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Measurement and Correlation of Diffusion Coefficients of Aromatic Compounds at Infinite Dilution in Alkane and Cycloalkane Solvents

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The Taylor dispersion technique was used to measure the diffusion coefficients of benzene, chlorobenzene, ethylbenzene, toluene, *p*-chlorotoluene, naphthalene, pyrene, and perylene at infinite dilution in mixtures of hexane + octane, hexane + decane, heptane + octane, heptane + decane, octane + decane, cyclohexane + hexane, cyclohexane + heptane, cyclohexane + octane, and cyclohexane + decane at 298.15 K. Experimental data were correlated satisfactorily by means of the Leffler−Cullinan equation using the measured values of solutes in the pure solvents and a group contribution method for estimating the viscosity of the solvent mixtures.

Introduction

Knowledge of diffusion coefficients of organic solutes in liquid mixtures is required in many chemical engineering designs.[1] The present paper is part of general contribution concerned with the acquisition of transport property data for binary and ternary systems and their modeling by means of literature equations.

The first step of our investigation[2] was concerned with the selection of literature models[3−9] for the correlation of diffusion coefficients D^{∞}_{1m} of aromatic compounds at infinite dilution in binary mixtures. For this purpose, characteristic mixtures (hexane−heptane, ethanol−hexane, and ethanol−acetone) were considered, and diffusion coefficient data were modeled by taking into account experimental values of the viscosities η_m of the solvent mixtures. It was shown[2] that the model of Perkins and Geankopolis,[3] which extends the Wilke and Chang equation[4] to mixed solvents, provides poor results in the case of nonideal solvent mixtures. The other literature models consider a linear dependence, either of $D^{\infty}_{1m}\eta_m$[5,6] or of its logarithm[7−9] with respect to the mole fraction of the mixed solvent. The results obtained with these models gave evidence that the use of the experimental values D^{∞}_{1p} of the solute in the pure solvent should always be taken into consideration, especially in the general case of nonideal mixtures. It was also observed[2] that the Leffler−Cullinan[7] equation provides the best correlation of experimental diffusion coefficients.

This second step of our general study is devoted to aromatic solutes in nonpolar binary solvent mixtures. Diffusion coefficients of benzene, chlorobenzene, ethylbenzene, toluene, *p*-chlorotoluene, naphthalene, pyrene, and perylene of aromatics at infinite dilution in binary mixtures containing hexane, heptane, octane, decane, and cyclohexane were measured at 298.15 K using the Taylor dispersion technique.[10]

In this work, the possibility of predicting diffusion coefficients in mixtures only from the properties of pure solvents was investigated. For this purpose, experimental data D^{∞}_{1m} were correlated by means of the Leffler−Cullinan[7] model, but taking into account viscosity values η_m predicted with a group contribution method.

Table 1. Comparison between Experimental Values of Infinite Dilution Diffusion Coefficients D^{∞}_{1p} at 298.15 K

		$10^5\ D^{\infty}_{1p}$/cm^2·s^{-1}	
solute	solvent	this work	literature
benzene	hexane	4.70	4.79,[7] 4.76,[11] 4.75[13]
benzene	heptane	3.75	3.40,[14] 3.87,[13] 3.53,[15a] 3.91[16]
benzene	octane	3.19	3.39[17b]
benzene	cyclohexane	1.92	1.90,[11] 1.86,[15a] 1.90,[16] 1.95[7]
toluene	hexane	4.12	4.62,[5] 4.06,[15a] 4.21[14]
toluene	heptane	3.42	3.24,[15a] 3.72[14]
toluene	octane	2.83	3.05[18b]
toluene	decane	1.93	2.24[5]
toluene	cyclohexane	1.66	1.65,[11] 1.63,[15a] 1.57[16]
naphthalene	octane	2.35	2.55[17b]
naphthalene	heptane	2.81	3.17[17b]

[a] Measurements performed at 297 K. [b] Measurements performed at 303 K.

