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# Studies on densities and viscosities of binary mixtures of alkyl benzoates in *n*-heptane

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## Abstract

Densities and viscosities have been determined for the two binary mixtures of methyl and ethyl benzoate in *n*-heptane at different concentrations and temperatures. The corresponding excess properties and the activation magnitudes were also calculated from the experimental data. All excess properties, including the excess Gibbs free energy of activation of flow, are negative over the entire range of compositions. The results for these binary mixtures are compared with those for methyl benzoate with *n*-nonane, the molecular interactions occurring in the mixtures being explained on the basis of the deviation from ideality of the magnitudes studied.

## INTRODUCTION

This paper is part of a broad program of research into the thermodynamic behavior of mixtures of esters and various solvents (*n*-alkanes, *n*-alcohols, and 1-chloroalkanes) that has been in progress at our laboratory for some time. The study of such behavior has so far been concerned with the different mixing properties, $h^E$, $g^E$, $v^E$, and the VLE values, for binary systems composed of aliphatic esters and a second component. The results have indicated the existence of specific interactions caused by the presence of the –COO– group. However, an earlier paper [1] which reported an initial study on the $v^E$, $\eta^E$ and $\Delta g^{*E}$ values of aromatic esters for the binary system methyl benzoate + *n*-nonane, did not consider this aspect. This paper, therefore, investigates the special behavior of the ester group on the benzene ring, using magnitudes that do not generate thermal effects, i.e. as if the large size of the benzoate molecule was the primary cause of the

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discrepancy with respect to the ideal behavior of the systems that contain them.

This second paper thus presents direct experimental values for density $\rho$ and viscosity $\eta$, and indirect values for the excess magnitudes for the two binary systems methyl benzoate + $n$-heptane and ethyl benzoate + $n$-heptane at four temperatures between 288.15 and 318.5 K. The thermodynamic activation functions that complete this study were calculated from the variation in $\rho$ and $\eta$ with temperature.

The $v^E$ values at 298.15 K for the two mixtures considered here, were found in the literature [2, 3] and will be used for purposes of comparison.

## EXPERIMENTAL

The density $\rho$ and viscosity $\eta$ values for the pure components and their mixtures were measured respectively in an Anton Paar 60/602 digital densimeter and in a Cannon–Fenske viscosimeter; the operation and calibration of these instruments were described in a previous paper [1]. The accuracy of the direct measurements of $\rho$ was $\pm 0.002\ \mathrm{kg\,m^{-3}}$ and that of $\eta$, $\pm 0.003$ mPa s. The precision of the magnitudes calculated indirectly was: for the concentrations $x$, $\pm 5 \times 10^{-5}$; for the excess volumes $v^E$, $\pm 2 \times 10^{-9}\ \mathrm{m^3\,mol^{-1}}$; and for the excess viscosities $\eta^E$, $\pm 0.005$ mPa s.

The components used in the present study did not undergo any further purification but were simply degassed ultrasonically for several hours and then dried in darkness on a molecular sieve (Fluka) prior to use. The $n$-heptane (puriss. p.a. >99.5 mol.%) was supplied by Fluka; the alkyl benzoates (+99 mol.%) were from Aldrich. Table 1 gives the values recorded for the most important properties of the components used in this experiment and also the values compiled from the literature for comparison. Even though the properties for methyl benzoate (Fluka) were reported in an earlier paper [1], the values were redetermined experimentally here because this time it was purchased from a different manufacturer. Using the expression $\alpha = -(\partial \ln \rho / \partial T)_p$, the mean coefficients of thermal expansion were also calculated from the density values at temperatures in the range 288.15–318.15 K. On the whole, the agreement between our experimental data and the literature values was good, with maximum errors of less than 4%.

