10713	−0.01561	12.9
0.8078	0.9910	1.48608	1231.2	665.7	−0.09716	−0.01298	8.7
0.9030	1.0427	1.50309	1247.9	615.8	−0.06636	−0.00821	4.3
0.9507	1.0707	1.51272	1257.3	590.8	−0.04330	−0.00472	2.0
Chlorobenzene + *n*-nonane							
0.0849	0.7332	1.40898	1205.9	937.9	0.02714	−0.00447	9.8
0.1221	0.7421	1.41156	1205.9	926.7	0.04460	−0.00637	13.3
0.2159	0.7660	1.41885	1205.8	897.8	0.07356	−0.01039	21.6
0.3149	0.7937	1.42730	1207.0	864.9	0.09219	−0.01388	27.9
0.3992	0.8196	1.43478	1208.8	835.0	0.09544	−0.01656	31.5
0.4998	0.8538	1.44550	1212.6	796.5	0.07350	−0.01797	32.9
0.6026	0.8929	1.45715	1218.3	754.6	0.05059	−0.01872	31.8
0.7045	0.9367	1.47033	1226.3	709.9	0.01203	−0.01782	27.5
0.8077	0.9870	1.48560	1237.2	662.0	−0.01456	−0.01499	20.4

(*continued*)

Table 2. Continued.

x	ρ (g cm^{-3})	n_D	u (m s^{-1})	κ_S (TPa^{-1})	(cm^3 M^{-1})	δn_D	$\delta\kappa_S$ (TPa^{-1})
0.9051	1.0410	1.50296	1250.8	614.0	−0.01567	−0.00938	11.1
0.9470	1.0665	1.51157	1257.9	592.6	−0.00745	−0.00582	6.3
Chlorobenzene + *n*-decane							
0.0723	0.7405	1.41391	1232.2	889.5	0.04399	−0.00394	10.1
0.1299	0.7528	1.41737	1230.9	876.8	0.07539	−0.00705	16.9
0.2161	0.7727	1.42324	1229.1	856.8	0.11477	−0.01103	26.0
0.3035	0.7948	1.42957	1227.9	834.5	0.14026	−0.01468	33.3
0.4138	0.8262	1.43881	1227.5	803.4	0.15077	−0.01803	39.6
0.5093	0.8569	1.44800	1228.2	773.6	0.14592	−0.01975	42.1
0.6048	0.8917	1.45795	1230.1	741.2	0.12887	−0.02070	42.1
0.7106	0.9359	1.47115	1235.1	700.5	0.10154	−0.01958	37.2
0.8066	0.9824	1.48478	1242.4	659.4	0.06757	−0.01692	28.7
0.8984	1.0340	1.50102	1252.2	616.8	0.03275	−0.01116	17.1
0.9528	1.0684	1.51241	1259.8	589.7	0.01345	−0.00598	8.4
Chlorobenzene + *n*-undecane							
0.0495	0.7453	1.41755	1256.4	850.0	0.03379	−0.00264	6.7
0.1115	0.7569	1.42026	1253.8	840.5	0.10091	−0.00668	15.4
0.1985	0.7747	1.42585	1250.5	825.5	0.16154	−0.01057	25.8
0.2952	0.7968	1.43218	1247.2	806.8	0.20450	−0.01478	35.4
0.4051	0.8254	1.44015	1244.5	782.3	0.23146	−0.01879	43.0
0.4989	0.8534	1.44826	1242.9	758.5	0.23471	−0.02091	46.7
0.6062	0.8904	1.45884	1242.2	727.9	0.21970	−0.02202	47.4
0.7095	0.9323	1.47093	1243.8	693.4	0.19056	−0.02119	43.1
0.8017	0.9762	1.48376	1247.5	658.2	0.15158	−0.01841	35.0
0.8997	1.0317	1.50072	1254.9	615.5	0.09145	−0.01213	20.9
0.9501	1.0649	1.51135	1260.4	591.1	0.03160	−0.00699	11.3
Chlorobenzene + *n*-dodecane							
0.0495	0.7453	1.41755	1256.4	850.0	0.03379	−0.00264	6.7
0.1115	0.7569	1.42026	1253.8	840.5	0.10091	−0.00668	15.4
0.1985	0.7747	1.42585	1250.5	825.5	0.16154	−0.01057	25.8
0.2952	0.7968	1.43218	1247.2	806.8	0.20450	−0.01478	35.4
0.4051	0.8254	1.44015	1244.5	782.3	0.23146	−0.01879	43.0
0.4989	0.8534	1.44826	1242.9	758.5	0.23471	−0.02091	46.7
0.6062	0.8904	1.45884	1242.2	727.9	0.21970	−0.02202	47.4
0.7095	0.9323	1.47093	1243.8	693.4	0.19056	−0.02119	43.1
0.8017	0.9762	1.48376	1247.5	658.2	0.15158	−0.01841	35.0
0.8997	1.0317	1.50072	1254.9	615.5	0.09145	−0.01213	20.9
0.9501	1.0649	1.51135	1260.4	591.1	0.03160	−0.00699	11.3

Table 4 presents the fitting parameters corresponding to these equations. The presented root mean square deviations were computed using Equation (7), where z is the value of the property, and n_{DAT} is the number of experimental data:

$$\sigma = \left(\frac{\sum_{i=1}^{n_{\mathrm{DAT}}} (z_{\mathrm{exp}} - z_{\mathrm{pred}})^2}{n_{\mathrm{DAT}}} \right)^{1/2}. \tag{7}$$

Figures 1–3 show the derived properties plotted against x_1 (chlorobenzene), as well as the curves fitted using Equation (4). For the binary mixtures, in these figures,

Table 3. Speeds of sound u, isentropic compressibilities κ_S and changes of isentropic compressibilities $\delta\kappa_S$ for the ternary mixtures chlorobenzene + n-hexane + (n-undecane, or n-dodecane) at 298.15 K.

