Measuring and modelling experimental densities and ultrasonic velocities of aromatic and halogenated environmental pollutants

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Abstract

The potential environmental impact of aromatic and halogenated chemicals from the petrochemical and steel industry is of growning concern. The present paper deals with the modelling and experimental determination of density and speed of sound at the range 278.15–323.15 of six aromatic and halogenated compounds (Benzene, Toluene, Ethylbenzene, Fluorobenzene, 2-Fluorotoluene and Chlorobenzene). Fitting equations were applied to the data in order to correlate for later computer based design. The estimation of the studied properties was made by the application of different theoretical procedures. The Mchaweh–Nasrifar–Moshfeghian model (MNM), an equation of state based on the generalized van der Waals theory which combines the Staverman–Guggenheim combinatorial term of lattice statistics with an attractive lattice gas expression and the Free Length Theory showed a good response at the studied conditions.
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1. Introduction

Reliable thermodynamic data of environmental pollutants are highly important from both practical and theoretical points of view. Environmental chemistry and engineering need this information for transfer modelling of organic pollutants in the environment, solve the remediation of contaminated soils and surface waters, minimize the presence of hazardous pollutants in aqueous effluents, develop new strategies for cheap and effective cleaning procedures and then, adequate decisions and remediation policies (Valsaraj, 2000). From a more fundamental point of view, thermodynamics are necessary for understanding the complex molecular interactions and mechanisms of solution and dispersion. The test of models and the development of new methods for prediction of thermodynamic functions, have a particular significance because they are the only way to ensure accurate results.

Halogenated and aromatic hydrocarbons are ubiquitous environmental pollutants, some of which are well known to exhibit carcinogenic/mutagenic characteristics. Most of them are emitted to the natural environment during anthropogenic activities such as petrochemical and chloro-alkali industries, mechanical industry cleaning procedures, partial combustion of organic material in waste incineration and motor vehicle (Taylor and Lenoir, 2001; Öberg and Öhrström, 2003). These emission sources are usually present in inhabited areas where an important number of

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chemical and petrochemical industries are placed as in the areas of Tarragona (Spain) and Salvador (Bahia – Brazil). The contamination of water supplies by these kind of organic chemicals is a problem of increasing concern due to the limited availability of hydric resources and the persistence of these pollutants in aqueous media. Particularly, halogenated and aromatic organic substances are recognized as a threat to public health that in some instances must be dealt by removing the chemicals from water through suitable treatment. Transfer to the atmosphere by air–water contact represents a convenient and possibly cost-effective treatment method for removing volatile compounds by an optimized procedure of residence time, turbulent regime and adequated temperature. Accurate and temperature-dependent knowledge of thermophysical properties are then necessary for an optimized modelation and simulation, as well as, a practical procedure of online concentration measurement tool. In response to this concern, our research group is evolved on determining the current levels of various organic/inorganic pollutants to establish the health risks for the population living in the neighborhood of industrial complexes, as well as, the measurement of accurate liquid properties and mass transfer coefficients in order to optimize simulation studies and understand the main mechanisms of dispersion (Nadal et al., 2005; Touriño et al., 2005). Then, this work is a part of a wider study related to theoretical and experimental analysis of environmental pollutants. Besides its own practical importance (Gupta and Olson, 2003), the density and ultrasonic velocity are closely linked with the determination of Henry's law constants and the air–water partition coefficients, mass transfer coefficient measurement and calorimetric studies by means of the Maxwell's coefficients (Mullins et al., 1998). These data are largely exploited in the calculation of vapor–liquid equilibria in aqueous systems, and then, of technological and environmental interest. A considerable amount of data are available for organic hydrocarbons in open databases, which are of major environmental and health concern. With the exception of several polyaromatic compounds, less attention has been paid to halogenated/aromatic hydrocarbons, for which only a limited number of experimental values are available in the literature, as well as, accurate studies related to the dependence of their properties with temperature or pressure. Moreover, it can be observed a considerable lack of accuracy or thermodynamic consistency in some data open literature, which is due to the early interest on environmental and the non-systematic efforts in what is referred to thermophysical characterization of pollutants until now. A worse perspective is obtained for mixture references owed to the recent development of accurate techniques, the relatively important non-ideality of such compounds in aqueous media as well as the time-consuming nature of the experimental procedures. Different previous published works report data compilations of physical and thermal properties of aromatic/halogenated pollutants but this information is not systematic, it can be found dis-

perse and many properties have not been studied in a wide extension. This kind of information is of high interest for the understanding of the evolution of flexibility, package trend, hydrophobicity and polar-hydrogen bond potential as a function of molecular structure, as well as, for the development of group contribution concepts for organic chemicals. All solutes selected for this study contain a Π-electron ring showing an aromatic molecular size, vapor pressure and volatility that occur as usual additives of fuels and solvents in mechanical industry, and then, environmental pollutants. Thermodynamics of these chemicals are conventional for application of mechanical oscillation and sing-around techniques for measurement of density and ultrasonic velocity, respectively, those of the highest accuracy nowadays, and allowing one to work at near-ambient conditions.

With these facts in mind, as a continuation of our scientific work investigating physical properties related to characterization of pollutants, we present the temperature dependence of density and ultrasonic velocity at the range of temperature 278.15–323.15 K and atmospheric pressure of a collection of halogenated and aromatic hydrocarbons (benzene, toluene, ethylbenzene, chlorobenzene, fluorobenzene and 2-fluorotoluene). From the experimental data, temperature dependent polynomials were fitted, the corresponding parameters being gathered. Because of the expense of the experimental measurement of such data and current processes design is strongly computer oriented, consideration was also given to how accurate different theoretical methods work by comparison with the experimental data. Different procedures were applied to the experimental data. For density estimation, a simplification of the Nasrifar–Moshfeghian liquid density correlation (MNM method) was applied, replacing the Mathias and Copeman temperature-dependent term with the original Soave–Redlich–Kwong equation of state (SRK EOS) (Soave, 1972) temperature-dependent term (Mchaweh et al., 2004). This replacement has overcome the limitations in use for the original model, which were due to the Mathias and Copeman vapor pressure dependent parameters. The Rackett equation of state and its modification was also tested (Rackett, 1970; Spencer and Danner, 1972) in order to analyze how accurate densities are predicted.

It was also applied a lattice type equation of state (EoS) to simultaneously correlate vapor pressure and densities in order to predict the non-ideal temperature dependence of these magnitudes at a wide range. The EoS is based on the generalized van der Waals theory and combines the Staverman–Guggenheim combinatorial term of lattice statistics with an attractive simplified lattice gas expression (Mattedi et al., 1998). The Free Length Theory was applied to estimate the isentropic compressibility of these compounds (Jacobson, 1952; Gonzalez et al., 2006) using the estimate intermolecular free length for pure compounds. Satisfactory predictions were obtained for both properties, a good accuracy being obtained for a wide range of temperatures.

2. Experimental

All chemical solvents used in the preparation of samples were of Merck quality with a purity better than 99.5 mol%. The pure components were stored in glass containers protected from sunlight at constant humidity and temperature. Usual manipulation and purification in our experimental works was applied (Resa et al., 2004). The molar mass, open literature data and experimental results at standard condition are shown in Table 1. The densities and ultrasonic velocities of pure components and their mixtures were measured with an Anton Paar DSA-48 vibrational tube densimeter and sound analyzer, with a resolution of 10^{-5} g cm^{-3} and 1 m s^{-1}. Apparatus calibration was performed periodically in accordance with vendor instructions using a double reference (Millipore quality water and ambient air at each temperature). Accuracy in the temperature of measurement was better than $\pm 10^{-2}$ K by means of a temperature control device that apply the Peltier principle to maintain isothermal conditions during the measurements. More details about techniques and procedure in our laboratory could be obtained from previously published works (Gonzalez et al., 1999).

For compact and smooth representation, the density and ultrasonic velocity of the chemicals were correlated as a function of temperature in accordance to Eq. (1)

$$P = \sum_{i=0}^{N} A_i T^i \tag{1}$$

where P is density (g cm^{-3}) or ultrasonic velocity (m s^{-1}), T is the absolute temperature in Kelvin and A_i are fitting parameters. N stands for the extension of the mathematical series which was optimized by means of the Bevington test. Densities and ultrasonic velocity are given in Table 2. The fitting parameters were obtained by the unweighted least squared method applying a fitting Marquardt algorithm. The root mean square deviations were computed using Eq. (2), where z is the value of the property, and n_{DAT} is the number of experimental data.

$$\sigma = \left(\frac{\sum_{i=1}^{n_{DAT}} \left(z_{i,exp} - z_{i,cal} \right)^2}{n_{DAT}} \right)^{1/2} \tag{2}$$

The fitting parameters and the corresponding deviations are gathered in Table 3. In Figs. 1 and 2, the temperature trend of density, ultrasonic velocity. These figures show a decrease in the packing efficiency of chemicals which results in a continuous diminution of density and ultrasonic velocity versus temperature. Halogenated compounds show the highest values of density and the lowest of ultrasonic velocity.