## RESULTS

The experimental data for density $\rho$ and dynamic viscosity $\eta$ for the mixtures $x_1C_6H_5COOC_uH_{2u+1} + x_2n\text{-}C_7H_{16}$, where $u$ is 1 or 2, at different concentrations and temperatures are given in Table 2, which also contains the excess values for the molar volumes, for the viscosity calculated using a non-logarithmic equation, and for the free activation energy of the viscous

TABLE 1

Properties of pure compounds at different temperatures and their comparison with literature data

| Property | 288.15 K | | 298.15 K | | 308.15 K | | 318.15 K | |
|---|---|---|---|---|---|---|---|---|
| | Exp. | Lit. | Exp. | Lit. | Exp. | Lit. | Exp. | Lit. |
| *n*-Heptane | | | | | | | | |
| $n_D$ | 1.3903 | | 1.3854 | 1.38511 [4]<br>1.3855 [5]<br>1.3852 [7] | 1,3805 | 1.3802 [5] | 1.3755 | 1.3750 [5] |
| $\rho/(\mathrm{kg\ m^{-3}})$ | 689.46 | | 679.28 | 679.46 [4, 6]<br>679.52 [5]<br>679.37 [7] | 670.62 | 671.07 [5] | 661.92 | 662.32 [5] |
| $\eta/(\mathrm{mPa\ s})$ | 0.441 | 0.441 [4]<br>0.440 [6] | 0.394 | 0.397 [4]<br>0.395 [6]<br>0.388 [7] | 0.353 | 0.3592 [4]<br>0.3581 [6] | 0.318 | 0.326 [6] |
| $\alpha/(\mathrm{K^{-1}})$ | 0.00134 | 0.00124 [4] | | | | | | |
| Methyl benzoate | | | | | | | | |
| $n_D$ | 1.5192 | 1.5190 [1] | 1.5145 | 1.51457 [4]<br>1.5144 [1] | 1.5101 | 1.5102 [1] | 1.5058 | 1.5056 [1] |
| $\rho/(\mathrm{kg\ m^{-3}})$ | 1092.62 | 1093.34 [4]<br>1091.85 [1] | 1083.60 | 1083.52 [1] | 1074.07 | 1073.29 [1] | 1064.52 | 1063.50 [1] |
| $\eta/(\mathrm{mPa\ s})$ | 2.246 | 2.298 [4]<br>2.250 [1] | 1.793 | 1.809 [1] | 1.485 | 1.476 [1] | 1.232 | 1.224 [1] |
| $\alpha/(\mathrm{K^{-1}})$ | 0.00087 | 0.000876 [4] | | | | | | |
| Ethyl benzoate | | | | | | | | |
| $n_D$ | 1.5071 | 1.50748 [4] | 1.5026 | 1.50348 [4] | 1.4985 | | 1.4940 | |
| $\rho/(\mathrm{kg\ m^{-3}})$ | 1050.42 | 1051.12 [4] | 1041.63 | 1042.1 [7] | 1032.55 | | 1023.00 | |
| $\eta/(\mathrm{mPa\ s})$ | 2.394 | 2.407 [4] | 1.906 | 1.990 [7] | 1.560 | | 1.294 | |
| $\alpha/(\mathrm{K^{-1}})$ | 0.00088 | 0.00089 (293.15 K) [4] | | | | | | |

TABLE 2

Densities $\rho$ viscosities $\eta$ and excess properties for the systems $x_1$ methyl (or ethyl) benzoate + $x_2$ $n$-heptane at several temperatures