x_1	x_2	u (m s^{-1})	κ_S (TPa^{-1})	$\delta\kappa_S$ (TPa^{-1})
Chlorobenzene + n-hexane + n-undecane				
0.0496	0.0427	1252.4	857.7	−5.0
0.0503	0.8992	1197.8	1221.3	−33.8
0.0968	0.3013	1215.8	714.5	−52.9
0.0985	0.1967	1229.9	886.6	−32.4
0.0987	0.6994	1140.2	1080.9	−68.5
0.0988	0.3964	1199.6	946.2	−64.3
0.1005	0.7986	1116.2	1142.3	−52.0
0.1017	0.4875	1183.6	979.4	−71.9
0.1023	0.0603	1247.9	853.2	−2.2
0.1925	0.7059	1127.3	1070.2	−54.8
0.1929	0.5076	1172.3	970.6	−63.3
0.1967	0.0968	1239.0	845.2	0.7
0.1994	0.3978	1191.2	929.8	−51.8
0.2009	0.2986	1209.7	795.3	−40.5
0.2017	0.1934	1223.3	869.9	−17.4
0.2979	0.2961	1204.9	873.5	−32.8
0.3010	0.3977	1185.6	906.2	−45.8
0.3017	0.6002	1141.8	988.9	−55.6
0.3019	0.0919	1235.5	822.9	11.4
0.3035	0.4929	1166.5	940.2	−54.6
0.3046	0.1910	1219.3	847.4	−8.7
0.3818	0.5281	1153.3	932.4	−55.7
0.3972	0.3978	1178.9	882.3	−42.5
0.4001	0.4995	1158.2	916.4	−53.2
0.4008	0.0948	1231.8	801.1	17.2
0.4015	0.1965	1215.8	823.7	−6.7
0.4356	0.2395	1208.0	823.7	−16.4
0.5006	0.4999	1160.0	870.5	−56.2
0.5011	0.2958	1195.8	818.4	−28.4
0.5018	0.3972	1175.8	846.6	−46.5
0.5019	0.1964	1213.1	795.0	−6.0
0.5025	0.0936	1226.9	777.1	23.5
0.6006	0.2985	1193.5	783.5	−35.4
0.6012	0.0974	1226.5	746.2	19.7
0.6021	0.1943	1213.7	758.9	−11.8
0.7037	0.1932	1214.7	743.7	3.2
0.7041	0.0938	1230.3	706.7	11.9
0.7991	0.1000	1233.7	667.3	−2.5
0.9022	0.0479	1249.9	615.1	−0.7
Chlorobenzene + n-hexane + n-dodecane				
0.0487	0.9040	1098.4	1218.9	−37.2
0.0505	0.0477	1271.5	823.6	−8.0
0.0961	0.8048	1119.3	1133.8	−61.0
0.0964	0.4000	1215.1	915.2	−79.1
0.0985	0.5094	1190.4	964.1	−83.9
0.0988	0.7014	1147.6	1061.3	−81.6
0.0989	0.0975	1262.1	829.4	−14.6

(*continued*)

Table 3. Continued.

x_1	x_2	u (m s^{-1})	κ_S (TPa^{-1})	$\delta\kappa_S$ (TPa^{-1})
0.0991	0.1997	1246.3	856.3	−38.2
0.1000	0.3069	1230.2	886.0	−61.4
0.1003	0.6040	1170.9	1006.8	−87.5
0.1365	0.6534	1155.1	1028.8	−80.7
0.1906	0.7073	1131.3	1060.0	−62.4
0.1956	0.0976	1256.3	817.0	−2.3
0.1958	0.3040	1223.1	872.4	−49.0
0.1966	0.2007	1240.8	842.0	−28.0
0.1987	0.4989	1183.3	946.0	−71.2
0.2012	0.4000	1201.2	909.4	−58.1
0.2350	0.1071	1252.8	813.4	0.0
0.2870	0.6137	1144.1	988.4	−63.0
0.2963	0.5074	1171.6	933.0	−63.4
0.2968	0.4053	1193.0	893.6	−52.1
0.2984	0.1996	1232.0	829.1	−14.4
0.2989	0.3009	1215.6	855.3	−38.2
0.3980	0.5025	1159.5	913.4	−54.5
0.3983	0.0961	1245.5	782.7	16.0
0.4027	0.3978	1185.9	868.6	−46.3
0.4035	0.2961	1208.8	833.4	−31.0
0.4053	0.1946	1226.7	806.6	−7.0
0.4993	0.3021	1200.6	812.4	−30.4
0.5000	0.4013	1176.8	845.5	−46.3
0.5018	0.0967	1240.8	760.4	19.9
0.5035	0.1966	1222.7	782.1	−7.4
0.5970	0.2033	1217.5	757.3	−11.7
0.5975	0.3034	1196.1	781.2	−37.2
0.6015	0.0976	1237.2	734.5	19.0
0.7071	0.0901	1237.4	699.2	14.5
0.8018	0.0956	1237.6	664.1	0.8
0.8997	0.0486	1250.8	616.2	1.2

the mixtures chlorobenzene + (*n*-hexane or *n*-heptane) show a contractive trend at any composition, due to the dispersive interactions among methylene groups and phenyl rings, and mainly polar interactions among chloride groups that reach a minimum for approximately equimolar mixtures. The mixtures chlorobenzene + (*n*-octane and *n*-nonane) present a sigmoidal trend, the former showing a slight expansive nature at low aromatic concentration and the latter showing a slight contractive tendency at high molar fraction of chlorobenzene. The increment of the haloaromatic solvent into the mixture leads to partial activation of the chloride groups. The polar interactions are strong enough to order the structure and contract the mixtures chlorobenzene + (*n*-octane or *n*-nonane) at high concentrations of chlorobenzene. Both the mixtures show a sigmoid tendency that disappear for higher molar weight alkanes. The rest of the functional family (chlorobenzene + (*n*-decane, *n*-undecane or *n*-dodecane)) shows expansive tendency at any concentration, this activation of the chloride group not being strong enough to order the mixture. In these mixtures, the steric hindrance avoids polar interactions, this effect being higher as molar weight rises.

Table 4. Fitting parameters of Equation (4) for the binary mixtures, Equation (5) for the ternary mixtures and root mean square deviations (σ).

