

# Supporting Information on Thermophysical Properties of Mixtures of 2-Ethylhexanoic Acid and Ethanol

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# Comparison of experimental pure component properties to literature data

Relative deviations are calculated between the measured data from this work as well as from the literature and the results of the empirical correlations from the main text. Since the procedure is exactly the same for the density, viscosity, thermal conductivity, and isobaric heat capacity, it is shown here using the exemplary property  $z$ :

$$\Delta_{\text{rel}}z = \frac{z^{\text{exp}} - z^{\text{fit}}}{z^{\text{fit}}}$$

Figure S1 shows the experimental results of this work for the density of pure EHA in comparison with experimental data from the literature. Since there are only two data points at atmospheric pressure from the literature, a deviation plot is not shown in this case. Table S1 lists the measurement results for the viscosity of pure EHA. Figures S2 show the experimental results of this work for the viscosity of pure EHA in comparison with experimental data from the literature. Again, a deviation plot is not shown because there are only two relevant data points for the comparison. Reasonable agreement is found but deviations increase with increasing temperature.

Figures S3 to S10 show the experimental results for the density, viscosity, thermal conductivity and isobaric heat capacity of pure ethanol in comparison with literature values.

Table S1: Results of the viscosity measurements for pure EHA <sup>a b</sup>

$T / \text{K}$	$\eta / \text{mPa s}$ ( $U(\eta) / \text{mPa s}$ )
293.15	7.529 (0.146)
303.15	5.354 (0.046)
313.15	3.961 (0.034)
323.15	3.042 (0.026)
333.15	2.413 (0.021)
343.15	1.961 (0.017)
353.15	1.629 (0.014)

<sup>a</sup> Viscosity  $\eta$  and temperature  $T$  at  $p = 101.3 \text{ kPa}$ . The combined expanded uncertainties are given in the table for  $U(\eta)$ ,  $u(p) = 3 \text{ kPa}$  and  $u(T) = 0.05 \text{ K}$ .

<sup>b</sup> Results for 293.15 to 333.15 K are repeated here for convenience. Results for 343.15 and 353.15 K are not shown in the main manuscript.