| $x_1$ | $\rho/(\mathrm{kg\,m^{-3}})$ | $v^E \times 10^6/(\mathrm{m^3\,mol^{-1}})$ | $\eta/(\mathrm{mPa\,s})$ | $\eta^E/(\mathrm{mPa\,s})$ | $\Delta g^{*E}/(\mathrm{kJ\,mol^{-1}})$ |
|---|---|---|---|---|---|
| Methyl benzoate(1) + $n$-heptane(2) | | | | | |
| 288.15 K | | | | | |
| 0.9017 | 1048.6 | −0.173 | 1.777 | −0.291 | −0.178 |
| 0.8033 | 1005.2 | −0.274 | 1.434 | −0.456 | −0.308 |
| 0.6984 | 959.9 | −0.315 | 1.149 | −0.553 | −0.430 |
| 0.5987 | 917.4 | −0.305 | 0.950 | −0.570 | −0.491 |
| 0.5004 | 877.5 | −0.262 | 0.814 | −0.530 | −0.482 |
| 0.3974 | 836.2 | −0.195 | 0.690 | −0.468 | −0.475 |
| 0.3001 | 798.5 | −0.124 | 0.607 | −0.375 | −0.400 |
| 0.1960 | 759.4 | −0.056 | 0.528 | −0.267 | −0.332 |
| 0.0999 | 724.5 | −0.012 | 0.480 | −0.142 | −0.187 |
| 298.15 K | | | | | |
| 0.9017 | 1039.4 | −0.204 | 1.435 | −0.221 | −0.184 |
| 0.8033 | 995.8 | −0.323 | 1.183 | −0.335 | −0.293 |
| 0.6984 | 950.2 | −0.373 | 0.968 | −0.403 | −0.396 |
| 0.5978 | 907.6 | −0.365 | 0.814 | −0.416 | −0.446 |
| 0.5004 | 867.4 | −0.320 | 0.701 | −0.393 | −0.449 |
| 0.3974 | 826.1 | −0.247 | 0.601 | −0.349 | −0.444 |
| 0.3001 | 788.3 | −0.169 | 0.533 | −0.282 | −0.379 |
| 0.1960 | 749.2 | −0.089 | 0.464 | −0.204 | −0.329 |
| 0.0999 | 714.3 | −0.032 | 0.425 | −0.109 | −0.187 |
| 308.15 K | | | | | |
| 0.9017 | 1030.0 | −0.236 | 1.197 | −0.176 | −0.190 |
| 0.8033 | 986.3 | −0.346 | 1.008 | −0.254 | −0.269 |
| 0.6984 | 940.9 | −0.411 | 0.839 | −0.305 | −0.353 |
| 0.5978 | 898.4 | −0.420 | 0.708 | −0.322 | −0.418 |
| 0.5004 | 858.3 | −0.382 | 0.616 | −0.303 | −0.414 |
| 0.3974 | 817.1 | −0.303 | 0.535 | −0.267 | −0.393 |
| 0.3001 | 779.4 | −0.210 | 0.472 | −0.221 | −0.358 |
| 0.1960 | 740.3 | −0.112 | 0.418 | −0.156 | −0.283 |
| 0.0999 | 705.5 | −0.039 | 0.382 | −0.084 | −0.163 |
| 318.15 K | | | | | |
| 0.9017 | 1020.6 | −0.262 | 1.024 | −0.118 | −0.139 |
| 0.8033 | 976.9 | −0.385 | 0.860 | −0.193 | −0.250 |
| 0.6984 | 931.5 | −0.457 | 0.720 | −0.238 | −0.341 |
| 0.5978 | 889.4 | −0.469 | 0.620 | −0.245 | −0.379 |
| 0.5004 | 849.1 | −0.430 | 0.539 | −0.236 | −0.395 |
| 0.3974 | 808.0 | −0.349 | 0.475 | −0.207 | −0.364 |
| 0.3001 | 770.4 | −0.250 | 0.422 | −0.171 | −0.328 |
| 0.1960 | 731.4 | −0.142 | 0.378 | −0.120 | −0.247 |
| 0.0999 | 696.7 | −0.057 | 0.346 | −0.064 | −0.138 |

TABLE 2 (continued)