Chlorobenzene + n-hexane				
V^E (cm^3 mol^{-1})	$A_0 = -2.082721$	$A_1 = -4.681165 \times 10^{-1}$	$A_2 = -2.039166 \times 10^{-1}$	$\sigma = 6 \times 10^{-3}$
δn_D	$A_0 = -3.488174 \times 10^{-2}$	$A_1 = -3.949050 \times 10^{-3}$	$A_2 = -8.788474 \times 10^{-3}$	
	$A_3 = -1.490360 \times 10^{-2}$			$\sigma = 10^{-4}$
$\delta\kappa_S$ (TPa^{-1})	$A_0 = -2.306290 \times 10^{2}$	$A_1 = -7.957901$	$A_2 = -6.690984$	
	$A_3 = 3.091474 \times 10^{1}$			$\sigma = 3 \times 10^{-1}$
Chlorobenzene + n-heptane				
V^E (cm^3 mol^{-1})	$A_0 = -9.704575 \times 10^{-1}$	$A_1 = -6.420816 \times 10^{-1}$	$A_2 = 1.286469 \times 10^{-1}$	$\sigma = 4 \times 10^{-3}$
δn_D	$A_0 = -5.222807 \times 10^{-2}$	$A_1 = -1.176311 \times 10^{-2}$	$A_2 = -1.590431 \times 10^{-2}$	
	$A_3 = -1.084609 \times 10^{-2}$			$\sigma = 9 \times 10^{-5}$
$\delta\kappa_S$ (TPa^{-1})	$A_0 = -3.470839 \times 10^{-1}$	$A_1 = -2.478998 \times 10^{1}$		$\sigma = 2 \times 10^{-1}$
Chlorobenzene + n-octane				
V^E (cm^3 mol^{-1})	$A_0 = -2.673145 \times 10^{-1}$	$A_1 = -5.552715 \times 10^{-1}$	$A_2 = -9.843823 \times 10^{-2}$	$\sigma = 2 \times 10^{-3}$
δn_D	$A_0 = -6.400685 \times 10^{-2}$	$A_1 = -1.717324 \times 10^{-2}$	$A_2 = -1.472762 \times 10^{-2}$	
	$A_3 = -1.318993 \times 10^{-2}$			$\sigma = 8 \times 10^{-5}$
$\delta\kappa_S$ (TPa^{-1})	$A_0 = 6.777673 \times 10^{1}$	$A_1 = -1.300111 \times 10^{1}$	$A_2 = -1.294989 \times 10^{-1}$	$\sigma = 10^{-1}$
Chlorobenzene + n-nonane				
V^E (cm^3 mol^{-1})	$A_0 = 3.053442 \times 10^{-1}$	$A_1 = -4.997629 \times 10^{-1}$	$A_2 = -3.253736 \times 10^{-1}$	
	$A_3 = 2.380149 \times 10^{-1}$			$\sigma = 3 \times 10^{-3}$
δn_D	$A_0 = -7.228009 \times 10^{-2}$	$A_1 = -2.430085 \times 10^{-2}$	$A_2 = -1.699335 \times 10^{-2}$	
	$A_3 = -1.142643 \times 10^{-2}$			$\sigma = 10^{-4}$
$\delta\kappa_S$ (TPa^{-1})	$A_0 = 1.319832 \times 10^{2}$	$A_1 = 3.32116$	$A_2 = -7.6780136$	$\sigma = 9 \times 10^{-2}$
Chlorobenzene + n-decane				
V^E (cm^3 mol^{-1})	$A_0 = 5.920530 \times 10^{-1}$	$A_1 = -2.004574 \times 10^{-1}$	$A_2 = -1.115094 \times 10^{-1}$	$\sigma = 10^{-3}$
δn_D	$A_0 = -7.879188 \times 10^{-2}$	$A_1 = -2.979046 \times 10^{-2}$	$A_2 = -1.991256 \times 10^{-2}$	
	$A_3 = -1.446161 \times 10^{-2}$			$\sigma = 9 \times 10^{-5}$
$\delta\kappa_S$ (TPa^{-1})	$A_0 = 1.687116 \times 10^{2}$	$A_1 = 2.642392 \times 10^{1}$		$\sigma = 2 \times 10^{-1}$

(*continued*)

Table 4. Continued.

Chlorobenzene + n-undecane				
V^E (cm^3 mol^{-1})	$A_0 = 9.510019 \times 10^{-1}$	$A_1 = -5.091970 \times 10^{-2}$		$\sigma = 7 \times 10^{-3}$
δn_D	$A_0 = -8.338097 \times 10^{-2}$	$A_1 = -3.516893 \times 10^{-2}$	$A_2 = -1.435496 \times 10^{-2}$	$\sigma = 2 \times 10^{-4}$
$\delta \kappa_S$ (TPa^{-1})	$A_0 = 1.875908 \times 10^{2}$	$A_1 = 4.819385 \times 10^{1}$	$A_2 = 8.194546$	$\sigma = 10^{-1}$
Chlorobenzene + n-dodecane				
V^E (cm^3 mol^{-1})	$A_0 = 1.101367$	$A_1 = 5.512629 \times 10^{-2}$	$A_2 = -1.666024 \times 10^{-1}$	$\sigma = 5 \times 10^{-3}$
δn_D	$A_0 = -8.700261 \times 10^{-2}$	$A_1 = -3.840632 \times 10^{-2}$	$A_2 = -2.760669 \times 10^{-2}$	
	$A_3 = -1.832565 \times 10^{-2}$			$\sigma = 8 \times 10^{-5}$
$\delta \kappa_S$ (TPa^{-1})	$A_0 = 1.978172 \times 10^{2}$	$A_1 = 6.242970 \times 10^{1}$	$A_2 = 1.596999 \times 10^{1}$	$\sigma = 9 \times 10^{-2}$
Chlorobenzene + n-hexane + n-undecane				
$\delta \kappa_S$ (TPa^{-1})	$B_0 = -0.1250$	$B_1 = -0.9500$	$B_2 = -0.0520$	
	$B_3 = 1.0367$	$B_4 = -0.6321$	$B_5 = 0.7336$	
	$B_6 = -0.2485$	$B_7 = 0.5867$	$B_8 = -0.1576$	$\sigma = 1.2698$
Chlorobenzene + n-hexane + n-dodecane				
$\delta \kappa_S$ (TPa^{-1})	$B_0 = -0.1870$	$B_1 = -1.5316$	$B_2 = -0.2254$	
	$B_3 = 2.6736$	$B_4 = -1.1380$	$B_5 = 1.9882$	
	$B_6 = -1.4257$	$B_7 = 1.5285$	$B_8 = -2.5097$	$\sigma = 1.4352$