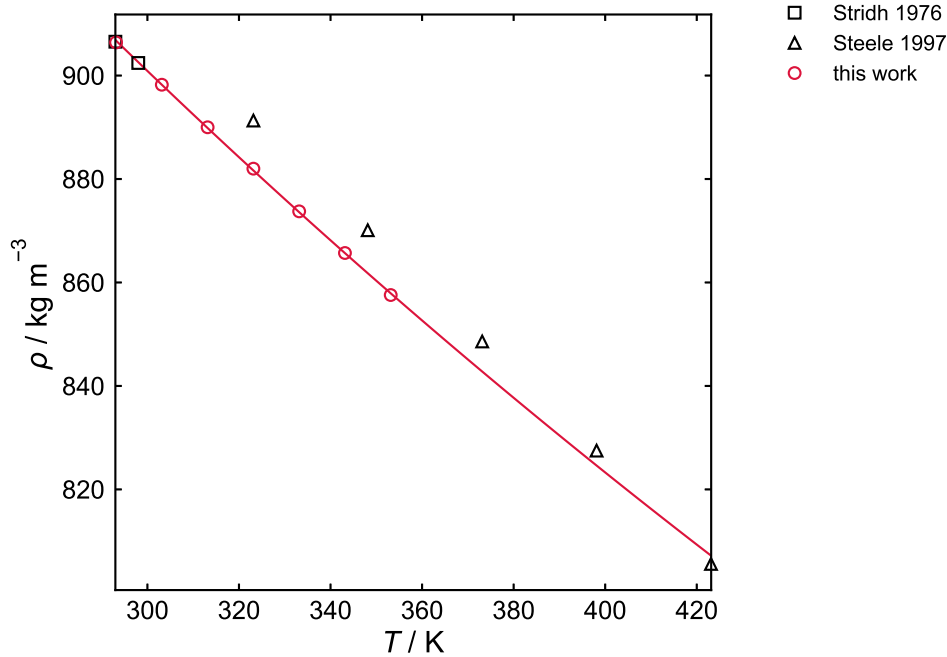


Figure S1: Density of pure EHA at 101.3 kPa (data of this work and data from Stridh<sup>1</sup>) or along the saturation line (data from Steele et al.<sup>2</sup>) as a function of temperature. Symbols are experimental results from this work and measurement data from the literature<sup>1,2</sup> as denoted in the legend. The line denotes the fit of the data of this work as described in the main text.

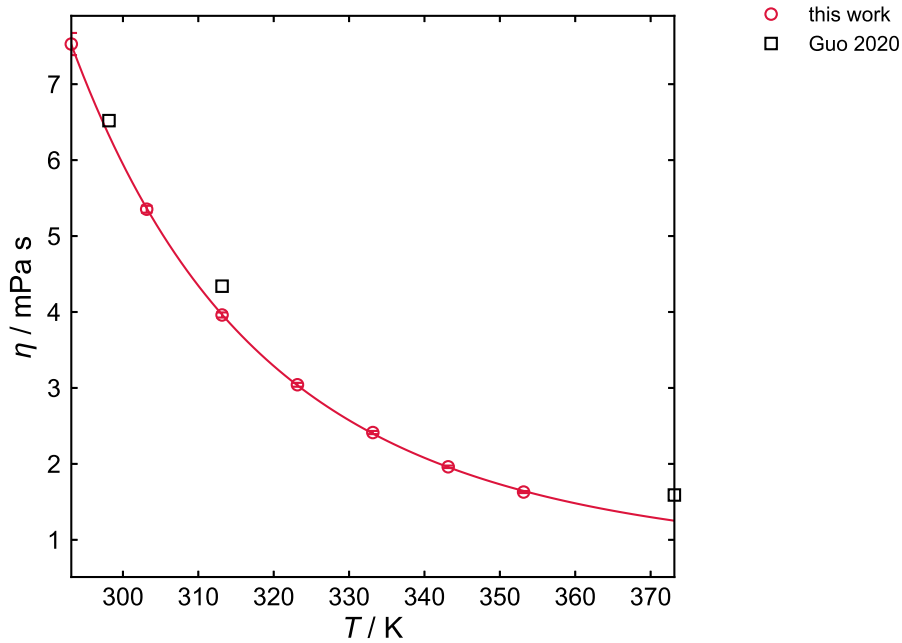


Figure S2: Viscosity of pure EHA at 101.3 kPa as a function of temperature. Symbols are experimental results from this work and measurement data from the literature<sup>25</sup> as denoted in the legend. The line denotes the fit of the data of this work as described in the main text.