Experimental Section

The Taylor dispersion technique[10] was used to determine diffusion coefficients at infinite dilution. The flow apparatus and procedures used for these measurements have been described previously.[2,11] It is based on the diffusive flow generated by the slow running of a solution, called carrier, in a long capillary tube and the dispersion of a very small amount of a solute injected into the carrier. In our case the flowing streams were the binary mixed solvents, and the limiting diffusion coefficients were obtained by injecting less than 10^{-4} g of solutes. A 655A liquid chromatographic pumping system (Merck-Hitachi, Tokyo, Japan) was used to provide the constant laminar flow; the temperature was kept at 298.15 K thanks to a thermostated bath (Karlsruhe, Germany). The detector was a Merck UV/vis filter photometer operating at 254 nm.

As previously reported,[2,11] the main sources of uncertainties in the calculation of the diffusion coefficients are the measurement of the retention time (0.5 %) and the determination of the width of the peak (1 %). Taking into account these imprecisions, the resulting uncertainty on the diffusion coefficients was estimated.

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Table 2. Experimental Infinite Dilution Diffusion Coefficients of Aromatics (1) in Hexane (2) + Octane (3) Mixtures[a]

	$10^5 D^{\infty}_{1m}/\mathrm{cm^2 \cdot s^{-1}}$							
x_2	benzene	chlorobenzene	ethylbenzene	toluene	*p*-chlorotoluene	naphthalene	pyrene	perylene
0.0000	3.19	2.89	2.58	2.83	2.62	2.35	1.81	1.58
0.1008	3.29	2.97	2.66	2.92	2.70	2.43	1.86	1.63
0.2033	3.41	3.07	2.74	3.01	2.78	2.52	1.92	1.68
0.3001	3.52	3.16	2.83	3.11	2.86	2.61	1.98	1.74
0.3997	3.65	3.27	2.92	3.22	2.95	2.71	2.04	1.80
0.5002	3.79	3.39	3.04	3.34	3.06	2.83	2.11	1.87
0.5991	3.94	3.52	3.15	3.47	3.17	2.94	2.19	1.94
0.7005	4.10	3.66	3.28	3.61	3.29	3.07	2.27	2.02
0.7984	4.29	3.81	3.41	3.76	3.43	3.22	2.37	2.10
0.8954	4.48	3.97	3.56	3.93	3.57	3.37	2.46	2.19
1.0000	4.70	4.16	3.73	4.12	3.74	3.55	2.58	2.30

[a] x_2 is the mole fraction of component (2) in the mixed solvent.

Table 3. Experimental Infinite Dilution Diffusion Coefficients of Aromatics (1) in Hexane (2) + Decane (3) Mixtures[a]

	$10^5 D^{\infty}_{1m}/\mathrm{cm^2 \cdot s^{-1}}$							
x_2	benzene	chlorobenzene	ethylbenzene	toluene	*p*-chlorotoluene	naphthalene	pyrene	perylene
0.0000	2.16	1.980	1.790	1.930	1.800	1.650	1.230	1.075
0.1927	2.406	2.200	1.984	2.143	1.980	1.834	1.357	1.191
0.4143	2.782	2.532	2.279	2.480	2.266	2.123	1.553	1.374
0.5131	2.995	2.719	2.444	2.670	2.429	2.284	1.668	1.477
0.7203	3.550	3.207	2.879	3.160	2.889	2.705	1.966	1.751
0.8935	4.190	3.715	3.352	3.690	3.350	3.167	2.315	2.047
1.0000	4.700	4.160	3.730	4.120	3.740	3.550	2.580	2.300

[a] x_2 is the mole fraction of component (2) in the mixed solvent.