| $x_1$ | $\rho/(\mathrm{kg\,m^{-3}})$ | $v^E \times 10^6/(\mathrm{m^3\,mol^{-1}})$ | $\eta/(\mathrm{mPa\,s})$ | $\eta^E/(\mathrm{mPa\,s})$ | $\Delta g^{*E}/(\mathrm{kJ\,mol^{-1}})$ |
|---|---|---|---|---|---|
| Ethyl benzoate(1) + *n*-heptane(2) | | | | | |
| 288.15 K | | | | | |
| 0.8972 | 1014.2 | −0.201 | 1.904 | −0.290 | −0.136 |
| 0.7984 | 978.6 | −0.281 | 1.532 | −0.469 | −0.258 |
| 0.6974 | 942.0 | −0.316 | 1.250 | −0.553 | −0.336 |
| 0.5985 | 906.1 | −0.317 | 1.041 | −0.569 | −0.374 |
| 0.4961 | 868.8 | −0.289 | 0.868 | −0.542 | −0.394 |
| 0.3941 | 831.7 | −0.239 | 0.733 | −0.478 | −0.385 |
| 0.2948 | 795.6 | −0.177 | 0.625 | −0.392 | −0.362 |
| 0.1952 | 759.6 | −0.112 | 0.547 | −0.275 | −0.277 |
| 0.0980 | 724.6 | −0.051 | 0.490 | −0.143 | −0.148 |
| 298.15 K | | | | | |
| 0.8972 | 1005.0 | −0.196 | 1.539 | −0.211 | −0.132 |
| 0.7984 | 969.3 | −0.314 | 1.263 | −0.338 | −0.238 |
| 0.6974 | 932.6 | −0.375 | 1.047 | −0.401 | −0.309 |
| 0.5985 | 896.5 | −0.387 | 0.882 | −0.417 | −0.347 |
| 0.4961 | 859.1 | −0.360 | 0.747 | −0.398 | −0.362 |
| 0.3941 | 821.8 | −0.305 | 0.638 | −0.353 | −0.354 |
| 0.2948 | 785.6 | −0.232 | 0.550 | −0.290 | −0.333 |
| 0.1952 | 749.5 | −0.151 | 0.484 | −0.205 | −0.257 |
| 0.0980 | 714.4 | −0.072 | 0.428 | −0.115 | −0.183 |
| 308.15 K | | | | | |
| 0.8972 | 995.7 | −0.218 | 1.286 | −0.150 | −0.107 |
| 0.7984 | 960.2 | −0.351 | 1.082 | −0.234 | −0.175 |
| 0.6974 | 923.5 | −0.423 | 0.912 | −0.282 | −0.230 |
| 0.5985 | 887.4 | −0.442 | 0.767 | −0.308 | −0.297 |
| 0.4961 | 850.0 | −0.418 | 0.655 | −0.296 | −0.310 |
| 0.3941 | 812.8 | −0.362 | 0.564 | −0.265 | −0.307 |
| 0.2948 | 776.7 | −0.285 | 0.492 | −0.216 | −0.274 |
| 0.1952 | 740.7 | −0.193 | 0.433 | −0.155 | −0.221 |
| 0.0980 | 705.6 | −0.097 | 0.387 | −0.084 | −0.139 |
| 318.15 K | | | | | |
| 0.8972 | 986.3 | −0.226 | 1.080 | −0.114 | −0.101 |
| 0.7984 | 950.8 | −0.373 | 0.913 | −0.184 | −0.181 |
| 0.6974 | 914.2 | −0.462 | 0.771 | −0.227 | −0.254 |
| 0.5985 | 878.3 | −0.469 | 0.662 | −0.240 | −0.292 |
| 0.4961 | 841.0 | −0.483 | 0.571 | −0.232 | −0.305 |
| 0.3941 | 803.9 | −0.431 | 0.498 | −0.205 | −0.285 |
| 0.2948 | 767.9 | −0.350 | 0.440 | −0.166 | −0.241 |
| 0.1952 | 731.9 | −0.245 | 0.393 | −0.116 | −0.169 |
| 0.0980 | 696.9 | −0.127 | 0.351 | −0.063 | −0.108 |

flow, obtained using

$$\Delta g^{*E} = RT(\ln \eta v - x_1 \ln \eta_1 v_1 - x_2 \ln \eta_2 v_2) \tag{1}$$

where $v$ is the molar volume and $\eta$ is the dynamic viscosity of the mixture, and the subscripts refer to the pure components; $R$ is the universal gas constant, and $T$ is absolute temperature. The excess magnitudes, here represented generically by $Y^E$, were correlated using the polynomial equation

$$Y^E = x_1 x_2 \sum_{i=0}^{n} A_i z^i \tag{2}$$

where

$$z = x_1/(x_1 + kx_2) \tag{3}$$

The $A_i$ coefficients were calculated in each case using a least-squares method to find the value of $k$ that minimized the standard deviation $s(Y^E)$ between the experimental data and eqn. (2). Table 3 presents the values thus obtained. Figures 1(a) and 1(b) depict the curves for $v^E$ and $\eta^E$ for the different cases of the two systems studied.