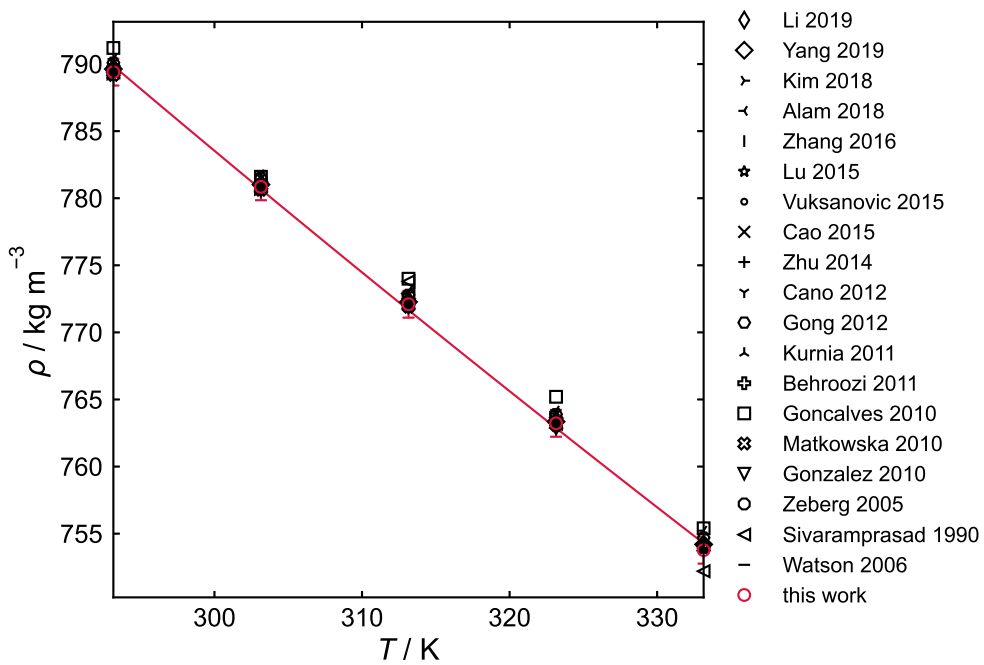


Figure S3: Density of pure ethanol at 101.3 kPa as a function of temperature. Symbols are experimental results from this work and measurement data from the literature<sup>3-21</sup> as denoted in the legend. The line denotes the fit of the data of this work as described in the main text.

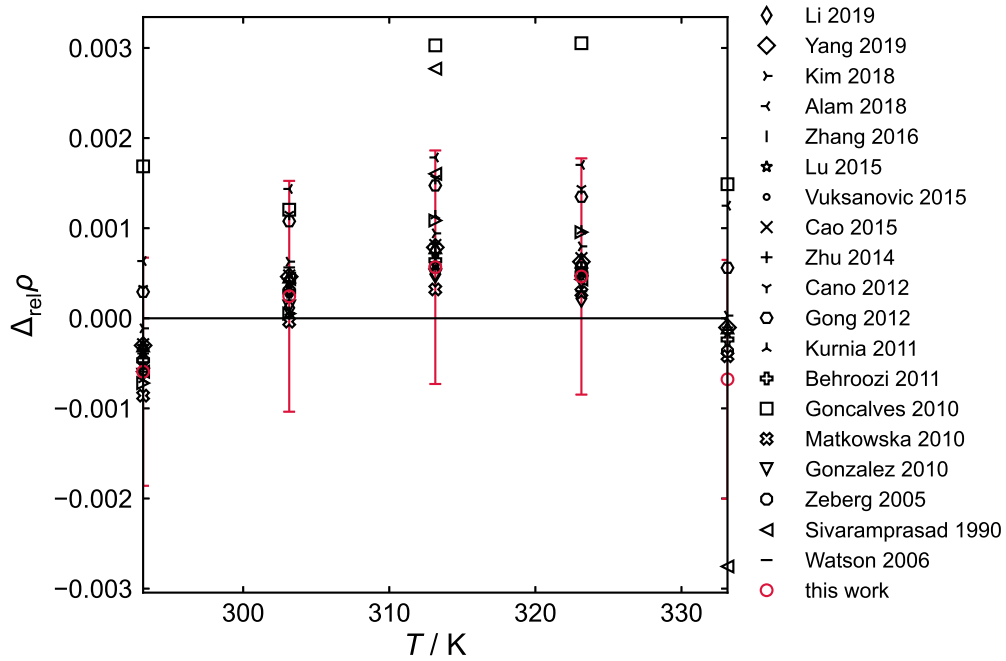


Figure S4: Relative deviation between experimental densities from this work or literature<sup>3-21</sup> as denoted in the legend and the fit to this work's data as described in the main text.