Table 4. Experimental Infinite Dilution Diffusion Coefficients of Aromatics (1) in Heptane (2) + Octane (3) Mixtures[a]

	$10^5 D^{\infty}_{1m}/\mathrm{cm^2 \cdot s^{-1}}$							
x_2	benzene	chlorobenzene	ethylbenzene	toluene	*p*-chlorotoluene	naphthalene	pyrene	perylene
0.0000	3.19	2.89	2.58	2.83	2.62	2.35	1.81	1.58
0.0992	3.23	2.93	2.63	2.88	2.66	2.39	1.84	1.61
0.2287	3.30	2.99	2.69	2.95	2.72	2.44	1.88	1.64
0.2924	3.33	3.02	2.72	2.98	2.74	2.47	1.90	1.66
0.4101	3.39	3.08	2.79	3.05	2.81	2.52	1.94	1.69
0.5052	3.44	3.13	2.84	3.10	2.84	2.56	1.97	1.72
0.6082	3.50	3.19	2.90	3.16	2.89	2.61	2.01	1.75
0.6973	3.55	3.24	2.95	3.22	2.94	2.65	2.04	1.78
0.7898	3.61	3.29	3.01	3.28	2.99	2.70	2.07	1.81
0.8954	3.68	3.36	3.08	3.35	3.05	2.75	2.12	1.85
1.0000	3.75	3.42	3.15	3.42	3.11	2.81	2.16	1.89

[a] x_2 is the mole fraction of component (2) in the mixed solvent.

Table 5. Experimental Infinite Dilution Diffusion Coefficients of Aromatics (1) in Heptane (2) + Decane (3) Mixtures[a]

	$10^5 D^{\infty}_{1m}/\mathrm{cm^2 \cdot s^{-1}}$							
x_2	benzene	chlorobenzene	ethylbenzene	toluene	*p*-chlorotoluene	naphthalene	pyrene	perylene
0.0000	2.16	1.98	1.79	1.93	1.80	1.65	1.23	1.08
0.1178	2.27	2.08	1.88	2.04	1.89	1.73	1.30	1.13
0.1784	2.32	2.13	1.92	2.10	1.94	1.78	1.33	1.16
0.3091	2.47	2.26	2.05	2.24	2.07	1.89	1.42	1.24
0.4135	2.59	2.38	2.16	2.36	2.17	1.98	1.49	1.30
0.4703	2.68	2.45	2.23	2.43	2.23	2.04	1.54	1.34
0.6041	2.88	2.64	2.41	2.62	2.40	2.19	1.66	1.45
0.6863	3.04	2.77	2.54	2.76	2.52	2.30	1.74	1.53
0.7595	3.18	2.89	2.65	2.90	2.63	2.40	1.82	1.60
0.8884	3.46	3.15	2.90	3.15	2.86	2.59	1.99	1.74
1.0000	3.75	3.42	3.15	3.42	3.11	2.81	2.16	1.89

[a] x_2 is the mole fraction of component (2) in the mixed solvent.

In order to determine the reliability of the technique, reference systems widely studied in literature were measured at 298.15 K. In Table 1, our measurements of diffusion coefficients at infinite dilution are compared with those from the literature. For each system where several data sources were available in literature, the scatter of published values corresponds to the "95 % confidence interval"; this interval varies from 1 % for benzene−hexane to 15 % for benzene−heptane

Table 6. Experimental Infinite Dilution Diffusion Coefficients of Aromatics (1) in Octane (2) + Decane (3) Mixtures[a]

	$10^5 D^{\infty}_{1m}$/cm^2·s^{-1}							
x_2	benzene	chlorobenzene	ethylbenzene	toluene	*p*-chlorotoluene	naphthalene	pyrene	perylene
0.0000	2.16	1.98	1.79	1.93	1.80	1.65	1.23	1.08
0.1384	2.27	2.07	1.87	2.02	1.88	1.72	1.29	1.13
0.2144	2.33	2.13	1.92	2.08	1.93	1.76	1.32	1.16
0.3015	2.40	2.19	1.97	2.14	1.99	1.81	1.37	1.19
0.4520	2.54	2.31	2.08	2.26	2.10	1.91	1.44	1.26
0.6010	2.69	2.45	2.20	2.39	2.22	2.01	1.53	1.34
0.6988	2.80	2.54	2.28	2.49	2.31	2.08	1.59	1.39
0.8208	2.95	2.67	2.39	2.61	2.43	2.18	1.67	1.46
0.8858	3.03	2.75	2.44	2.69	2.49	2.24	1.72	1.50
1.0000	3.19	2.89	2.58	2.83	2.62	2.35	1.81	1.58

[a] x_2 is the mole fraction of component (2) in the mixed solvent.