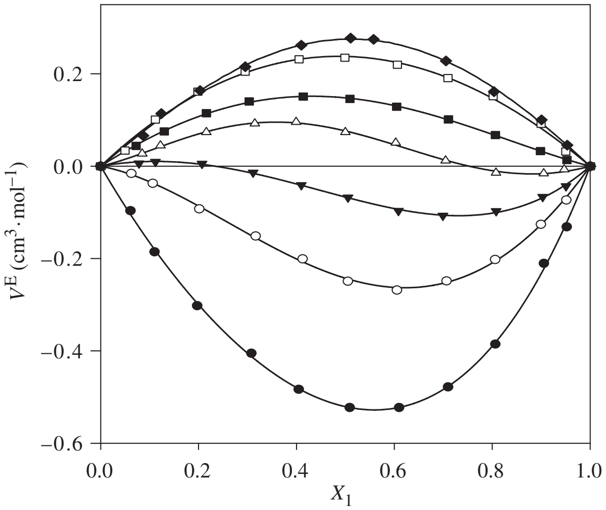

Figure 1. Dependence of excess molar volumes (cm^3 mol^{-1}) with mole fraction at 298.15 K for chlorobenzene + ((●) *n*-hexane + (○) *n*-heptane, (▼) *n*-octane, (▽) *n*-nonane, (■) *n*-decane, (□) *n*-undecane, or (◆) *n*-dodecane) and (——, Equation (4)) fitting curves.

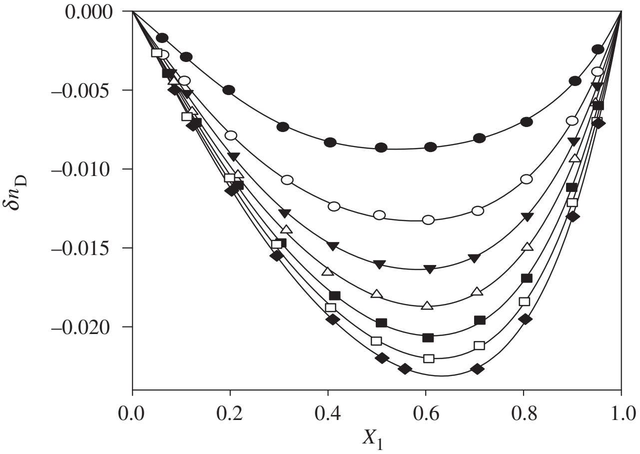

Figure 2. Dependence of change of refractive indices with mole fraction at 298.15 K for chlorobenzene + ((●) *n*-hexane + (○) *n*-heptane, (▼) *n*-octane, (▽) *n*-nonane, (■) *n*-decane, (□) *n*-undecane, or (◆) *n*-dodecane) and (——, Equation (4)) fitting curves.

In what is referred to previous studies on these mixtures, only earlier data were found for excess molar volumes on the mixtures of chlorobenzene + (*n*-hexane [15], *n*-heptane [16–18], *n*-octane [15,16], *n*-nonane [16], *n*-decane [15], and *n*-dodecane [15]).

An adequate coincidence has been found for chlorobenzene + *n*-heptane from the previously used data. The disposable excess molar volumes for the systems chlorobenzene + (*n*-octane or *n*-nonane) show poor quality and a different trend

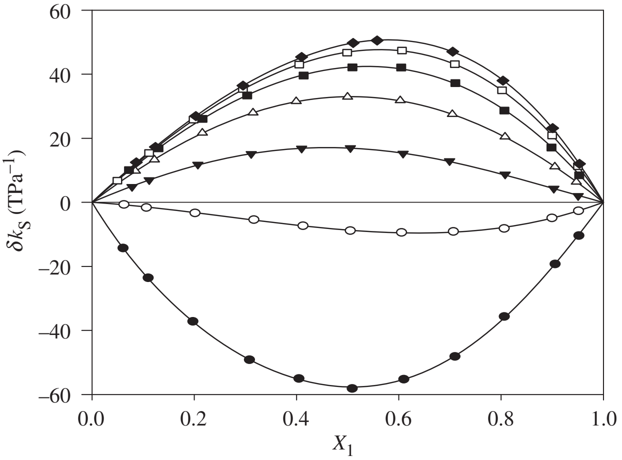

Figure 3. Dependence of change of isentropic compressibilities (TPa^{-1}) with mole fraction at 298.15 K for chlorobenzene + ((●) *n*-hexane + (○) *n*-heptane, (▼) *n*-octane, (▽) *n*-nonane, (■) *n*-decane, (□) *n*-undecane, or (◆) *n*-dodecane) and (——, Equation (4)) fitting curves.

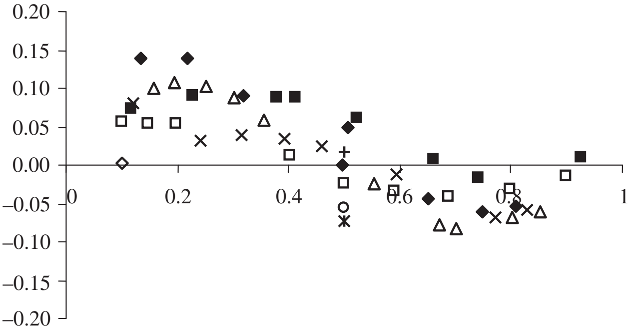

Figure 4. Comparison of excess molar volume between previously published data and experimental data for the systems chlorobenzene + (*n*-hexane (⁎, [15]), *n*-heptane (◆, [16]; □, [18]; △, [17]), *n*-octane (■, [16]; ◇, [15]), *n*-nonane (×, [16]); *n*-decane (○, [15]), and *n*-dodecane (+, [15]).

from that observed in this study. The work of Dominguez *et al.* [15], gathers only values for the systems chlorobenzene + (*n*-hexane, *n*-octane, *n*-decane or *n*-dodecane) at equimolar composition. These literature data are compared with the experimental ones as shown in Figure 4, in terms of relative deviation.