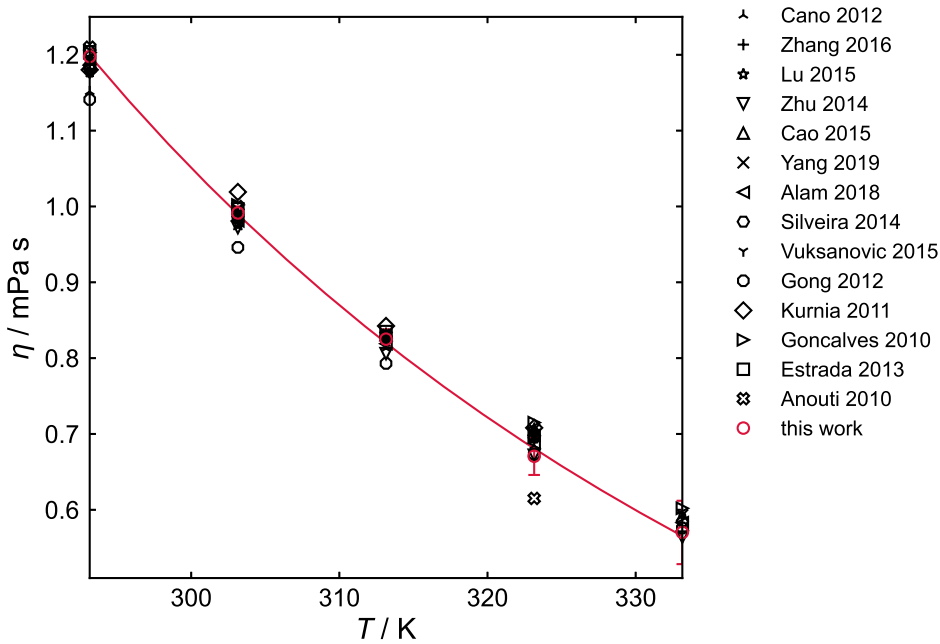


Figure S5: Viscosity of pure ethanol at 101.3 kPa as a function of temperature. Symbols are experimental results from this work and measurement data from the literature<sup>4,6-14,16,22-24</sup> as denoted in the legend. The line denotes the fit of the data of this work as described in the main text.

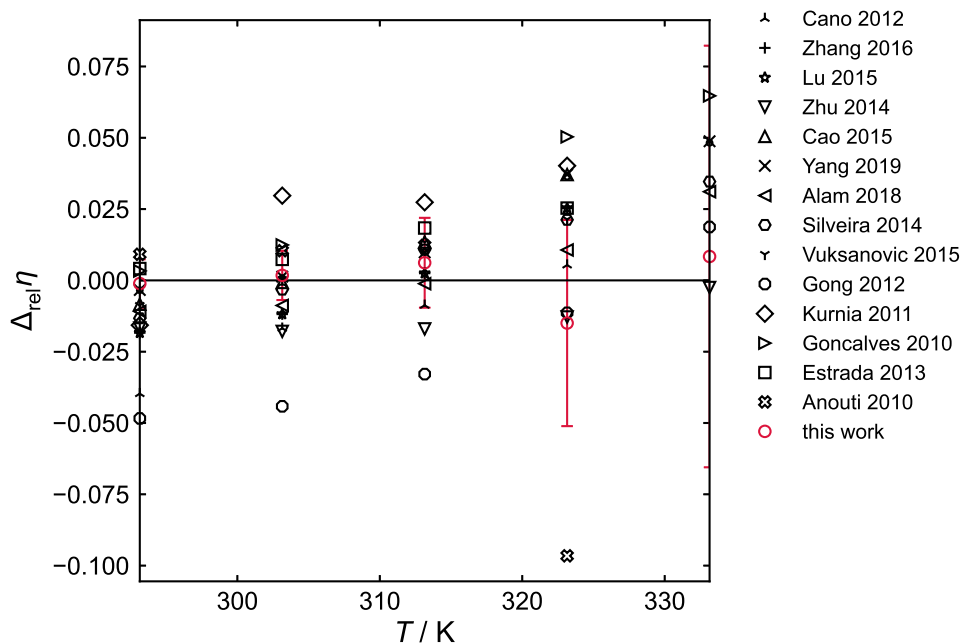


Figure S6: Relative deviation between experimental viscosities from this work or literature<sup>4,6–14,16,22–24</sup> as denoted in the legend and the fit to this work’s data as described in the main text.