3. Theoretical

3.1. Estimation of density

3.1.1. The Mchaweh–Nasrifar–Moshfeghian model (MNM) and Rackett EoS (R)

Increasingly, modern process design involves the use of computer aided process design procedures. The physical property packages used in chemical simulators typically rely on generalized equations for predicting properties as a function of temperature, pressure, etc. Despite the success developing several procedures of density estimation for pure compounds or mixtures, only a few of them may be of real application for chemicals of nonideal trend or high molar mass. An important criteria for estimating the density of these substances, is to understand the complex mechanisms of mixing process, commonly related to number and kind of selected "active" molecular groups, and the molecular configuration in terms of 3D structure. Second, the estimation strategy must be account for the strong temperature dependency of density. Both criteria are important for the design of clean processing facilities and policies that are frequently missing or not taken into account carefully. Perhaps the second criteria is more difficult to develop due to a set of factors are related as branching, molecular flexibility and disperse forces for this kind of compounds which obstruct to translate these facts into

Table 1
Comparison of experimental with literature data for the used chemicals at 298.15 K

Compound	Molecular mass (g mol^{-1})	Exp. density (g cm^{-3})	Lit. density (g cm^{-3})	Exp. ultrasonic velocity (m s^{-1})	Lit. ultrasonic velocity (m s^{-1})
Benzene	78.114[a]	0.87351	0.87360[c]	1297.85	1299[c]
Toluene	92.141[a]	0.86222	0.86219[c]	1303.03	1304[c]
Ethylbenzene	106.168[a]	0.86312	0.86252[c]	1312.66	1318[c]
Chlorobenzene	112.559[a]	1.10086	1.10094[d]	1265.54	1267.9[d]
2-Fluorotoluene	110.132[b]	1.00688[e]	1.00123[b,e]	1205.98	–
Fluorobenzene	96.104[a]	1.01901	1.01879[d]	1163.75	1166[d]

[a] Poling et al. (2001).
[b] Riddick et al. (1986).
[c] George and Nandhibatla (2003).
[d] Gascón et al. (2005).
[e] at 290.40.

Table 2
Densities (ρ), ultrasonic sound (u) of the used chemicals in the range of temperature 278.15–323.15 K

T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹
Benzene																	
323.150	0.84920	1186.96	314.900	0.85682	1222.32	306.650	0.86488	1258.75	298.399	0.87325	1296.64	290.150	0.88181	1335.76	281.900	0.89061	1377.31
322.900	0.84940	1187.82	314.650	0.85706	1223.40	306.400	0.86514	1259.91	298.150	0.87351	1297.85	289.900	0.88209	1337.02	281.650	0.89087	1378.60
322.650	0.84962	1188.80	314.400	0.85730	1224.47	306.150	0.86539	1261.01	297.900	0.87377	1299.07	289.650	0.88234	1338.15	281.400	0.89114	1379.94
322.400	0.84986	1189.92	314.150	0.85754	1225.61	305.900	0.86564	1262.17	297.650	0.87402	1300.22	289.400	0.88261	1339.43	281.150	0.89142	1381.29
322.150	0.85009	1190.97	313.900	0.85778	1226.66	305.650	0.86589	1263.27	297.400	0.87428	1301.43	289.150	0.88287	1340.62	280.900	0.89168	1382.53
321.900	0.85031	1191.98	313.650	0.85801	1227.81	305.400	0.86613	1264.35	297.150	0.87454	1302.59	288.900	0.88313	1341.83	280.650	0.89195	1383.80
321.650	0.85053	1193.10	313.400	0.85825	1228.92	305.150	0.86639	1265.52	296.900	0.87481	1303.79	288.650	0.88340	1343.07	280.400	0.89223	1385.33
321.400	0.85076	1194.17	313.150	0.85849	1229.93	304.900	0.86664	1266.62	296.650	0.87506	1304.94	288.400	0.88367	1344.31	280.150	0.89250	1386.51
321.150	0.85099	1195.25	312.899	0.85873	1230.98	304.650	0.86689	1267.75	296.400	0.87531	1306.07	288.150	0.88393	1345.58	279.900	0.89276	1387.79
320.900	0.85122	1196.33	312.650	0.85897	1232.14	304.400	0.86714	1268.91	296.150	0.87556	1307.17	287.900	0.88419	1346.77	279.650	0.89302	1389.03
320.650	0.85144	1197.38	312.400	0.85921	1233.29	304.150	0.86740	1269.99	295.900	0.87583	1308.43	287.650	0.88446	1348.02	279.400	0.89330	1390.44
320.400	0.85166	1198.38	312.150	0.85947	1234.41	303.900	0.86765	1271.12	295.650	0.87609	1309.58	287.400	0.88472	1349.25	279.150	0.89356	1391.63
320.150	0.85190	1199.58	311.900	0.85970	1235.46	303.650	0.86790	1272.28	295.400	0.87634	1310.77	287.150	0.88497	1350.44	278.900	0.89385	1393.15
319.900	0.85213	1200.59	311.650	0.85995	1236.61	303.400	0.86815	1273.36	295.150	0.87661	1311.97	286.900	0.88524	1351.60	278.650	0.89411	1394.42
319.650	0.85236	1201.73	311.400	0.86019	1237.69	303.150	0.86840	1274.48	294.900	0.87687	1313.12	286.650	0.88552	1353.06	278.400	0.89439	1395.82
319.400	0.85259	1202.75	311.150	0.86044	1238.82	302.900	0.86866	1275.63	294.650	0.87713	1314.32	286.400	0.88578	1354.25	278.150	0.89466	1397.35
319.150	0.85282	1203.87	310.900	0.86066	1239.79	302.650	0.86891	1276.75	294.400	0.87737	1315.44	286.150	0.88606	1355.53			
318.900	0.85305	1204.93	310.650	0.86092	1241.04	302.400	0.86916	1277.90	294.150	0.87764	1316.65	285.900	0.88630	1356.67			
318.650	0.85329	1206.06	310.400	0.86117	1242.11	302.150	0.86942	1279.05	293.900	0.87789	1317.83	285.650	0.88657	1357.97			
318.400	0.85353	1207.15	310.150	0.86142	1243.27	301.900	0.86968	1280.21	293.650	0.87816	1319.01	285.400	0.88683	1359.24			
318.150	0.85373	1208.10	309.900	0.86166	1244.34	301.650	0.86992	1281.30	293.400	0.87843	1320.22	285.150	0.88712	1360.52			
317.900	0.85406	1209.73	309.650	0.86190	1245.42	301.400	0.87018	1282.49	293.150	0.87868	1321.37	284.900	0.88739	1361.93			
317.650	0.85429	1210.99	309.400	0.86216	1246.59	301.150	0.87043	1283.60	292.900	0.87894	1322.54	284.650	0.88765	1363.14			
317.400	0.85453	1212.05	309.150	0.86240	1247.67	300.900	0.87082	1284.07	292.650	0.87920	1323.75	284.400	0.88791	1364.36			
317.150	0.85469	1212.46	308.900	0.86265	1248.74	300.650	0.87108	1285.09	292.400	0.87947	1324.95	284.150	0.88818	1365.65			
316.900	0.85494	1213.62	308.650	0.86290	1249.85	300.400	0.87133	1286.20	292.150	0.87972	1326.12	283.900	0.88843	1366.79			
316.650	0.85517	1214.71	308.400	0.86314	1250.94	300.150	0.87147	1288.42	291.900	0.87998	1327.33	283.650	0.88873	1368.27			
316.400	0.85539	1215.75	308.150	0.86339	1252.06	299.900	0.87171	1289.60	291.650	0.88023	1328.50	283.400	0.88900	1369.55			
316.150	0.85564	1216.85	307.900	0.86364	1253.20	299.650	0.87198	1290.82	291.400	0.88050	1329.71	283.150	0.88926	1370.79			
315.900	0.85587	1218.00	307.650	0.86389	1254.31	299.400	0.87223	1291.98	291.150	0.88077	1330.90	282.900	0.88953	1372.06			
315.650	0.85609	1218.95	307.400	0.86414	1255.42	299.150	0.87249	1293.18	290.900	0.88103	1332.11	282.650	0.88980	1373.47			
315.400	0.85634	1220.12	307.150	0.86438	1256.53	298.900	0.87274	1294.36	290.650	0.88128	1333.34	282.400	0.89007	1374.72			
315.150	0.85657	1221.16	306.900	0.86463	1257.65	298.650	0.87300	1295.48	290.400	0.88156	1334.56	282.150	0.89033	1375.98			
Toluene																	
323.150	0.84124	1201.38	314.400	0.84815	1235.93	305.650	0.85560	1271.61	296.900	0.86334	1308.39	288.150	0.87128	1346.99	279.400	0.87947	1388.34
322.900	0.84138	1202.07	314.150	0.84834	1237.02	305.400	0.85584	1272.62	296.650	0.86357	1309.47	287.900	0.87150	1348.12	279.150	0.87970	1389.60
322.650	0.84157	1203.12	313.900	0.84857	1237.93	305.150	0.85604	1273.69	296.400	0.86378	1310.55	287.650	0.87174	1349.26	278.900	0.87993	1390.87
322.400	0.84178	1203.98	313.650	0.84878	1239.00	304.900	0.85626	1274.70	296.150	0.86402	1311.61	287.400	0.87197	1350.44	278.650	0.88017	1392.10
322.150	0.84198	1205.02	313.400	0.84898	1240.02	304.650	0.85649	1275.70	295.900	0.86424	1312.71	287.150	0.87220	1351.55	278.400	0.88040	1393.32
321.900	0.84217	1205.95	313.150	0.84919	1240.94	304.400	0.85670	1276.77	295.650	0.86447	1313.74	286.900	0.87243	1352.69	278.150	0.88060	1394.57
321.650	0.84236	1206.97	312.900	0.84940	1242.08	304.150	0.85691	1277.80	295.400	0.86468	1314.87	286.650	0.87266	1353.86			
321.400	0.84255	1207.93	312.650	0.84962	1242.98	303.900	0.85713	1278.85	295.150	0.86491	1315.94	286.400	0.87289	1354.95			
321.150	0.84276	1208.97	312.400	0.84982	1244.05	303.650	0.85736	1279.88	294.900	0.86514	1316.98	286.150	0.87312	1356.16			
320.900	0.84295	1210.01	312.150	0.85004	1245.08	303.400	0.85757	1280.92	294.650	0.86537	1318.10	285.900	0.87335	1357.30			
320.650	0.84313	1210.90	311.900	0.85023	1246.12	303.150	0.85780	1281.99	294.400	0.86559	1319.17	285.650	0.87359	1358.48			
320.400	0.84334	1211.91	311.650	0.85046	1247.09	302.900	0.85801	1283.03	294.150	0.86582	1320.25	285.400	0.87382	1359.63			
320.150	0.84353	1212.91	311.400	0.85068	1248.10	302.650	0.85823	1284.08	293.900	0.86604	1321.36	285.150	0.87404	1360.69			
319.900	0.84371	1213.89	311.150	0.85088	1249.12	302.400	0.85845	1285.12	293.650	0.86626	1322.42	284.900	0.87429	1362.02			
319.650	0.84391	1214.85	310.900	0.85109	1250.05	302.150	0.85866	1286.19	293.400	0.86649	1323.53	284.650	0.87453	1363.08			
319.400	0.84411	1215.84	310.650	0.85130	1251.04	301.900	0.85888	1287.22	293.150	0.86672	1324.66	284.400	0.87474	1364.32			
319.150	0.84432	1217.01	310.400	0.85152	1252.10	301.650	0.85911	1288.24	292.900	0.86695	1325.75	284.150	0.87500	1365.47			