Figures 5 and 6 show the trend of changes in isentropic compressibilities for the ternary mixtures. The mathematical structure of Equation (5) leads to the analysis of the ternary contribution ΔQ_{ter} (simultaneous interactions among all compounds in the mixture) in what is referred to shape and sign (Figure 7(a) and (b)), and then, its effect on total non-ideality. This contribution poses two questions: first, the considerable contribution to the derived property by ternary molecular interactions (around 10%); second, the approximate equimolecular maximum in ternary contribution with only negative values for the chlorobenzene corner.

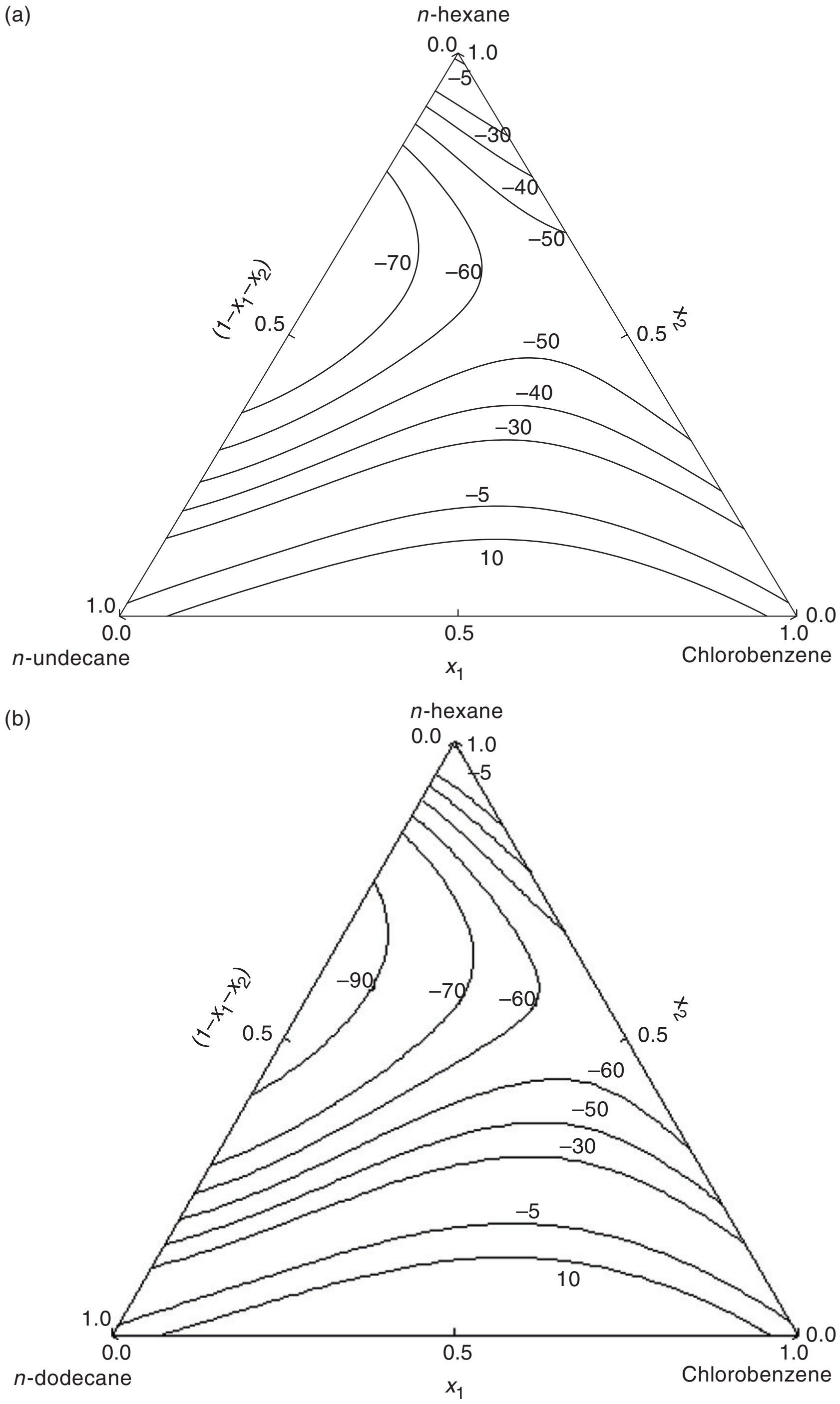

Figure 5. Constant value lines of ternary changes of isentropic compressibilities correlated using Equations (5) and (6), at the temperature 298.15 K for the system chlorobenzene + *n*-hexane + (a) *n*-undecane and (b) *n*-dodecane.