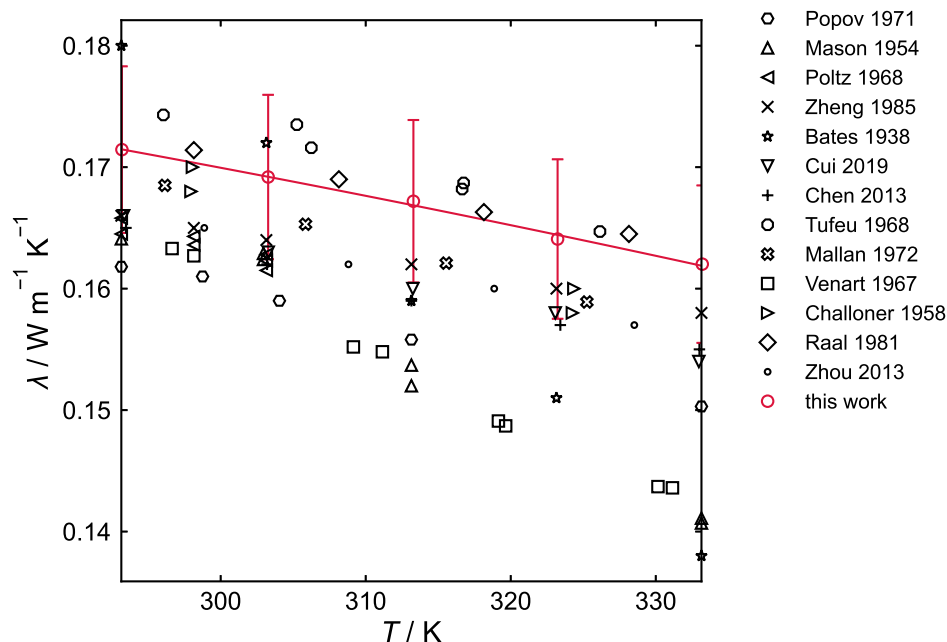


Figure S7: Thermal conductivity of pure ethanol at 101.3 kPa as a function of temperature. Symbols are experimental results from this work and measurement data from the literature<sup>26–38</sup> as denoted in the legend. The line denotes the fit of the data of this work as described in the main text.