Table 2 (*continued*)

T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹
318.900	0.84452	1217.95	310.150	0.85172	1253.17	301.400	0.85933	1289.30	292.650	0.86718	1326.86	283.900	0.87521	1366.83						
318.650	0.84472	1218.93	309.900	0.85192	1254.11	301.150	0.85955	1290.06	292.400	0.86739	1327.95	283.650	0.87546	1367.97						
318.400	0.84492	1219.85	309.649	0.85215	1255.12	300.900	0.85979	1291.17	292.150	0.86763	1329.04	283.400	0.87570	1369.09						
318.150	0.84508	1220.98	309.400	0.85237	1256.22	300.650	0.86000	1292.25	291.900	0.86785	1330.18	283.150	0.87592	1370.27						
317.900	0.84526	1221.77	309.150	0.85258	1257.29	300.400	0.86023	1293.33	291.650	0.86809	1331.25	282.900	0.87614	1371.52						
317.650	0.84547	1222.87	308.900	0.85282	1258.26	300.150	0.86045	1294.33	291.400	0.86831	1332.36	282.650	0.87640	1372.55						
317.400	0.84567	1223.83	308.650	0.85301	1259.34	299.900	0.86067	1295.60	291.150	0.86854	1333.47	282.400	0.87662	1373.91						
317.150	0.84586	1224.81	308.400	0.85324	1260.28	299.650	0.86088	1296.69	290.900	0.86876	1334.59	282.150	0.87686	1375.13						
316.900	0.84609	1225.95	308.150	0.85344	1261.35	299.400	0.86110	1297.77	290.650	0.86899	1335.72	281.900	0.87712	1376.20						
316.650	0.84629	1226.82	307.900	0.85367	1262.38	299.150	0.86133	1298.80	290.400	0.86922	1336.79	281.650	0.87735	1377.55						
316.400	0.84652	1227.95	307.650	0.85387	1263.44	298.900	0.86155	1299.85	290.150	0.86945	1338.00	281.400	0.87758	1378.72						
316.150	0.84671	1228.78	307.400	0.85409	1264.36	298.650	0.86178	1300.93	289.900	0.86967	1339.07	281.150	0.87781	1379.96						
315.900	0.84690	1229.87	307.150	0.85430	1265.44	298.400	0.86200	1302.00	289.650	0.86990	1340.17	280.900	0.87803	1380.96						
315.650	0.84712	1230.87	306.900	0.85452	1266.47	298.150	0.86222	1303.03	289.400	0.87013	1341.34	280.650	0.87828	1382.16						
315.400	0.84732	1231.91	306.650	0.85474	1267.47	297.900	0.86244	1304.11	289.150	0.87037	1342.46	280.400	0.87852	1383.57						
315.150	0.84751	1233.00	306.400	0.85497	1268.52	297.650	0.86267	1305.18	288.900	0.87059	1343.57	280.150	0.87877	1384.72						
314.900	0.84773	1233.95	306.150	0.85517	1269.54	297.400	0.86289	1306.22	288.650	0.87081	1344.75	279.900	0.87900	1385.77						
314.650	0.84795	1234.93	305.900	0.85538	1270.59	297.150	0.86312	1307.32	288.400	0.87105	1345.89	279.650	0.87923	1387.16						