As mentioned in the introduction, the literature contains $v^E$ values for the two mixtures (methyl benzoate or ethyl benzoate + $n$-heptane) at 298.15 K. Figure 2 shows the differences between these data and our $v^E$ data fitted by eqn. (2). The mean error between our data and the values reported by Grolier et al. [2] was 39% for the mixture methyl benzoate + $n$-heptane and 30.6% for the mixture ethyl benzoate + $n$-heptane; the mean error with respect to the values reported by Dussart et al. [3] was 22.3% for methyl benzoate + $n$-heptane and 22.2% for ethyl benzoate + $n$-heptane.

Viscosity may be related to the thermodynamic activation magnitudes for the mixtures using the equation of Eyring et al. [8]

$$\eta = \frac{hN}{v} \exp[\Delta h^{\neq}/RT - \Delta s^{\neq}/R] \tag{4}$$

from which the thermodynamic activation values $\Delta h^{\neq}$ and $\Delta s^{\neq}$ can be calculated. It follows that $\Delta g^{\neq}$ can then be obtained, because $\Delta g^{\neq} = \Delta h^{\neq} - T\,\Delta s^{\neq}$. These values appear in Table 3.

## DISCUSSION

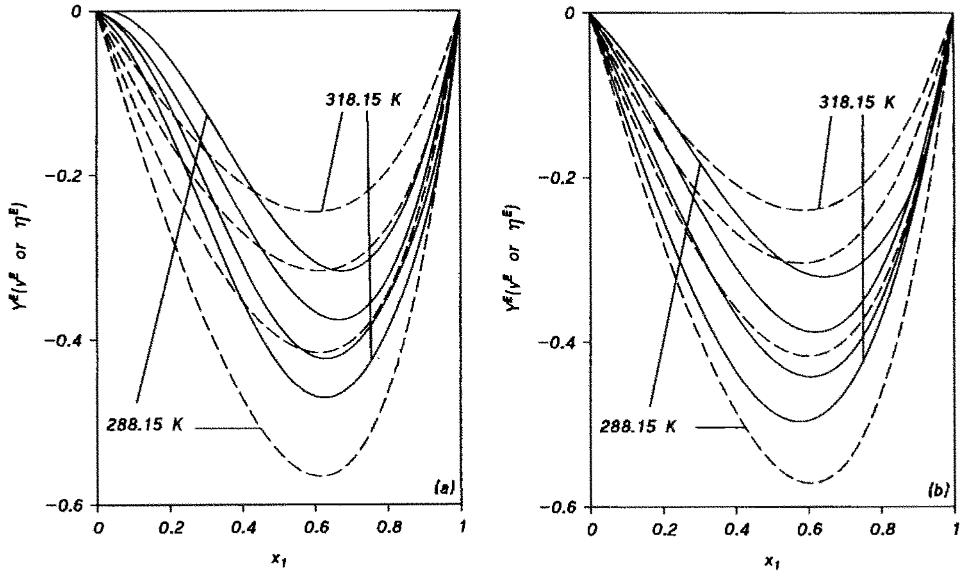
The qualitative representations of the excess magnitudes $v^E$ and $\eta^E$ presented in Figs. 1(a) and (b) reveal certain important characteristics of mixtures of alkyl benzoate + $n$-heptane. Firstly, higher volumetric contractions could be expected in these mixtures as compared to those in mixtures with $n$-nonane [1]: the possibility of interstitial accommodation of the

TABLE 3

Coefficients $k$, $A_i$ and standard deviations obtained for eqn. (2)