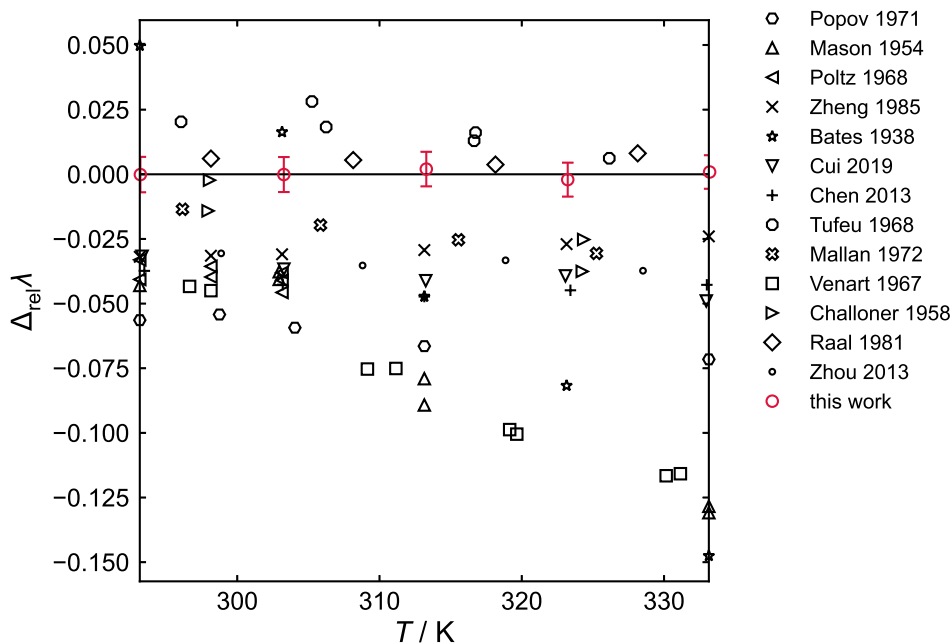


Figure S8: Relative deviation between experimental thermal conductivities from this work or literature<sup>26–38</sup> as denoted in the legend and the fit to this work’s data as described in the main text.

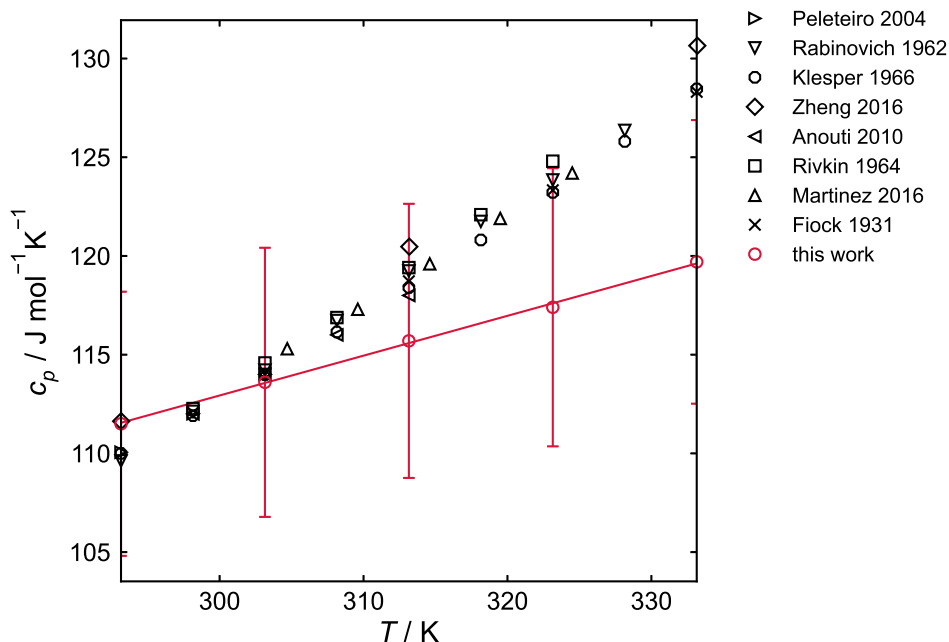


Figure S9: Isobaric heat capacity of pure ethanol at 101.3 kPa as a function of temperature. Symbols are experimental results from this work and measurement data from the literature<sup>24,39–45</sup> as denoted in the legend. The line denotes the fit of the data of this work as described in the main text.