Table 7. Experimental Infinite Dilution Diffusion Coefficients of Aromatics (1) in Cyclohexane (2) + Hexane (3) Mixtures[a]

	$10^5 D^{\infty}_{1m}$/cm^2·s^{-1}							
x_2	benzene	chlorobenzene	Ethylbenzene	toluene	*p*-chlorotoluene	naphthalene	pyrene	perylene
0.0000	4.70	4.16	3.73	4.12	3.74	3.55	2.58	2.30
0.1884	4.26	3.62	3.29	3.71	3.25	3.16	2.34	2.05
0.3882	3.78	3.07	2.85	3.30	2.76	2.71	2.03	1.76
0.4918	3.46	2.74	2.58	3.02	2.49	2.43	1.84	1.57
0.5857	3.18	2.46	2.34	2.76	2.25	2.19	1.67	1.41
0.6988	2.85	2.13	2.04	2.47	1.97	1.88	1.46	1.24
0.7914	2.50	1.85	1.81	2.18	1.74	1.66	1.30	1.09
0.8977	2.21	1.60	1.60	1.91	1.51	1.44	1.13	0.94
1.0000	1.92	1.34	1.36	1.66	1.28	1.18	0.95	0.79

[a] x_2 is the mole fraction of component (2) in the mixed solvent.

Table 8. Experimental Infinite Dilution Diffusion Coefficients of Aromatics (1) in Cyclohexane (2) + Heptane (3) Mixtures[a]

	$10^5 D^{\infty}_{1m}$/cm^2·s^{-1}							
x_2	benzene	chlorobenzene	ethylbenzene	toluene	*p*-chlorotoluene	naphthalene	pyrene	perylene
0.0000	3.75	3.42	3.15	3.42	3.11	2.81	2.16	1.89
0.1013	3.68	3.26	3.07	3.30	3.00	2.72	2.10	1.82
0.2027	3.53	3.05	2.90	3.14	2.84	2.57	1.99	1.70
0.4037	3.24	2.64	2.56	2.87	2.51	2.26	1.75	1.51
0.4998	3.05	2.44	2.38	2.69	2.32	2.08	1.63	1.40
0.6018	2.83	2.20	2.18	2.52	2.10	1.90	1.48	1.28
0.8024	2.39	1.75	1.77	2.12	1.68	1.53	1.22	1.04
0.9002	2.22	1.58	1.57	1.92	1.50	1.38	1.11	0.93
1.0000	1.92	1.34	1.36	1.66	1.28	1.18	0.95	0.79

[a] x_2 is the mole fraction of component (2) in the mixed solvent.

Table 9. Experimental Infinite Dilution Diffusion Coefficients of Aromatics (1) in Cyclohexane (2) + Octane (3) Mixtures[a]

	$10^5 D^{\infty}_{1m}$/cm^2·s^{-1}							
x_2	benzene	chlorobenzene	ethylbenzene	toluene	*p*-chlorotoluene	naphthalene	pyrene	perylene
0.0000	3.19	2.89	2.58	2.83	2.62	2.35	1.81	1.58
0.2042	3.02	2.60	2.40	2.66	2.39	2.15	1.67	1.45
0.4044	2.80	2.31	2.17	2.47	2.14	1.93	1.52	1.30
0.5017	2.72	2.17	2.07	2.38	2.03	1.83	1.45	1.24
0.6029	2.60	2.02	1.94	2.26	1.89	1.71	1.36	1.16
0.8014	2.32	1.72	1.72	2.01	1.63	1.48	1.19	0.99
0.8971	2.14	1.55	1.54	1.85	1.47	1.34	1.08	0.90
1.0000	1.92	1.34	1.36	1.66	1.28	1.18	0.95	0.79

[a] x_2 is the mole fraction of component (2) in the mixed solvent.

or toluene−heptane. As can be observed in Table 1, our measurements are in agreement with literature data since they do not move away from more than 15 % of the published values.