| $T$/K | $k$ | $A_0$ | $A_1$ | $A_2$ | $A_3$ | $s(Y^E)$ |
|---|---|---|---|---|---|---|
| Methyl benzoate + $n$-heptane | | | | | | |
| $v^E \times 10^6/(m^3\ mol^{-1})$ | | | | | | |
| 288.15 | 0.998 | 0.091 | −2.271 | – | – | 0.0054 |
| 298.15 | 1.127 | −0.135 | −2.433 | – | – | 0.0067 |
| 308.15 | 3.046 | −0.154 | −8.487 | 14.305 | −9.926 | 0.0034 |
| 318.15 | 3.005 | −0.350 | −8.285 | 13.594 | −9.550 | 0.0057 |
| $\eta^E/(mPa\ s)$ | | | | | | |
| 288.15 | 2.268 | −1.441 | −2.296 | – | – | 0.0048 |
| 298.15 | 3.079 | −1.145 | −1.764 | – | – | 0.0031 |
| 308.15 | 3.716 | −0.906 | −1.429 | – | – | 0.0043 |
| 318.15 | 1.941 | −0.663 | −0.824 | – | – | 0.0012 |
| $\Delta g^{*E}/(kJ\ mol^{-1})$ | | | | | | |
| 288.15 | 0.190 | −1.990 | – | – | – | 0.0127 |
| 298.15 | 0.597 | −2.440 | 2.039 | −1.659 | – | 0.0117 |
| 308.15 | 2.900 | −1.834 | 1.139 | −1.836 | – | 0.0120 |
| 318.15 | 0.190 | −1.570 | – | – | – | 0.0059 |
| Ethyl benzoate + $n$-heptane | | | | | | |
| $v^E \times 10^6/(m^3\ mol^{-1})$ | | | | | | |
| 288.15 | 3.084 | −0.446 | −3.997 | 5.436 | −4.327 | 0.0051 |
| 298.15 | 1.090 | −0.664 | −1.638 | – | – | 0.0059 |
| 308.15 | 1.256 | −0.974 | −1.592 | – | – | 0.0047 |
| 318.15 | 1.056 | −1.325 | −1.260 | – | – | 0.0055 |
| $\eta^E(mPa\ s)$ | | | | | | |
| 288.15 | 2.217 | −1.534 | −2.101 | – | – | 0.0040 |
| 298.15 | 2.454 | −1.179 | −1.468 | – | – | 0.0029 |
| 308.15 | 1.954 | −0.896 | −0.850 | – | – | 0.0028 |
| 318.15 | 1.379 | −0.640 | −0.688 | – | – | 0.0010 |
| $\Delta g^{*E}/(kJ\ mol^{-1})$ | | | | | | |
| 288.15 | 0.342 | −1.876 | 0.361 | – | – | 0.0094 |
| 298.15 | 0.144 | −3.446 | 4.190 | −2.201 | – | 0.0064 |
| 308.15 | 0.412 | −1.634 | 0.574 | – | – | 0.0079 |
| 318.15 | 0.190 | −1.183 | – | – | – | 0.0090 |

hydrocarbon molecules among the ester molecules increases with decreasing $n$-alkane chain length. However, the $v^E$ values became more negative as the number of carbon atoms in the benzoate increases, resulting in lower polarity and a weakening of the associations between ester molecules, thereby enabling induced dipole–dipole complexes to form between the benzoate and the $n$-heptane, which in turn gave rise to endothermic effects



(a) (b)

Fig. 1. ——, Excess molar volumes $v^E \times 10^6/(\mathrm{m^3\,mol^{-1}})$ and – – –, excess viscosities $\eta^E/(\mathrm{mPa\,s})$ for the binary systems (a) $x_1$ methyl benzoate + $x_2$ *n*-heptane and (b) $x_1$ ethyl benzoate + $x_2$ *n*-heptane, as a function of temperature.

in the mixing process [2]. The contraction in the volume increased significantly as temperature increased.

However, the $\eta^E$ and $\Delta g^{*E}$ values became less negative as the temperature rose; this behavior was similar to that in the system studied previously [1]. Because of the above arguments and in accordance with the Arrhenius theory, the negative values of the activation entropies (Table 4)