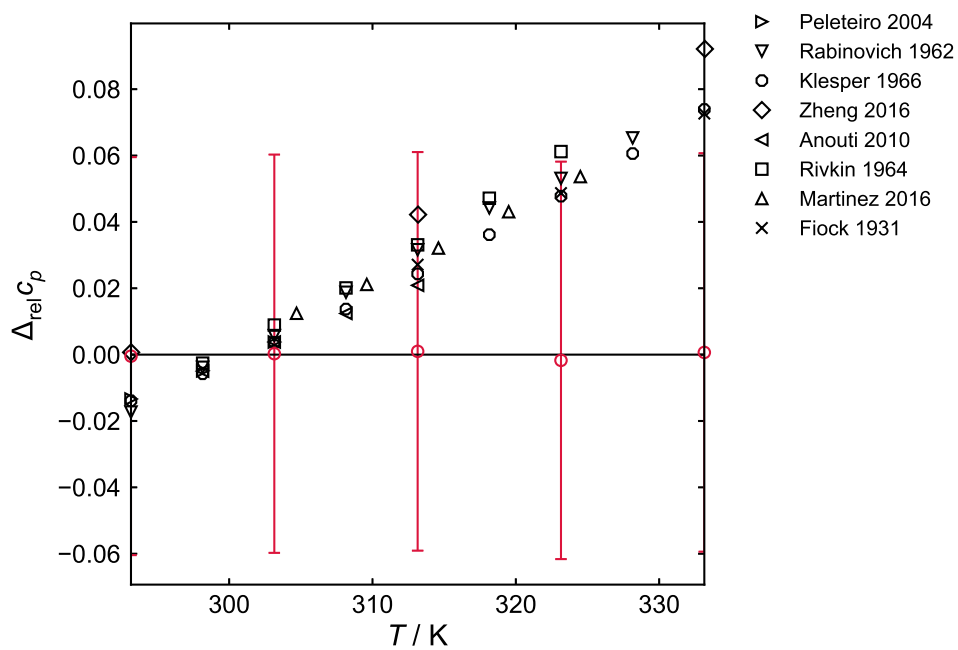


Figure S10: Relative deviation between experimental isobaric heat capacities from this work or literature<sup>24,39-45</sup> as denoted in the legend and the fit to this work's data as described in the main text.

## Self-diffusion coefficients of the pure components

The results of the self-diffusion coefficient measurements of pure ethanol at 101.3 kPa and temperatures between 298.15 and 333.15 K are given in Table S2. As evident from Figure S11, this work's results for the self-diffusion coefficient of pure ethanol are in excellent agreement with literature data.

Table S2: Results of the self-diffusion coefficient measurements for pure ethanol<sup>a</sup>

$T / \text{K}$	$D_{\text{EtOH}} / 10^{-9} \text{ m}^2 \text{ s}^{-1}$ ( $U(D_{\text{EtOH}}) / 10^{-9} \text{ m}^2 \text{ s}^{-1}$ )
298.15	1.071 (0.001)
303.15	1.199 (0.002)
313.15	1.494 (0.002)
323.15	1.843 (0.007)
333.15	2.251 (0.003)

<sup>a</sup> Self-diffusion coefficient  $D_{\text{EtOH}}$  and temperature  $T$  at  $p = 101.3 \text{ kPa}$ . The combined expanded uncertainties of the self-diffusion coefficient  $U(D_{\text{EtOH}})$  ( $k = 2$ ) are given in the table and  $u(T) = 0.1 \text{ K}$  and  $u(p) = 3 \text{ kPa}$ .