The experimental diffusion coefficients of aromatic solutes D^{∞}_{1m} are presented in Tables 2 to 6 for mixed alkane solvents and in Tables 7 to 10 for cyclohexane + alkane solvents.

Materials. All solutes were of the highest purity research grade, available from Merck (Darmstadt, Germany). The solvents (Merck) were the highest purity Lichrosolv grade.

Results and Discussion

Diffusion coefficient data D^{∞}_{1m} were correlated by means of the Leffler−Cullinan[7] equation, which is expressed for a binary solvent mixture by the following relation:

$$\ln(D^{\infty}_{1m}\eta_m) = x_2 \ln(D^{\infty}_{12}\eta_2) + x_3 \ln(D^{\infty}_{13}\eta_3), \quad x_3 \approx 1 - x_2 \qquad (1)$$

where η_m and η_p are respectively the viscosities of the mixture and the pure solvent p. In this work, the viscosity η_m was

Table 10. Experimental Infinite Dilution Diffusion Coefficients of Aromatics (1) in Cyclohexane (2) + Decane (3) Mixtures[a]

	$10^5\, D^{\infty}_{1m}/\mathrm{cm^2 \cdot s^{-1}}$							
x_2	benzene	chlorobenzene	ethylbenzene	toluene	*p*-chlorotoluene	naphthalene	pyrene	perylene
0.0000	2.16	1.98	1.79	1.93	1.80	1.65	1.23	1.08
0.2065	2.12	1.85	1.71	1.90	1.70	1.57	1.18	1.02
0.4003	2.10	1.74	1.65	1.86	1.61	1.48	1.13	0.97
0.5005	2.09	1.68	1.62	1.84	1.57	1.43	1.11	0.94
0.7045	2.06	1.54	1.53	1.79	1.46	1.33	1.05	0.89
0.9001	2.00	1.41	1.43	1.72	1.35	1.23	0.99	0.83
1.0000	1.92	1.34	1.36	1.66	1.28	1.18	0.95	0.79

[a] x_2 is the mole fraction of component (2) in the mixed solvent.

Table 11. Average Absolute Percent Deviations AAD for the Prediction of Diffusion Coefficients of Aromatics at Infinite Dilution in Binary Alkane Mixtures Using the Leffler−Cullinan Equation with the Experimental Values of D^{∞}_{1p}

solutes	hexane + octane	hexane + decane	heptane + octane	heptane + decane	octane + decane	mean values
benzene	0.76	1.33	0.48	1.51	0.58	0.90
chlorobenzene	0.86	0.75	0.41	1.51	0.72	0.86
ethylbenzene	0.81	0.73	0.40	1.68	0.77	0.90
toluene	0.82	0.80	0.31	0.95	0.69	0.70
p-chlorotoluene	0.88	1.36	0.37	1.37	0.71	0.90
naphthalene	0.87	1.06	0.35	1.07	0.76	0.80
pyrene	0.87	1.52	0.33	1.26	0.67	0.88
perylene	0.72	1.40	0.48	1.58	0.79	0.96
mean values	0.82	1.12	0.39	1.37	0.71	

Table 12. Average Absolute Percent Deviations AAD for the Prediction of Diffusion Coefficients of Aromatics at Infinite Dilution in Binary Cyclohexane + Alkane Mixtures Using the Leffler−Cullinan Equation with the Experimental Values of D^{∞}_{1p}

solutes	cyclohexane + hexane	cyclohexane + heptane	cyclohexane + octane	cyclohexane + decane	mean values
benzene	1.92	1.87	1.49	2.08	1.84
chlorobenzene	2.46	1.67	1.63	1.83	1.91
ethylbenzene	1.35	2.57	1.53	1.39	1.74
toluene	1.92	1.85	1.29	1.68	1.70
p-chlorotoluene	1.24	3.03	1.67	1.54	1.90
naphthalene	4.49	2.35	1.28	2.00	2.62
pyrene	3.70	1.94	1.58	2.04	2.37
perylene	3.13	2.38	1.48	2.22	2.34
mean values	2.53	2.21	1.49	1.85	