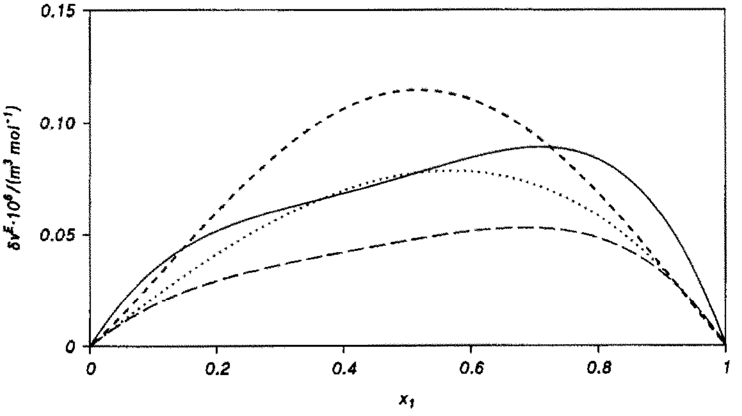


Fig. 2. Deviations $\delta v^E = (v^E - v^E_{\mathrm{cal}})$ from eqn. (2) of the values obtained by other authors at 298.15 K for the mixture $x_1$ methyl benzoate + $x_2$ *n*-heptane: ——, Grolier et al. [2]; — — —, Dusart et al. [3]; and for $x_1$ ethyl benzoate + $x_2$ *n*-heptane: – – –, Grolier et al. [2]; · · ·, Dusart et al. [3].

TABLE 4

Activation parameters for $x_1$ methyl (or ethyl) benzoate + $x_2$*n*-heptane

| $x_1$ | $\Delta g^{\neq}/(\mathrm{kJ\ mol^{-1}})$ | | | | $\Delta s^{\neq}/(\mathrm{J\ K^{-1}\ mol^{-1}})$ | $\Delta h^{\neq}/(\mathrm{kJ\ mol^{-1}})$ |
|---|---|---|---|---|---|---|
| | 288.15 | 298.15 | 308.15 | 318.15 | | |
| Methyl benzoate(1) + *n*-hepane(2) | | | | | | |
| 1.0000 | 65.3 | 67.1 | 68.9 | 70.6 | −176.4 | 14.5 |
| 0.9017 | 64.8 | 66.6 | 68.4 | 70.1 | −178.7 | 13.3 |
| 0.8033 | 64.3 | 66.1 | 67.9 | 69.8 | −180.9 | 12.2 |
| 0.6984 | 63.8 | 65.7 | 67.5 | 69.3 | −183.4 | 11.0 |
| 0.5978 | 63.4 | 65.3 | 67.1 | 69.0 | −185.3 | 10.0 |
| 0.5004 | 63.1 | 65.0 | 66.8 | 68.7 | −185.8 | 9.6 |
| 0.3974 | 62.7 | 64.6 | 66.5 | 68.4 | −188.0 | 8.6 |
| 0.3001 | 62.5 | 64.3 | 66.2 | 68.1 | −187.8 | 8.4 |
| 0.1960 | 62.2 | 64.1 | 66.0 | 67.9 | −189.8 | 7.5 |
| 0.0999 | 62.0 | 63.9 | 65.8 | 67.7 | −189.7 | 7.3 |
| 0.0000 | 61.8 | 63.7 | 65.6 | 67.5 | −189.2 | 7.3 |
| Ethyl benzoate(1) + *n*-heptane(2) | | | | | | |
| 1.0000 | 65.6 | 67.3 | 69.1 | 70.9 | −175.8 | 14.9 |
| 0.8972 | 65.0 | 66.8 | 68.6 | 70.4 | −179.3 | 13.3 |
| 0.7984 | 64.6 | 66.4 | 68.2 | 70.0 | −181.4 | 12.3 |
| 0.6974 | 64.1 | 65.9 | 67.8 | 69.6 | −183.1 | 11.3 |
| 0.5985 | 63.7 | 65.5 | 67.4 | 69.2 | −184.1 | 10.6 |
| 0.4961 | 63.3 | 65.1 | 67.0 | 68.8 | −185.7 | 9.8 |
| 0.3941 | 62.9 | 64.8 | 66.6 | 68.5 | −187.3 | 8.9 |
| 0.2948 | 62.5 | 64.4 | 66.3 | 68.2 | −189.5 | 7.9 |
| 0.1952 | 62.3 | 64.2 | 66.1 | 68.0 | −190.2 | 7.5 |
| 0.0980 | 62.0 | 63.9 | 65.8 | 67.7 | −189.5 | 7.4 |
| 0.0000 | 61.8 | 63.7 | 65.6 | 67.5 | −189.3 | 7.3 |

and the high $\Delta h^{\neq}$ values suggest the existence of molecular interactions that give rise to a more rigid molecular arrangement.

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