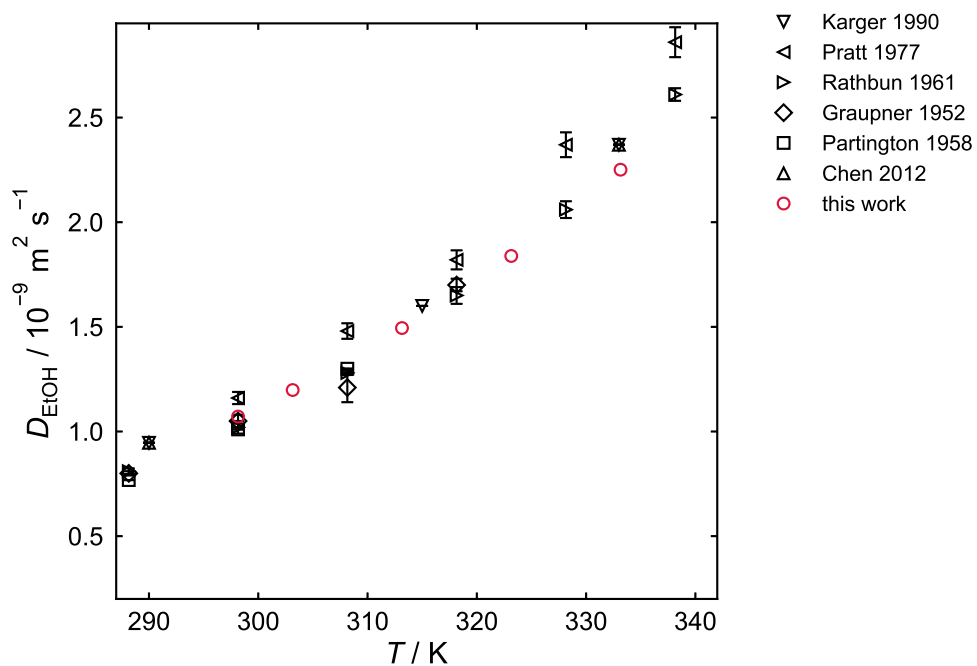


Figure S11: Self-diffusion coefficient of pure ethanol at 101.3 kPa as a function of temperature. Symbols are experimental results from this work and measurement data from the literature<sup>46–51</sup> as denoted in the insert legend. Error bars are with symbol size.

Table S3 gives the measurement results for the self-diffusion coefficient of pure EHA at 101.3 kPa and temperatures between 298.15 and 353.15 K. Additionally, the results are depicted in Figure S12.

Table S3: Results of the self-diffusion coefficient measurements for pure EHA <sup>a</sup>

$T / \text{K}$	$D_{\text{EHA}} / 10^{-9} \text{ m}^2 \text{ s}^{-1}$
298.15	0.126
303.15	0.152
313.15	0.213
323.15	0.287
333.15	0.375
343.15	0.477
353.15	0.596

<sup>a</sup> Self-diffusion coefficient  $D_{\text{EHA}}$  and temperature  $T$  at  $p = 101.3 \text{ kPa}$ . The combined expanded uncertainty of the self-diffusion coefficient of EHA is  $U(D_{\text{EHA}}) (k = 2) = 10^{-12} \text{ m}^2 \text{ s}^{-1}$  and  $u(T) = 0.1 \text{ K}$  and  $u(p) = 3 \text{ kPa}$ .

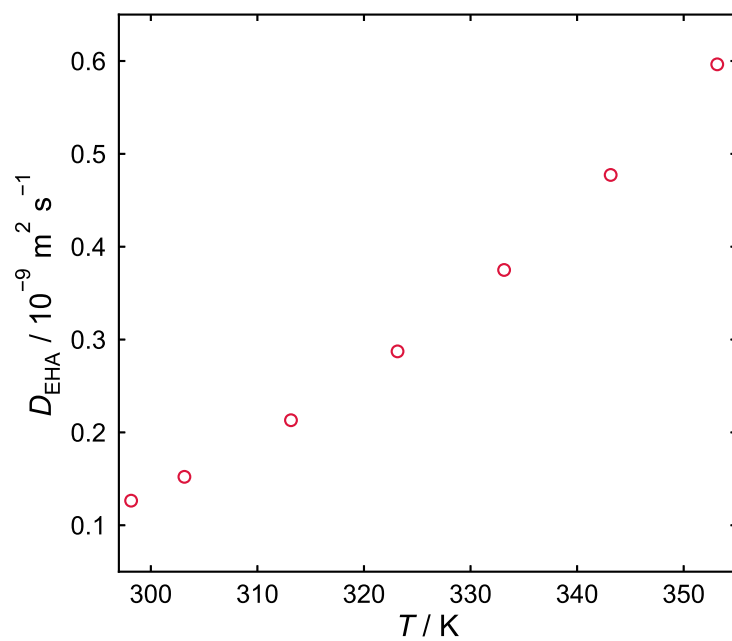


Figure S12: Self-diffusion coefficient of pure EHA at 101.3 kPa as a function of temperature. Symbols are experimental results from this work. Error bars are within symbol size.

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