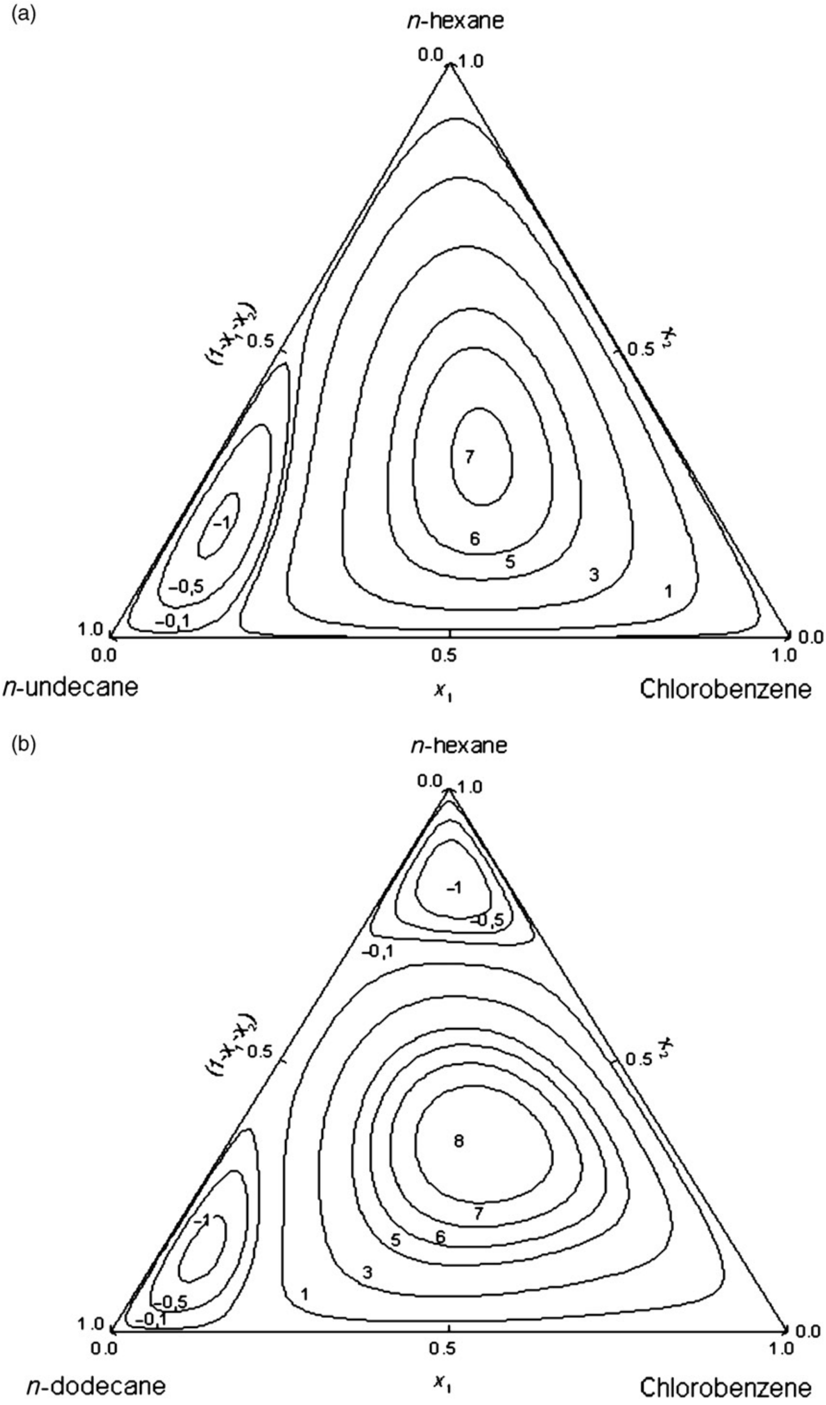

Figure 6. Constant value lines of change of isentropic compressibility ternary contribution in accordance with the Equation (6), at the temperature 298.15 K for the system chlorobenzene + *n*-hexane + (a) *n*-undecane and (b) *n*-dodecane.

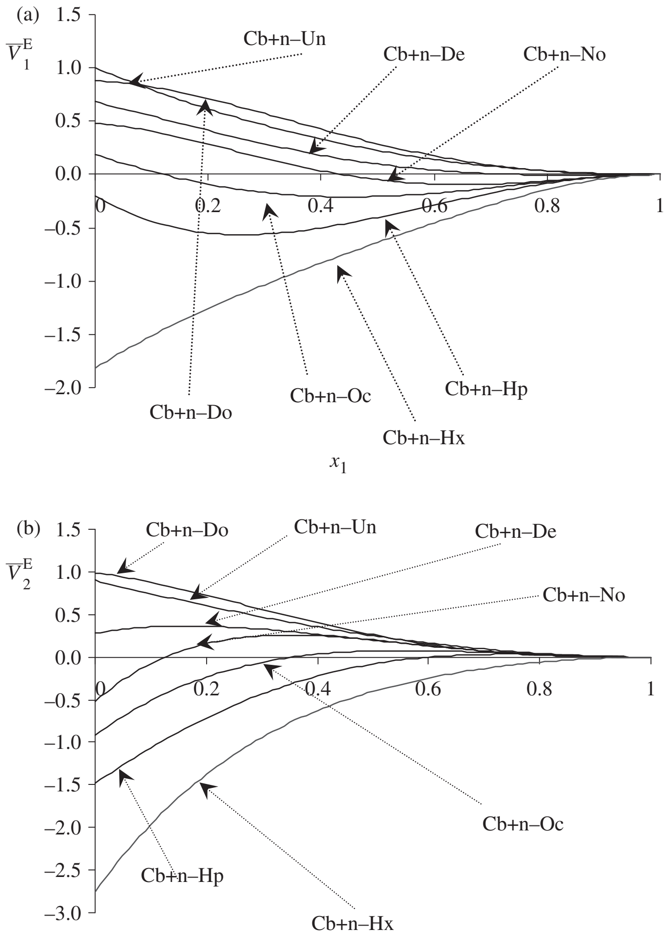

Figure 7. Partial excess molar volumes ($\text{cm}^3\,\text{mol}^{-1}$) of the binary systems. (a) $\overline{V}_1^E$ and (b) $\overline{V}_2^E$ at 298.15 K (Cb, chlorobenzene; *n*-Hp, *n*-heptane; *n*-Oc, *n*-octane; *n*-No, *n*-nonane; *n*-De, *n*-decane; *n*-Un, *n*-undecane; *n*-Do, *n*-dodecane).

3.2. *Partial excess molar volumes*

Partial molar quantities are important in the study of the dependence of an extensive property on the phase composition at constant pressure and temperature, because the trend is shown with molar fraction variation. They should be applied to any extensive property of a single-phase system, such as volume, Gibbs energy or any other. If E represents any extensive property of a single phase which is a function of pressure, temperature and mole numbers of the components, the differential of E should be expressed as

$$\delta E = \left(\frac{\partial E}{\partial T}\right)_{P,n} \mathrm{d}T + \left(\frac{\partial E}{\partial P}\right)_{T,n} \mathrm{d}P + \sum_{i=1}^{N} \left(\frac{\partial E}{\partial n_i}\right)_{T,P,n} \mathrm{d}n_i, \tag{8}$$

where the quantity $(\partial E/\partial n_i)_{T,P,n}$ is defined as the partial molar quantity of the ith component in the phase, the value n refers to all the other components present,

Table 5. Partial excess molar volumes at infinite dilution of the binary mixtures at 298.15 K.