Ethylbenzene

T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹
323.150	0.84339	1215.35	314.400	0.84987	1248.23	305.650	0.85687	1282.32	296.900	0.86417	1317.83	288.150	0.87168	1355.66	279.400	0.87947	1398.37			
322.900	0.84354	1216.24	314.150	0.85006	1249.25	305.400	0.85708	1283.29	296.650	0.86438	1318.86	287.900	0.87190	1356.79	279.150	0.87968	1399.52			
322.650	0.84372	1217.09	313.900	0.85028	1250.28	305.150	0.85729	1284.33	296.400	0.86460	1319.92	287.650	0.87212	1357.96	278.900	0.87992	1400.99			
322.400	0.84390	1218.15	313.650	0.85045	1251.12	304.900	0.85749	1285.33	296.150	0.86480	1320.95	287.400	0.87235	1359.13	278.650	0.88013	1402.23			
322.150	0.84407	1219.01	313.400	0.85066	1252.11	304.650	0.85769	1286.27	295.900	0.86502	1322.03	287.150	0.87256	1360.30	278.400	0.88035	1403.42			
321.900	0.84426	1219.91	313.150	0.85086	1253.07	304.400	0.85791	1287.31	295.650	0.86523	1323.04	286.900	0.87277	1361.34	278.150	0.88055	1404.65			
321.650	0.84444	1220.87	312.900	0.85105	1254.01	304.150	0.85811	1288.31	295.400	0.86543	1324.07	286.650	0.87299	1362.49						
321.400	0.84462	1221.85	312.650	0.85126	1255.01	303.900	0.85831	1289.29	295.150	0.86566	1325.18	286.400	0.87321	1363.65						
321.150	0.84481	1222.73	312.400	0.85145	1256.00	303.650	0.85852	1290.29	294.900	0.86586	1326.20	286.150	0.87343	1364.73						
320.900	0.84498	1223.71	312.150	0.85165	1256.97	303.400	0.85873	1291.28	294.650	0.86608	1327.29	285.900	0.87366	1365.95						
320.650	0.84517	1224.58	311.900	0.85185	1257.95	303.150	0.85894	1292.35	294.400	0.86630	1328.36	285.650	0.87388	1367.20						
320.400	0.84535	1225.61	311.650	0.85204	1258.87	302.900	0.85914	1293.37	294.150	0.86651	1329.47	285.400	0.87410	1368.32						
320.150	0.84554	1226.53	311.400	0.85223	1259.77	302.650	0.85935	1294.36	293.900	0.86672	1330.48	285.150	0.87432	1369.53						
319.900	0.84573	1227.45	311.150	0.85243	1260.81	302.400	0.85956	1295.34	293.650	0.86694	1331.60	284.900	0.87455	1370.80						
319.650	0.84589	1228.32	310.900	0.85263	1261.70	302.150	0.85976	1296.33	293.400	0.86715	1332.63	284.650	0.87477	1372.03						
319.400	0.84608	1229.34	310.650	0.85285	1262.83	301.900	0.85997	1297.34	293.150	0.86737	1333.69	284.400	0.87498	1373.13						
319.150	0.84626	1230.16	310.400	0.85305	1263.73	301.650	0.86018	1298.35	292.900	0.86757	1334.76	284.150	0.87520	1374.23						
318.900	0.84646	1231.29	310.150	0.85323	1264.63	301.400	0.86039	1299.40	292.650	0.86779	1335.84	283.900	0.87543	1375.49						
318.650	0.84665	1232.15	309.900	0.85344	1265.71	301.150	0.86060	1300.36	292.400	0.86800	1336.97	283.650	0.87564	1376.70						
318.400	0.84681	1233.00	309.649	0.85363	1266.57	300.900	0.86081	1301.39	292.150	0.86822	1338.02	283.400	0.87586	1377.87						
318.150	0.84701	1234.08	309.400	0.85384	1267.69	300.650	0.86101	1302.39	291.900	0.86844	1339.12	283.150	0.87609	1379.22						
317.900	0.84721	1235.06	309.150	0.85406	1268.72	300.400	0.86123	1303.40	291.650	0.86865	1340.23	282.900	0.87632	1380.40						
317.650	0.84739	1235.99	308.900	0.85424	1269.57	300.150	0.86144	1304.43	291.400	0.86886	1341.31	282.650	0.87654	1381.60						
317.400	0.84757	1236.89	308.650	0.85444	1270.54	299.900	0.86164	1305.43	291.150	0.86908	1342.40	282.400	0.87677	1382.92						
317.150	0.84776	1237.80	308.400	0.85464	1271.43	299.650	0.86186	1306.50	290.900	0.86930	1343.50	282.150	0.87698	1384.08						
316.900	0.84796	1238.82	308.150	0.85485	1272.54	299.400	0.86207	1307.53	290.650	0.86951	1344.60	281.900	0.87722	1385.50						
316.650	0.84814	1239.66	307.900	0.85504	1273.44	299.150	0.86227	1308.53	290.400	0.86973	1345.69	281.650	0.87744	1386.83						
316.400	0.84832	1240.59	307.650	0.85524	1274.44	298.900	0.86248	1309.58	290.150	0.86994	1346.80	281.400	0.87768	1388.17						
316.150	0.84852	1241.59	307.400	0.85545	1275.40	298.650	0.86269	1310.57	289.900	0.87016	1347.88	281.150	0.87789	1389.37						
315.900	0.84872	1242.59	307.150	0.85565	1276.44	298.400	0.86290	1311.61	289.650	0.87039	1349.03	280.900	0.87812	1390.67						
315.650	0.84890	1243.37	306.900	0.85587	1277.49	298.150	0.86312	1312.66	289.400	0.87059	1350.10	280.650	0.87835	1391.90						
315.400	0.84911	1244.56	306.650	0.85607	1278.48	297.900	0.86333	1313.66	289.150	0.87082	1351.25	280.400	0.87857	1393.22						
315.150	0.84930	1245.50	306.400	0.85626	1279.37	297.650	0.86353	1314.70	288.900	0.87103	1352.32	280.150	0.87879	1394.50						
314.900	0.84953	1246.73	306.150	0.85647	1280.33	297.400	0.86376	1315.78	288.650	0.87125	1353.42	279.900	0.87902	1395.75						
314.650	0.84968	1247.40	305.900	0.85668	1281.37	297.150	0.86395	1316.79	288.400	0.87147	1354.53	279.650	0.87924	1396.98						

Chlorobenzene

323.150	1.07715	1178.24	314.150	1.08510	1208.90	305.150	1.09378	1240.33	296.150	1.10292	1272.91	287.150	1.11239	1307.32	278.150	1.12220	1344.58
322.900	1.07733	1178.89	313.900	1.08534	1209.77	304.900	1.09403	1241.25	295.900	1.10318	1273.84	286.900	1.11264	1308.24			
322.650	1.07755	1179.75	313.650	1.08556	1210.56	304.650	1.09429	1242.11	295.650	1.10344	1274.79	286.650	1.11292	1309.27			
322.400	1.07775	1180.59	313.400	1.08581	1211.48	304.400	1.09454	1243.04	295.400	1.10370	1275.71	286.400	1.11318	1310.23			
322.150	1.07794	1181.41	313.150	1.08603	1212.38	304.150	1.09479	1243.92	295.150	1.10396	1276.66	286.150	1.11346	1311.26			
321.900	1.07816	1182.26	312.900	1.08628	1213.27	303.900	1.09503	1244.80	294.900	1.10422	1277.57	285.900	1.11369	1312.13			
321.650	1.07837	1183.09	312.650	1.08651	1214.06	303.650	1.09528	1245.70	294.650	1.10447	1278.50	285.650	1.11398	1313.22			
321.400	1.07859	1184.01	312.400	1.08674	1214.93	303.400	1.09553	1246.56	294.400	1.10473	1279.40	285.400	1.11426	1314.29			
321.151	1.07877	1184.71	312.150	1.08696	1215.76	303.150	1.09578	1247.49	294.150	1.10500	1280.37	285.150	1.11453	1315.30			
320.900	1.07901	1185.64	311.900	1.08722	1216.70	302.900	1.09603	1248.36	293.900	1.10526	1281.32	284.900	1.11481	1316.35			
320.650	1.07923	1186.48	311.650	1.08745	1217.61	302.650	1.09629	1249.27	293.650	1.10552	1282.26	284.650	1.11507	1317.35			
320.400	1.07946	1187.34	311.400	1.08769	1218.46	302.400	1.09652	1250.11	293.400	1.10579	1283.18	284.400	1.11533	1318.29			
320.150	1.07967	1188.22	311.151	1.08790	1219.16	302.150	1.09679	1251.07	293.150	1.10604	1284.10	284.150	1.11561	1319.30			
319.900	1.07989	1189.13	310.900	1.08818	1220.22	301.900	1.09704	1251.93	292.900	1.10630	1285.04	283.900	1.11588	1320.43			
319.650	1.08012	1189.96	310.650	1.08842	1221.03	301.650	1.09729	1252.88	292.650	1.10657	1285.98	283.650	1.11615	1321.51			
319.400	1.08034	1190.86	310.400	1.08865	1221.95	301.400	1.09755	1253.76	292.400	1.10682	1286.92	283.400	1.11643	1322.46			
319.150	1.08055	1191.66	310.150	1.08889	1222.79	301.150	1.09780	1254.66	292.150	1.10709	1287.90	283.150	1.11671	1323.55			
318.900	1.08077	1192.58	309.900	1.08913	1223.65	300.900	1.09804	1255.53	291.900	1.10735	1288.82	282.900	1.11697	1324.43			
318.650	1.08100	1193.39	309.650	1.08937	1224.51	300.650	1.09829	1256.42	291.650	1.10762	1289.79	282.650	1.11723	1325.48			
318.401	1.08119	1194.10	309.400	1.08962	1225.40	300.400	1.09856	1257.40	291.400	1.10789	1290.70	282.400	1.11752	1326.61			
318.150	1.08144	1195.08	309.150	1.08986	1226.29	300.150	1.09882	1258.30	291.150	1.10814	1291.69	282.150	1.11780	1327.75			
317.900	1.08166	1195.94	308.900	1.09010	1227.13	299.900	1.09906	1259.17	290.900	1.10841	1292.65	281.900	1.11806	1328.58			
317.650	1.08190	1196.80	308.650	1.09034	1227.98	299.650	1.09932	1260.12	290.650	1.10867	1293.63	281.650	1.11835	1329.72			
317.400	1.08211	1197.64	308.400	1.09060	1228.91	299.400	1.09958	1261.01	290.400	1.10894	1294.59	281.400	1.11860	1330.60			
317.150	1.08236	1198.59	308.150	1.09083	1229.76	299.150	1.09984	1261.94	290.150	1.10919	1295.52	281.150	1.11888	1331.78			
316.900	1.08259	1199.46	307.900	1.09108	1230.64	298.900	1.10009	1262.83	289.900	1.10946	1296.51	280.900	1.11917	1332.85			
316.650	1.08278	1200.15	307.650	1.09132	1231.52	298.650	1.10035	1263.75	289.650	1.10973	1297.48	280.650	1.11943	1333.86			
316.400	1.08304	1201.13	307.400	1.09156	1232.37	298.400	1.10061	1264.65	289.400	1.10998	1298.41	280.400	1.11970	1334.85			
316.150	1.08324	1201.87	307.150	1.09182	1233.26	298.150	1.10086	1265.54	289.150	1.11026	1299.43	280.150	1.12000	1336.05			
315.900	1.08350	1202.87	306.900	1.09205	1234.15	297.900	1.10112	1266.49	288.900	1.11052	1300.39	279.900	1.12026	1336.97			
315.650	1.08372	1203.73	306.650	1.09230	1235.06	297.650	1.10137	1267.37	288.650	1.11078	1301.41	279.650	1.12054	1338.16			
315.400	1.08395	1204.54	306.400	1.09255	1235.91	297.400	1.10164	1268.33	288.400	1.11106	1302.35	279.400	1.12081	1339.13			
315.150	1.08418	1205.41	306.150	1.09279	1236.80	297.150	1.10189	1269.22	288.150	1.11131	1303.34	279.150	1.12108	1340.17			
314.900	1.08440	1206.24	305.900	1.09304	1237.67	296.900	1.10215	1270.13	287.900	1.11158	1304.33	278.900	1.12137	1341.32			
314.650	1.08463	1207.03	305.650	1.09330	1238.59	296.650	1.10240	1271.07	287.650	1.11185	1305.30	278.650	1.12164	1342.33			
314.400	1.08486	1207.98	305.400	1.09354	1239.47	296.400	1.10267	1272.01	287.400	1.11211	1306.28	278.399	1.12193	1343.58			