estimated with the group contribution method proposed by Grunberg and Nissan[12] according to the Eyring theory:[8]

$$\ln(\eta_m) = x_2 \ln(\eta_2) + x_3 \ln(\eta_3) + x_2 x_3 G_m \tag{2}$$

which leads to the following expression of eq 1:

$$\ln(D^{\infty}_{1m}) = x_2 \ln(D^{\infty}_{12}) + x_3 \ln(D^{\infty}_{13}) - x_2 x_3 G_m \tag{3}$$

The Leffler−Cullinan equation allows therefore correlating diffusion coefficients independently of viscosity data.

According to the Grunberg−Nissan method G_m is expressed as:

$$G_m = \sum \Delta_3 - \sum \Delta_2 + W \tag{4}$$

$\Sigma\Delta_i$ and W are estimated from the group contributions proposed by the authors. In this work, the value of the cyclohexane group parameter was modified: $\Delta_{\text{cyclohexane ring}} = 0.616$ instead of 0.416.

The results of the correlation presented in Table 11 for mixed alkane solvents and in Table 12 for cyclohexane + alkane solvents were obtained by using in eq 3 the experimental values of D^{∞}_{12} and D^{∞}_{13} given in Tables 2 to 10. AAD is the average absolute percent deviation:

$$\mathrm{AAD} = \frac{100}{n} \sum \left| \frac{D^{\infty\mathrm{exp}}_{1m} - D^{\infty\mathrm{calc}}_{1m}}{D^{\infty\mathrm{exp}}_{1m}} \right| \tag{5}$$

where n is the number of experimental points.

For all mixed solvents the correlation of diffusion data is quite satisfactory. Indeed, deviations reported in Tables 11 and 12 are less than 3 %, which means that it is in the range of the experimental uncertainties. Figures 1 and 2 illustrate the good agreement between experimental and calculated data. It is worth recalling that, as was pointed out in the previous paper,[2] such results can only be obtained by taking into consideration in the

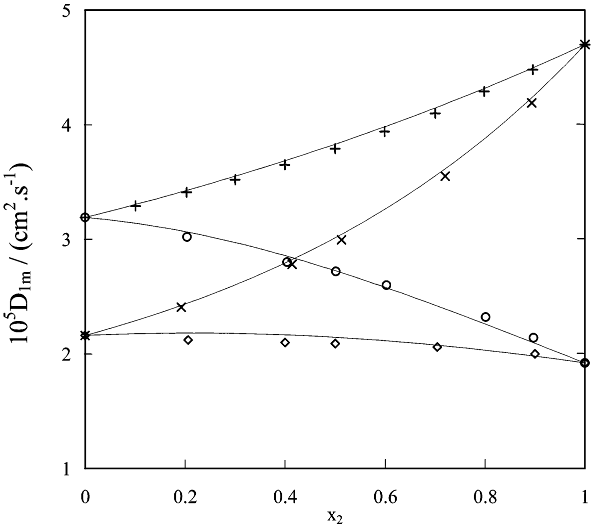

Figure 1. Correlation of diffusion coefficients D^{∞}_{1m} of benzene (1) at infinite dilution in various mixed solvents: +, hexane (2) + octane (3); ×, hexane (2) + decane (3); ○, cyclohexane (2) + octane (3); ◇, cyclohexane (2) + decane (3).