	$\overline{V}_1^{\mathrm{E},\infty}$ ($\mathrm{cm^3\,mol^{-1}}$)	$\overline{V}_2^{\mathrm{E},\infty}$ ($\mathrm{cm^3\,mol^{-1}}$)
Chlorobenzene + *n*-hexane	−1.8185	−2.7548
Chlorobenzene + *n*-heptane	−0.1997	−1.4839
Chlorobenzene + *n*-octane	0.1895	−0.9210
Chlorobenzene + *n*-nonane	0.4797	−0.5198
Chlorobenzene + *n*-decane	0.6810	0.2801
Chlorobenzene + *n*-undecane	1.0019	0.9001
Chlorobenzene + *n*-dodecane	0.8793	0.9903

showing the finite change in the property on the addition of 1 mol of the component *i* in an infinite quantity of solution at constant temperature and pressure. The partial excess molar volume of a component in a binary mixture can be determined from the excess molar volume data; we have applied the Redlich–Kister expression to fit the data. This way the parameters given in Table 4 for Equation (4) are applied. The expression for the partial excess molar volume can be written as follows:

$$\overline{V}_i^E = (1 - x_i)^2 \left[\sum_{p=0}^{m} B_p (2x_1 - 1)^p + x_i \sum_{p=1}^{m} (-2)^{i-1} p B_p (2x_1 - 1)^{p-1} \right], \tag{9}$$

where the parameters are as explained above. From Equation (9), the corresponding limiting partial excess molar volumes should be determined by considering x_i rule for each case, such limiting values being dependent only on these correlation parameters. Table 5 presents the values of limiting partial excess molar volumes at 298.15 K for the binary mixtures. These values show the strong influence of the aliphatic chain on the excess molar volumes of similar compounds in the chlorobenzene environment.

3.3. *Estimation of derived magnitudes*

Due to the strong dependence of design and optimisation of chemical processes on computation, the availability of accurate, simple and tested methods, as well as the corresponding necessary parameters is of increasing relevance. In this case, consideration was given to the Rackett equation of state [19,20] in order to analyse how accurate the densities are predicted. On observing these models, the density can be described as follows:

$$\rho = \left(\frac{MP_{\mathrm{C}}}{RT_{\mathrm{C}}} \right) \beta^{-\left[1+(1-T_{\mathrm{r}})^{2/7}\right]}, \tag{10}$$

where T_{r} is the reduced temperature for the mixture, T_{C} and P_{C} are the pseudocritical mixing properties and β is the compressibility factor or an acentric factor dependent parameter, which varies according to a molecular structure parameter [21]. The selected mixing rule to compute the density was proposed by Kay (modified combination of Prausnitz–Gunn) [22,23]. In order to predict the mixing density, critical properties are required for each compound; the open

Table 6. Critical values from the open literature compounds into mixtures.

Compound	P_c (atm)	T_c (K)	Z_c	ω
Chlorobenzene	44.61	632.40	0.265	0.2490
n-hexane	23.73	507.43	0.264	0.3047
n-heptane	27.00	540.26	0.263	0.3494
n-octane	24.54	568.83	0.259	0.3962
n-nonane	22.75	595.65	0.255	0.4368
n-decane	20.95	618.45	0.249	0.4842
n-undecane	19.40	638.76	0.243	0.5362
n-dodecane	18.00	658.20	0.238	0.5752

Table 7. Root mean square deviations (σ) for estimated density by Rackett (R) or modified Rackett (mR) with respect to experimental density for the binary mixtures.

	σ	
Compound	*R*	mR
Chlorobenzene + *n*-hexane	0.0148	0.0149
Chlorobenzene + *n*-heptane	0.0234	0.0235
Chlorobenzene + *n*-octane	0.0238	0.0302
Chlorobenzene + *n*-nonane	0.0338	0.0344
Chlorobenzene + *n*-decane	0.0406	0.0405
Chlorobenzene + *n*-undecane	0.0463	0.0451
Chlorobenzene + *n*-dodecane	0.0476	0.0465

Table 8. Root mean square deviations (σ) or estimation of refractive index on mixing (Lorentz–Lorenz rule) with respect to experimental refractive indices for the binary mixtures.

Compound	σ
Chlorobenzene + *n*-hexane	0.00167
Chlorobenzene + *n*-heptane	0.00068
Chlorobenzene + *n*-octane	0.00049
Chlorobenzene + *n*-nonane	0.00076
Chlorobenzene + *n*-decane	0.00092
Chlorobenzene + *n*-undecane	0.00109
Chlorobenzene + *n*-dodecane	0.00123

literature or estimative methods should be used. Table 6 presents the open literature critical values [21] for the compounds involved in the studied mixtures. In Table 7, a comparison between the binary experimental and estimated densities is shown in terms of the root mean square deviations, as explained before. Attending to these values, it is observed that Rackett and modified Rackett equation provide adequate predictions for these binary mixtures, similar results are shown with these equations. Unfavourable results are obtained for the heaviest mixtures. In what is referred to as the refractive indices on mixing, the experimental data are compared with the results by the mixing rule proposed by Lorentz–Lorenz [24]. In Table 8, the root mean

Table 9. Root mean square deviations (σ) of isentropic compressibilities (TPa^{-1}) obtained by applying the CFT with respect experimental isentropic compressibilities for the binary mixtures.

Compound	σ
Chlorobenzene + *n*-hexane	0.0124
Chlorobenzene + *n*-heptane	0.0175
Chlorobenzene + *n*-octane	0.0149
Chlorobenzene + *n*-nonane	0.0078
Chlorobenzene + *n*-decane	0.0124
Chlorobenzene + *n*-undecane	0.0124
Chlorobenzene + *n*-dodecane	0.0100

Table 10. Parameters of the CFT and the FLT applied in the estimations of the isentropic compressibilities of the ternary mixture chlorobenzene + *n*-hexane + (*n*-undecane or *n*-dodecane).