Fluorobenzene

323.150	0.99166	1066.02	314.150	1.00104	1100.32	305.150	1.01101	1135.66	296.150	1.02133	1171.99	287.150	1.03193	1210.33	278.150	1.04277	1250.98
322.900	0.99188	1066.68	313.900	1.00132	1101.32	304.900	1.01129	1136.64	295.900	1.02162	1172.99	286.900	1.03223	1211.46			
322.650	0.99212	1067.55	313.650	1.00157	1102.22	304.650	1.01157	1137.61	295.650	1.02191	1174.03	286.650	1.03253	1212.60			
322.400	0.99238	1068.54	313.400	1.00184	1103.23	304.400	1.01185	1138.61	295.400	1.02220	1175.05	286.400	1.03282	1213.63			
322.150	0.99264	1069.46	313.150	1.00212	1104.25	304.150	1.01215	1139.64	295.150	1.02250	1176.08	286.150	1.03312	1214.76			
321.900	0.99290	1070.49	312.900	1.00241	1105.26	303.900	1.01242	1140.59	294.900	1.02278	1177.09	285.900	1.03340	1215.74			
321.650	0.99315	1071.44	312.651	1.00264	1106.01	303.650	1.01271	1141.60	294.650	1.02307	1178.12	285.650	1.03372	1216.93			
321.400	0.99341	1072.40	312.400	1.00294	1107.16	303.400	1.01300	1142.63	294.400	1.02337	1179.18	285.400	1.03401	1218.04			
321.150	0.99366	1073.34	312.150	1.00321	1108.11	303.150	1.01328	1143.59	294.150	1.02366	1180.24	285.150	1.03432	1219.18			
320.900	0.99393	1074.31	311.900	1.00348	1109.04	302.900	1.01356	1144.59	293.900	1.02396	1181.27	284.900	1.03460	1220.21			
320.650	0.99417	1075.18	311.650	1.00376	1110.15	302.650	1.01385	1145.62	293.650	1.02424	1182.28	284.650	1.03491	1221.35			
320.400	0.99443	1076.25	311.400	1.00403	1111.00	302.400	1.01413	1146.59	293.400	1.02454	1183.33	284.400	1.03519	1222.38			
320.150	0.99469	1077.19	311.150	1.00431	1112.02	302.150	1.01442	1147.63	293.150	1.02483	1184.35	284.150	1.03550	1223.55			
319.900	0.99496	1078.18	310.900	1.00459	1112.99	301.900	1.01471	1148.62	292.900	1.02511	1185.39	283.900	1.03581	1224.68			
319.650	0.99521	1079.12	310.650	1.00485	1113.96	301.650	1.01498	1149.64	292.650	1.02541	1186.44	283.650	1.03612	1225.80			
319.400	0.99547	1080.06	310.400	1.00514	1114.94	301.400	1.01527	1150.61	292.400	1.02571	1187.50	283.400	1.03641	1226.91			
319.150	0.99573	1081.02	310.150	1.00542	1115.98	301.150	1.01557	1151.65	292.150	1.02600	1188.57	283.150	1.03671	1228.11			
318.900	0.99599	1081.93	309.900	1.00570	1116.99	300.900	1.01585	1152.64	291.900	1.02629	1189.61	282.900	1.03702	1229.24			

Table 2 (continued)