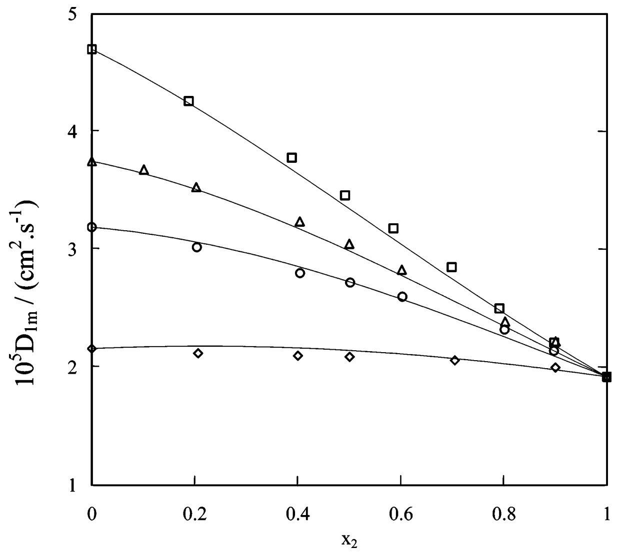

Figure 2. Correlation of experimental diffusion coefficients D_{1m}^{∞} of benzene (1) at infinite dilution in various mixed solvents of cyclohexane (2) with component (3): □, hexane; Δ, heptane; ○, octane; ◇, decane. —, Leffler–Cullinan equation using experimental values of D_{1p}^{∞}.

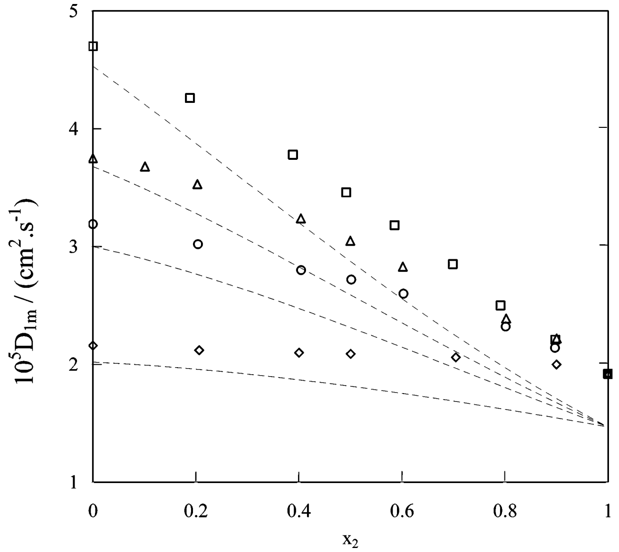

Figure 3. Correlation of experimental diffusion coefficients D_{1m}^{∞} of benzene (1) at infinite dilution in various mixed solvents of cyclohexane (2) with component (3): □, hexane; Δ, heptane; ○, octane; ◇, decane. – –, Leffler–Cullinan equation using for D_{1p}^{∞} the Wilke–Chang predictions.

Leffler–Cullinan equation (eqs 1 or 3) the experimental values of the diffusion coefficients D_{1p}^{∞} of the solutes in the pure solvents. In Figure 3, we have plotted the curves obtained with the same equation, but using for D_{1p}^{∞} the values calculated from the Wilke–Chang equation[4] (which depends, at a given temperature, on the solvent molar mass and viscosity and on the solute molar volume); the deterioration of results obtained in this case is essentially due to the poor prediction of D_{1p}^{∞}.

The Grunberg–Nissan method[12] is known to be a rough technique for calculating viscosity data; however, as is observed in this work, this equation turned out to be sufficient for correlating saturated hydrocarbon solvent mixtures.

Conclusions

Diffusion coefficients of several aromatics at infinite dilution in binary mixtures containing hexane, heptane, octane, decane, and cyclohexane were measured at 298.15 K by using the Taylor dispersion technique. As was suggested in a previous work,[2] experimental data were correlated by means of the Leffler–Cullinan equation taking into account the experimental values of diffusion coefficients in the pure solvents. Thanks to the Grunberg–Nissan method, it was possible to calculate diffusion coefficients independently of viscosities. In the case of the alkane and cycloalkane solvents considered in this work, the agreement between experimental and calculated values is quite satisfactory; indeed, deviations are always less than 3 %, in the range of the experimental uncertainties.

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