	CFT	
	B (characteristic molecular volume, cm^3)	*S* (collision factor, ms^{-1})
	298.15 K	298.15 K
Chlorobenzene	24.14	3.35
n-hexane	30.60	2.89
n-heptane	43.28	3.02
n-octane	43.74	3.11
n-nonane	44.13	3.19
n-decane	44.78	3.25
n-undecane	45.34	3.31
n-dodecane	45.92	3.35
	FLT	
	Y (liquid internal surface, cm^2)	*L* (free length, cm)
	298.15 K	298.15 K
Chlorobenzene	0.341×10^{-2}	4.89×10^{-9}
n-hexane	0.400×10^{-2}	7.46×10^{-9}
n-heptane	0.433×10^{-2}	6.98×10^{-9}
n-octane	0.466×10^{-2}	6.64×10^{-9}
n-nonane	0.497×10^{-2}	6.38×10^{-9}
n-decane	0.528×10^{-2}	6.18×10^{-9}
n-undecane	0.558×10^{-2}	6.02×10^{-9}
n-dodecane	0.587×10^{-2}	5.89×10^{-9}

square deviations for the binary mixtures are presented, where the higher values are usually obtained in those mixtures of the highest non-ideality and expansive trend.

The CFT method [25–27] was applied to the isentropic compressibilities estimation. The application of the CFT shows lower deviation values when predicting the changes of isentropic compressibilities in the binary mixtures.

Table 11. Root mean square deviations (TPa^{-1}) from experimental data for the estimation of the excess volume by the Soave–Redlich–Kwong (SRK) state equation and the Peng–Robinson (PR) state equation for the ternary mixture chlorobenzene + *n*-hexane + (*n*-undecane or *n*-dodecane) at the temperature of 298.15 K.

*R*1	*R*2	*R*3	*R*4
SRK			
Chlorobenzene + *n*-hexane + *n*-undecane			
0.31649	0.30336	0.30336	0.30326
Chlorobenzene + *n*-hexane + *n*-dodecane			
0.33703	0.30195	0.30196	0.24040
PR			
Chlorobenzene + *n*-hexane + *n*-undecane			
0.29673	0.30201	0.30202	0.30812
Chlorobenzene + *n*-hexane + *n*-dodecane			
0.31159	0.29975	0.29975	0.24116

Table 9 presents the CFT values, and the estimation was realised for all the components; chlorobenzene, *n*-hexane, *n*-heptane, *n*-octane, *n*-nonane, *n*-decane, *n*-undecane and *n*-dodecane. For binary mixtures, the unfavourable results are of the binary mixture chlorobenzene + *n*-dodecane. This is one exception as the results of the derived properties of the mixtures of chlorobenzene + *n*-alkane, are in good agreement, and all values are similar. If one were to study the binary mixtures, when there is a link between halogenated aromatic compound and aliphatic compound, the number of the results of the derived properties increases with the size of the alkane, but there is one exception – *n*-dodecane. If one had studied this binary system, the number of results is the smallest of all and that of *n*-dodecane being the largest. From Table 10, it could be observed that the size of the aliphatic compounds increases as the values of the theory and the values of the two theories CFT and FLT for ternary mixtures are presented, both of theories arrive at similar results. Table 11 presents the deviations from experimental data by the Soave–Redlich–Kwong and Peng–Robinson state equations, the best results are obtained with the Peng–Robinson equation.

4. Results and conclusions

In earlier papers [3,28–30], we reported the thermodynamic behaviour of different alkanes in the chlorobenzene environment related to the separation of the haloaromatic compounds. The importance of such type of compounds, due to their presence as hazardous chemicals in the environment, leads us to investigate their different thermodynamic properties to understand the intermolecular weak bonds among the donors and acceptors and the influence of length of aliphatic chain on steric hindrance effects. Previously, different authors have experimentally demonstrated that the aromatic compounds form weak complexes with a variety of polar solvents, the latter acting as acceptors and the former as donors. Nevertheless, no complex formation with saturated hydrocarbons have been observed to explain the contractive tendency with short saturated hydrocarbons (as *n*-hexane or *n*-heptane).

In this work, the densities, refractive indices and speeds of sound at 298.15 K for different chlorobenzene + *n*-alkane mixtures and speeds of sound for ternary mixtures chlorobenzene + *n*-hexane + (*n*-heptane, *n*-octane, *n*-nonane, *n*-decane, *n*-undecane, or *n*-dodecane) have been measured. The derived properties were calculated from the experimental measurements, the data being correlated with polynomial expressions which fitted the data well. In general, the derived data reported in this study on the binary systems chlorobenzene + (*n*-hexane, *n*-heptane, *n*-octane, *n*-nonane, *n*-decane, *n*-undecane, or *n*-dodecane) at 298.15 K and atmospheric pressure are the only data that disagree with those reported earlier by other researchers as the systems chlorobenzene + (*n*-octane or *n*-nonane) follow sigmoid trend. Not surprisingly, the systems exhibited a non-ideal behaviour, which is dependent on the molar weight of *n*-alkane with an increasing expansive trend as the aliphatic chain rises. It is well known that when non-polar compounds mix, slight variations in the intermolecular interactions take place. The new specific dispersive interactions that appear should be suitably measured by combining volumetric or calorimetric techniques, presented here. Usually these mixtures show a moderate non-ideal behaviour, which is severely conditioned by the difference in molecular volume. In this case, the steric hindrance is the most important factor in mixing thermodynamics. This fact is noted by an initial contractive trend in mixtures (*n*-hexane and *n*-heptane) except for the cases of dilution of long-chain alkane environment, where a slight expansive effect is reflected. Besides the steric hindrance effect of interaction phenyl/aliphatic chain, the activation–deactivation of the chloride group plays a main role in what is referred to as the dipole interaction and induction of dipole. As shown in previous paper [15], the order breaking ability for aliphatic alkanes of chlorobenzene is identical to that of other aromatic compounds, being dependent mainly on the shape rather than polarity power. As it could be observed, the higher deviations were obtained for any mixture at the dilute condition of chlorobenzene.

Figures 5(a) and (b) show the negative behaviour with *n*-heptane and the positive near the binary alkanes; the character contractive is small. Figures 6(a) and (b) show same behaviour for all the alkanes, but there is a place near the binary chlorobenzene + *n*-hexane where the character contractive is the most important in the ternary mixture. As the quantity of *n*-alkane increases, the ternary mixture is slightly contractive for the reduction of dipolar link, and the link with aliphatic alkanes are very difficult.

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