T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹	T/K	ρ/g cm⁻³	u/m s⁻¹
318.650	0.99624	1082.90	309.650	1.00597	1117.92	300.650	1.01613	1153.68	291.650	1.02659	1190.66	282.650	1.03730	1230.32						
318.400	0.99650	1083.84	309.400	1.00624	1118.89	300.400	1.01641	1154.64	291.400	1.02688	1191.71	282.400	1.03759	1231.39						
318.150	0.99677	1084.85	309.150	1.00653	1119.90	300.150	1.01671	1155.66	291.150	1.02722	1193.33	282.150	1.03791	1232.57						
317.900	0.99702	1085.75	308.900	1.00681	1120.86	299.900	1.01699	1156.65	290.900	1.02751	1194.35	281.900	1.03821	1233.70						
317.650	0.99731	1086.84	308.650	1.00708	1121.80	299.650	1.01728	1157.67	290.650	1.02780	1195.37	281.650	1.03852	1234.87						
317.400	0.99757	1087.74	308.400	1.00735	1122.80	299.400	1.01757	1158.72	290.400	1.02810	1196.42	281.400	1.03881	1235.95						
317.150	0.99782	1088.68	308.150	1.00764	1123.81	299.150	1.01786	1159.72	290.150	1.02838	1197.51	281.150	1.03911	1237.04						
316.900	0.99809	1089.70	307.900	1.00791	1124.76	298.900	1.01814	1160.71	289.900	1.02868	1198.56	280.900	1.03942	1238.26						
316.650	0.99835	1090.64	307.650	1.00820	1125.76	298.650	1.01843	1161.72	289.650	1.02898	1199.63	280.650	1.03971	1239.31						
316.400	0.99863	1091.57	307.400	1.00848	1126.73	298.400	1.01872	1162.73	289.400	1.02928	1200.71	280.400	1.04002	1240.47						
316.150	0.99889	1092.55	307.150	1.00877	1127.73	298.150	1.01901	1163.75	289.150	1.02956	1201.73	280.150	1.04033	1241.64						
315.900	0.99916	1093.56	306.900	1.00903	1128.70	297.900	1.01930	1164.80	288.900	1.02986	1202.83	279.900	1.04064	1242.85						
315.650	0.99944	1094.61	306.650	1.00932	1129.70	297.650	1.01959	1165.80	288.650	1.03016	1203.91	279.650	1.04092	1243.85						
315.400	0.99970	1095.48	306.400	1.00960	1130.70	297.400	1.01989	1166.85	288.400	1.03046	1204.99	279.400	1.04123	1245.11						
315.150	0.99996	1096.44	306.150	1.00988	1131.70	297.150	1.02016	1167.83	288.150	1.03075	1206.05	279.150	1.04154	1246.24						
314.900	1.00023	1097.35	305.900	1.01016	1132.67	296.900	1.02046	1168.90	287.900	1.03104	1207.13	278.900	1.04186	1247.46						
314.650	1.00051	1098.50	305.650	1.01044	1133.64	296.650	1.02074	1169.87	287.650	1.03134	1208.21	278.650	1.04217	1248.73						
314.400	1.00078	1099.40	305.400	1.01072	1134.63	296.400	1.02105	1170.96	287.400	1.03163	1209.27	278.400	1.04246	1249.72						
2-Fluorotoluene																				
323.150	0.97477	1111.62	314.150	0.98298	1145.04	305.150	0.99178	1179.10	296.150	1.00092	1213.93	287.150	1.01029	1250.55				278.149	1.01991	1289.69
322.900	0.97500	1112.63	313.900	0.98321	1145.91	304.900	0.99200	1179.85	295.900	1.00117	1214.89	286.900	1.01056	1251.61						
322.650	0.97520	1113.46	313.650	0.98345	1146.91	304.650	0.99227	1180.99	295.650	1.00142	1215.85	286.650	1.01081	1252.61						
322.400	0.97543	1114.39	313.400	0.98370	1147.84	304.400	0.99251	1181.83	295.400	1.00168	1216.86	286.400	1.01109	1253.76						
322.150	0.97566	1115.33	313.150	0.98393	1148.74	304.150	0.99276	1182.74	295.150	1.00194	1217.87	286.150	1.01134	1254.74						
321.900	0.97587	1116.26	312.900	0.98418	1149.72	303.900	0.99301	1183.75	294.900	1.00220	1218.85	285.900	1.01161	1255.78						
321.650	0.97609	1117.16	312.650	0.98442	1150.61	303.650	0.99325	1184.67	294.650	1.00245	1219.84	285.650	1.01188	1256.95						
321.400	0.97631	1118.05	312.400	0.98467	1151.62	303.400	0.99351	1185.64	294.400	1.00272	1220.87	285.400	1.01214	1257.96						
321.150	0.97652	1118.99	312.150	0.98489	1152.40	303.150	0.99376	1186.59	294.150	1.00297	1221.86	285.150	1.01241	1259.06						
320.900	0.97675	1119.90	311.900	0.98513	1153.38	302.900	0.99402	1187.57	293.900	1.00323	1222.85	284.900	1.01267	1260.10						
320.650	0.97698	1120.82	311.650	0.98539	1154.45	302.650	0.99426	1188.53	293.650	1.00350	1223.90	284.650	1.01293	1261.20						
320.400	0.97721	1121.74	311.400	0.98562	1155.37	302.400	0.99451	1189.50	293.400	1.00376	1224.89	284.400	1.01320	1262.28						
320.150	0.97742	1122.68	311.150	0.98586	1156.27	302.150	0.99477	1190.44	293.150	1.00402	1225.86	284.151	1.01346	1263.32						
319.900	0.97765	1123.60	310.900	0.98609	1157.15	301.900	0.99503	1191.43	292.900	1.00428	1226.87	283.900	1.01372	1264.36						
319.650	0.97787	1124.51	310.650	0.98634	1158.13	301.650	0.99526	1192.36	292.650	1.00454	1227.88	283.650	1.01400	1265.57						
319.400	0.97811	1125.49	310.400	0.98658	1159.06	301.400	0.99553	1193.36	292.399	1.00480	1228.90	283.400	1.01426	1266.66						
319.150	0.97833	1126.39	310.150	0.98682	1160.00	301.150	0.99578	1194.36	292.150	1.00505	1229.87	283.150	1.01453	1267.67						
318.900	0.97856	1127.34	309.900	0.98707	1160.94	300.900	0.99604	1195.30	291.900	1.00532	1230.93	282.900	1.01481	1268.82						
318.650	0.97878	1128.20	309.650	0.98732	1161.89	300.650	0.99629	1196.26	291.650	1.00557	1231.91	282.650	1.01507	1269.91						
318.400	0.97901	1129.18	309.400	0.98755	1162.83	300.400	0.99654	1197.24	291.400	1.00584	1232.94	282.400	1.01533	1271.00						
318.150	0.97924	1130.10	309.150	0.98781	1163.84	300.150	0.99680	1198.19	291.150	1.00610	1233.99	282.150	1.01561	1272.14						
317.900	0.97947	1131.01	308.900	0.98804	1164.69	299.900	0.99706	1199.16	290.900	1.00636	1234.97	281.900	1.01588	1273.18						
317.650	0.97971	1131.93	308.650	0.98829	1165.70	299.650	0.99732	1200.14	290.650	1.00662	1236.01	281.650	1.01615	1274.31						
317.400	0.97993	1132.85	308.400	0.98853	1166.56	299.400	0.99757	1201.10	290.400	1.00688	1237.01	281.400	1.01642	1275.36						
317.150	0.98016	1133.83	308.150	0.98879	1167.60	299.150	0.99782	1202.07	290.150	1.00714	1238.04	281.150	1.01668	1276.50						
316.900	0.98041	1134.77	307.900	0.98904	1168.57	298.900	0.99808	1203.07	289.900	1.00740	1239.07	280.900	1.01696	1277.66						
316.650	0.98064	1135.79	307.650	0.98927	1169.43	298.650	0.99834	1204.05	289.650	1.00766	1240.09	280.650	1.01723	1278.73						
316.400	0.98085	1136.58	307.400	0.98952	1170.35	298.400	0.99859	1205.03	289.400	1.00794	1241.20	280.400	1.01750	1279.85						
316.150	0.98109	1137.51	307.150	0.98977	1171.30	298.150	0.99885	1205.98	289.150	1.00819	1242.19	280.150	1.01777	1280.94						
315.900	0.98133	1138.50	306.900	0.99002	1172.30	297.900	0.99910	1206.99	288.900	1.00845	1243.26	279.900	1.01804	1282.02						
315.650	0.98156	1139.33	306.650	0.99026	1173.21	297.650	0.99936	1207.93	288.650	1.00872	1244.29	279.650	1.01833	1283.31						
315.400	0.98179	1140.33	306.400	0.99052	1174.28	297.400	0.99962	1208.93	288.400	1.00897	1245.28	279.400	1.01860	1284.36						
315.150	0.98204	1141.25	306.150	0.99077	1175.20	297.150	0.99988	1209.97	288.150	1.00923	1246.31	279.150	1.01887	1285.52						
314.900	0.98228	1142.19	305.900	0.99101	1176.15	296.900	1.00013	1210.93	287.900	1.00950	1247.37	278.900	1.01915	1286.61						
314.650	0.98251	1143.17	305.650	0.99126	1177.09	296.650	1.00039	1211.92	287.650	1.00977	1248.46	278.650	1.01941	1287.70						
314.400	0.98274	1144.08	305.400	0.99151	1178.11	296.400	1.00066	1212.88	287.400	1.01001	1249.43	278.400	1.01967	1288.81						

Table 3
Parameters of Eq. (1) for density and ultrasonic velocity in the range 283.15–323.15 K and root mean square deviations (σ)

	A_0	A_1	A_2	A_3	σ
$\rho/(\text{g cm}^{-3})$					
Benzene	0.900023	−0.00108	3.26E−07	1.9E−08	2.523E−05
Toluene	0.885297	−0.00094	1.19E−07	2.03E−08	2.256E−05
Ethylbenzene	0.885048	−0.0009	5.13E−07	1.64E−08	1.791E−05
Chlorobenzene	1.127633	−0.0011	4.21E−07	2.65E−08	2.036E−05
Fluorobenzene	1.04876	−0.00121	9.17E−08	2.39E−08	1.472E−05
2-Fluorotoluene	1.025255	−0.00107	−6.6E−09	2.49E−08	1.735E−05
$u/(\text{m s}^{-1})$					
Benzene	1424.179	−5.54432	0.022653	−0.00014	0.180
Toluene	1419.827	−5.18646	0.024847	−0.00017	0.078
Ethylbenzene	1431.306	−5.55901	0.039871	−0.0003	0.164
Chlorobenzene	1366.533	−4.52668	0.023766	−0.00017	0.066
Fluorobenzene	1274.858	−4.87737	0.020953	−0.00014	0.095
2-Fluorotoluene	1313.131	−4.75568	0.023074	−0.00017	0.062
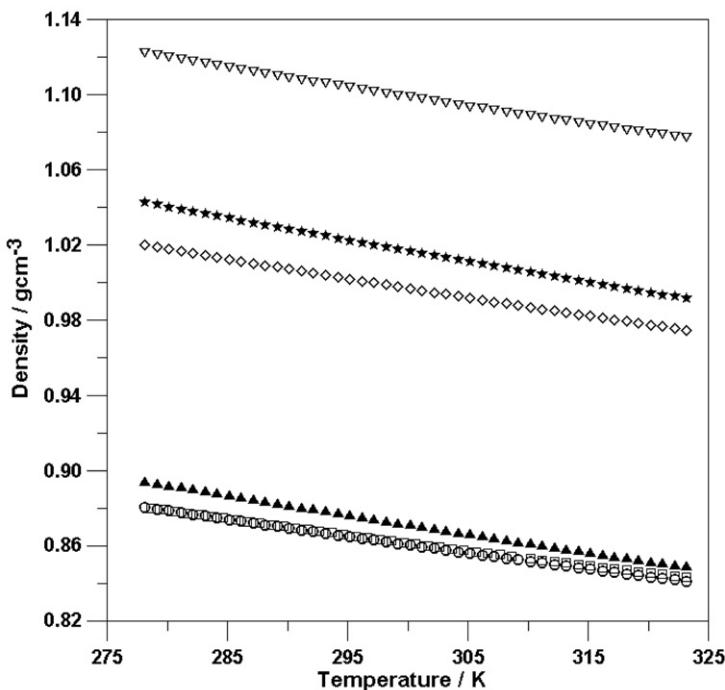
Fig. 1. Curves of density (g cm^{-3}) of benzene (▲), toluene (○), ethylbenzene (□), chlorobenzene (▽), fluorobenzene (★) and 2-flurotoluene (◇) at the range of temperatures 278.15–323.15 K.

model. In this case, a simplification for the Nasrifar–Moshfeghian liquid density correlation was applied, replacing the Mathias and Copeman temperature-dependent term with the original Soave–Redlich–Kwong equation of state (SRK EOS) (Soave, 1972) temperature-dependent term. This replacement has overcome the limitations in use for the original model which were due to the Mathias and Copeman vapor pressure dependent parameters (Mchaweh et al., 2004). The Nasrifar–Moshfeghian model (NM) (Nasrifar and Moshfeghian, 1999) requires three parameters for each compound, that are not readily available for all compounds. In the absence of these three parameters, the NM correlation fails to predict the density of pure compounds and their mixtures. The modification of this model, Mcha-

weh–Nasrifar–Moshfeghian model (MNM), overcomes this barrier by replacing the PSRK parameter α with the original SRK term α_{SRK}. The parameter α_{SRK} is defined in terms of reduced temperature (T_r):

$$\alpha_{SRK} = [1 + m(1 - \sqrt{T_r})]^2 \tag{3}$$

where m is given by the following relation as a function of acentric factor (ω):

$$m = 0.480 + 1.574\omega - 0.176\omega^2 \tag{4}$$

The revised model after replacement has the following general formula:
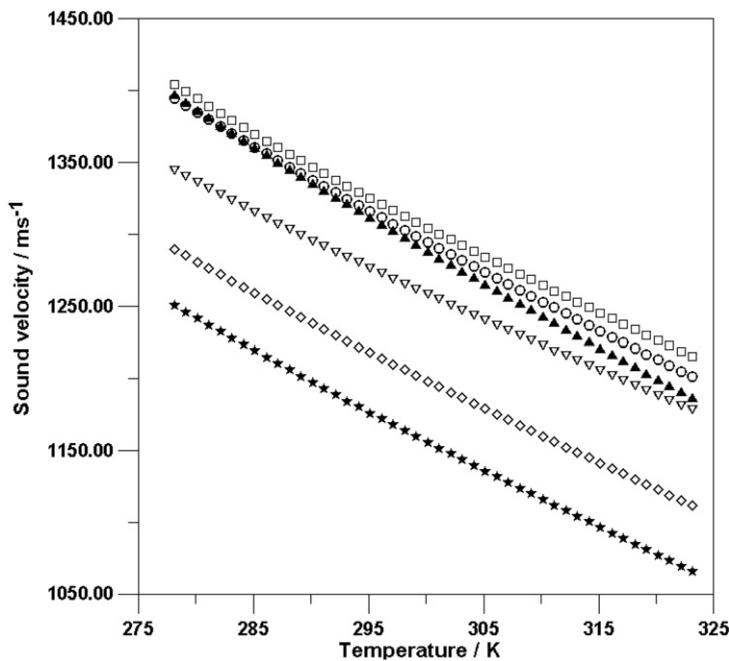
Fig. 2. Curves of ultrasonic velocity (m s^{-1}) of benzene (▲), toluene (○), ethylbenzene (□), chlorobenzene (∇), fluorobenzene (★) and 2-flurotoluene (◇) at the range of temperatures 278.15–323.15 K.

$$\rho_S = \rho_C \rho_0 \lfloor 1 + \delta_{SRK}(\alpha_{SRK} - 1)^{1/3} \rfloor \qquad (5)$$

where ρ_C is the critical density and the parameter δ_{SRK} is a new characteristic parameter for each compound. The parameter ρ_0 is the reference density and calculated by the following equation:

$$\rho_0 = 1 + 1.169\tau^{1/3} + 1.818\tau^{2/3} - 2.658\tau^{3/3} + 2.161\tau^{4/3} \qquad (6)$$

where the temperature-dependent variable τ is defined as

$$\tau = 1 - \frac{T_r}{\alpha_{SRK}} \qquad (7)$$

The critical properties and acentric factors required for different compounds were taken from referenced open literature (Poling et al., 2001).

In those cases where δ_{SRK} is not available, Mchaweh et al. (2004) proposed a general correlation as a function of acentric factor

$$\delta_{SRK} = 0.1596\omega - 0.0319 \qquad (8)$$

The deviation of these methods with respect to experimental data has been gathered into Table 4 together with the Rackett equation of state deviations, in accordance with the following expression:

$$\rho = \left(\frac{MP_C}{RT_C}\right)\beta^{[1+(1-T_r)^{2/7}]} \qquad (9)$$

where T_r is the reduced temperature, T_C and P_C are the critical properties of mixture, M is the molecular weight and β is the compressibility factor or an acentric factor dependent parameter which varies attending to a molecular structure parameter (Rackett, 1970; Spencer and Danner,

Table 4
Root mean square deviations for predictive density values by Rackett (R), modified Rackett (mR) or simplified Nasrifar and Moshfeghian (NM) and for predictive speed of sound values by means of Free Lengh Theory (FLT) with respect to corresponding experimental data the range 278.15–323.15 K

	R	mR	NM	FLT
Benzene	0.0012	0.0002	0.0019	52.666
Toluene	0.0010	0.0031	0.0008	41.288
Ethylbenzene	0.0010	0.0024	0.0035	38.928
Chlorobenzene	0.0007	0.0007	0.0039	28.596
2-Fluorotoluene	0.0133	0.0154	0.0028	28.007
Fluorobenzene	0.0061	0.0012	0.0008	45.471

1972) accurate results being obtained for the applied methods.

3.1.2. MTC lattice gas EOS

In the last few years, many researchers have applied and modify cubic equations of state to almost any situation for thermodynamic studies of pure chemicals and mixtures, although the success is always strongly dependent of a wide understanding of how molecules interact in terms of space and energy (Valderrama, 2003). However, in the last few years the interest related to non-cubic theoretically based EoS for prediction of fluid phase equilibria or others thermodynamical properties has increased. In this work, the lattice gas EOS developed by Mattedi et al. (1998) was also used to describe volumetric trend of these chemicals. The EoS is normally written in group contribution form, which is:

$$z = \tilde{v}r \ln\left[\frac{\tilde{v}}{\tilde{v}-1}\right] + \frac{Z}{2}\tilde{v}r \ln\left[\frac{\tilde{v}-1+(q/r)}{\tilde{v}}\right] + l$$
$$- \frac{\tilde{v}\Psi(q/r)}{\tilde{v}-1+(q/r)}\sum_{i=1}^{n_c}\sum_{a=1}^{n_g} x_i v_i^a Q^a \frac{(\Gamma^a - 1)}{\tilde{v}-1+(q/r)\Gamma^a} \quad (10)$$

where z is the compressibility factor, v_i^a is the number of type a groups in a molecule of type i, Q^a is the surface area of group a, $l = (Z/2)(r-q) - (r-1)$ and Ψ is a constant of the lattice structure, set to 1. The average number of segments occupied by a molecule in the lattice (r), the mean number of nearest neighbours (Zq) and the reduced molar volume ($\tilde{v}$) are given by:

$$r = \sum_{i=1}^{n_c} x_i \sum_{a=1}^{n_g} v_i^a R^a \quad (11)$$

$$Zq = \sum_{i=1}^{n_c} x_i \sum_{a=1}^{n_g} v_i^a Z Q^a \quad (12)$$

$$\tilde{v} = \frac{V}{NrV^*} = \frac{v}{rv^*} \quad (13)$$

$$rV^* = \sum_{i=1}^{n_c} x_i \sum_{a=1}^{n_g} v_i^a V^a \quad (14)$$

$$rv^* = \sum_{i=1}^{n_c} x_i \sum_{a=1}^{n_g} v_i^a v^a \quad (15)$$

Here, R^a and V^a are the group-contribution parameters for the number of segments and hard-core volume, respectively; v^a is the molar hard-core volume parameter for a group of type a. There was also defined:

$$\Gamma^a = \sum_{m=1}^{n_g} S^m \gamma^{ma} \quad (16)$$

$$S^m = \frac{\sum_{i=1}^{n_c} v_i^m x_i Q^m}{q} \quad (17)$$

$$\gamma^{ma} = \exp(-u^{ma}/(RT)) \quad (18)$$

where u^{ma} is the interaction energy between groups m and a. The fugacity coefficient derived for the model is

$$\ln\hat{\phi}_i = -r_i \ln\left[\frac{\tilde{v}-1}{\tilde{v}-1+(q/r)}\right] + (1-l_i)$$
$$\times \ln\left[\frac{\tilde{v}}{\tilde{v}-1+(q/r)}\right] + \frac{\Psi(q/r)(q_i - r_i)}{\tilde{v}-1+(q/r)}$$
$$+ \Psi\sum_{a=1}^{n_g} v_i^a Q^a \ln\left[\frac{\tilde{v}-1+(q/r)}{\tilde{v}-1+(q/r)\Gamma^a}\right] - \frac{\Psi}{r}\sum_{k=1}^{n_c}$$
$$\times \sum_{a=1}^{n_g} x_k v_k^a Q^a \frac{\left(\sum_{e=1}^{n_g} v_i^e Q^e \gamma^{ea} - r_i\right)}{\tilde{v}-1+(q/r)\Gamma^a} - \ln z \quad (19)$$

It was assumed in previous works that u^{ba} are given by:

$$\frac{u^{ba}}{R} = \frac{u_0^{ba}}{R}\left(1 + \frac{B^{ba}}{T}\right) \quad (20)$$

In summary, the equation of state has four parameters for each group (v^a, Q^a, u_0^{aa}/R and B^{aa}) and two parameters for interactions between unlike groups (u_0^{ba}/R and B^{ba}). The cell volume v^* is fixed in 5 cm³ mol⁻¹ was used as suggested by Mattedi et al. (1998). Although the EoS is written in a group contribution form, in this work there was used a molecular approach, and so each compound were considered as a group. Pure parameters were fitted using the simplex algorithm of Nelder and Mead (Press et al., 1989), in order to minimize the objective function:

$$F = \frac{\sum_{i=1}^{N}\left[\left(\frac{P_{i,cal}^{sat} - P_{i,pex}^{sat}}{P_{i,pex}^{sat}}\right)^2 + \left(\frac{\rho_{i,cal}^{liq\_sat} - \rho_{i,pex}^{liq\_sat}}{\rho_{i,pex}^{liq\_sat}}\right)^2\right]}{N} \quad (21)$$

where P^{sat} is the vapor pressure and ρ^{liq_sat} is the saturated molar liquid density. The subscripts cal and pex indicate calculated and pseudo-experimental values and N is the number of data points used. Pseudo-experimental data was generated through DIPPR correlation (Daubert and Danner, 1985) to 180 points with temperature ranging from 278.15 to 323.15 K. For 2-fluorotoluene, experimental data for vapor pressures from Boublík et al. (1984) and Stull (1947) (only 14 temperatures varying from 248.95 to 387.15 K) and experimental liquid densities from this work were used instead of DIPPR correlation as the coefficients were not available. Table 5 presents the obtained parameters, the root mean square deviations between vapor pressure and saturated molar liquid density

Table 5
Obtained parameters for EoS, mean deviation between calculated and pseudo-experimental values for vapor pressure (P^{sat}) and saturated liquid molar density (ρ^{sat}) and mean deviation between calculated and experimental densities (ρ)

Substances	Parameters				$\sigma(P^{sat})$	$\sigma(\rho^{sat})$	$\sigma(\rho)$
	v^a/cm³/mol	Q^a	B^{aa}/K	$u_0^{aa}/R/K$			
Benzene	58.073	9.3285	1.6001	−456.118	0.0003	0.06356	0.00465
Toluene	75.514	10.540	0.40161	−456.336	0.0001	0.01131	0.00281
Ethylbenzene	88.703	12.022	0.39747	−446.155	0.0001	0.00865	0.00249
Chlorobenzene	81.796	9.5814	47.917	−391.179	0.0001	0.02598	0.00269
Fluorobenzene	64.946	9.3983	1.3668	−459.507	0.0002	0.02455	0.00259
2-Fluorotoluene	82.256	10.785	1.0975	−437.335	0.0132	–	0.01889

calculated by the EoS and by DIPPR correlation and also the mean square root deviations between experimental liquid densities and the values calculated by the EoS. The numerical values for the obtained parameters are coherent. As expected, similar parameters for all substances have the same magnitude. Only B^{aa} value for chlorobenzene is much higher than for others compounds. But this parameter represent the energy temperature dependence and it could have different magnitude. Volume and surface parameters (v^a and Q^a) increases with the carbon number for the aromatics and from fluorobenzene to 2-fluorotoluene. From the presented results it could be seen that a very good agreement between experimental and calculated density values as the calculated deviation was always less than 0.005 except for 2-fluorotoluene, moreover the vapor pressure is also very well described in the range of temperature studied as the obtained deviation was always less 0.0005. Although the deviations from experimental data for 2-fluorotoluene are higher than for the others compounds, it could be explained as few experimental data points for vapor pressures in the considered range was used to parameter fitting however the obtained results indicate that the equation is also able to represent its behavior.

3.2. Estimation of ultrasonic velocity

3.2.1. Free length theory

In the last few years, Free Length Theory (FLT) has proved its applicability for multicomponent estimation and accurate results for molecules of different nature. The experimental data for the isentropic compressibility of the chemicals studied here were compared with values determined by the theoretical procedures. This model could be expressed as follows (Jacobson, 1952; Gonzalez et al., 2006):

$$\kappa_S = \left(\frac{L_f^2}{K^2}\right) \qquad (22)$$

where k_s is the isentropic compressibility that is calculated with the speed of sound (u) and density (ρ), through the next expression:

$$\kappa_S = \left(\frac{1}{u^2 \cdot \rho}\right) \qquad (23)$$

The L_f is intermolecular free length and K is a temperature dependent constant ($K = (93.875 + 0.375 \cdot T) \times 10^{-8}$). The pertinent relations in these calculations and its theoretical basis were described in the literature cited above. The free length theory estimates the isentropic compressibility attending to the free displacement of molecules as a main function of temperature. The deviations of each procedure for the studied compounds are gathered into Table 4, giving the FLT acceptable results in terms of quantity and sign at every studied case.

4. Conclusions

It is well known that thermodynamic properties govern the behaviour of contaminants in the environment. Values of basic magnitudes as density, ultrasonic velocities and isentropic compressibilities can thus be applied to model and predict the displacement, distribution, and fate of contaminants into natural media. In this paper, original data for the temperature dependence of density and ultrasonic velocity at the range of temperature 278.15–323.15 K and atmospheric pressure of a collection of halogenated and aromatic hydrocarbons (benzene, toluene, ethylbenzene, chlorobenzene, fluorobenzene and 2-fluorotoluene), have been measured.

In order to provide correlative methods to be used in computer-aided design, data were directly correlated with polynomial functions. Moreover, density data were compared with predictions of corresponding states theories. Density and vapor pressures were simultaneously correlated by a lattice equation of state. Ultrasonic velocity were compared through isentropic compressibility description with Free Length theory. Satisfactory results were obtained with all predictive and correlative models.

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