Investigation of supercooled liquids

Intrigued by an inspiring question by an anonymous reviewer, we investigated how our correlation performs for supercooled liquids. Only for few substances there was sufficient experimental data at supercooled conditions available: few n-alkanes, 1-propanol and water. The experimental reduced viscosities are presented in fig. 1. Interestingly, the reduced viscosities of the five investigated substances still show a monovariable dependence on the residual entropy $s_{res}$. Though, for the self-associating substances (i.e. water and 1-propanol), viscosities at supercooled conditions show a steep increase which was not captured by our

*To whom correspondence should be addressed
correlation. For the investigated \( n \)-alkanes, we did not find that steep increase of the viscosity at supercooled conditions: experimental data align well along our correlation result.

Figure 1: Experimental viscosities of selected substances (symbols) together with the calculated viscosities (red lines) using the parameters given in Table 1 of the publication. Additionally to the data used in the publication (black symbols), we added data at supercooled conditions (blue symbols) of water, \(^1\!-\!^4\) 1-propanol\(^5\!\!^6\) and three \( n \)-alkanes.\(^7\)
References of experimental data

Table 1: Overview of investigated \( n \)-alkanes with their range of conditions and references

<table>
<thead>
<tr>
<th>Substance</th>
<th>Pressure range MPa</th>
<th>Temperature range K</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane</td>
<td>0.0007 - 1002.40</td>
<td>78.25 - 1050.00</td>
<td>8–86</td>
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<tr>
<td>Ethane</td>
<td>0.0267 - 78.45</td>
<td>100.00 - 523.15</td>
<td>9,26,39,87–94</td>
</tr>
<tr>
<td>Propane</td>
<td>0.0267 - 144.65</td>
<td>88.15 - 510.93</td>
<td>26,39,45,57,67,91,94–98</td>
</tr>
<tr>
<td>( n )-Butane</td>
<td>0.0267 - 69.17</td>
<td>140.00 - 510.93</td>
<td>26,39,99–104</td>
</tr>
<tr>
<td>( n )-Pentane</td>
<td>0.0001 - 784.53</td>
<td>293.15 - 548.15</td>
<td>26,39,99,105–113</td>
</tr>
<tr>
<td>( n )-Hexane</td>
<td>0.1000 - 500.00</td>
<td>178.15 - 623.15</td>
<td>99,104,106,114–121</td>
</tr>
<tr>
<td>( n )-Heptane</td>
<td>0.0060 - 248.88</td>
<td>185.00 - 548.15</td>
<td>112,116,122–127</td>
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<tr>
<td>( n )-Octane</td>
<td>0.0981 - 505.50</td>
<td>273.15 - 573.15</td>
<td>104,106,126,128–132</td>
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<tr>
<td>( n )-Nonane</td>
<td>0.0989 - 69.00</td>
<td>303.15 - 463.15</td>
<td>122,133</td>
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<tr>
<td>( n )-Decane</td>
<td>0.1000 - 300.00</td>
<td>288.95 - 574.50</td>
<td>26,106,134–140</td>
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<tr>
<td>( n )-Undecane</td>
<td>2.4520 - 62.42</td>
<td>292.75 - 520.15</td>
<td>122,141,142</td>
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<td>( n )-Dodecane</td>
<td>0.1000 - 501.60</td>
<td>298.15 - 473.15</td>
<td>129,143,144</td>
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<tr>
<td>( n )-Tridecane</td>
<td>0.0980 - 100.00</td>
<td>293.15 - 542.65</td>
<td>145,146</td>
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<td>( n )-Tetradecane</td>
<td>0.0980 - 60.00</td>
<td>302.65 - 524.45</td>
<td>145,147</td>
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<tr>
<td>( n )-Pentadecane</td>
<td>0.0980 - 320.00</td>
<td>303.95 - 515.75</td>
<td>143,148–150</td>
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<tr>
<td>( n )-Hexadecane</td>
<td>0.0980 - 425.10</td>
<td>318.15 - 531.95</td>
<td>119,145,151,152</td>
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<tr>
<td>( n )-Heptadecane</td>
<td>0.0980 - 49.15</td>
<td>324.65 - 522.65</td>
<td>141,142,153</td>
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<td>0.1000 - 360.00</td>
<td>319.85 - 507.15</td>
<td>142–144,154</td>
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<td>350.45 - 534.25</td>
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<td>0.0980 - 49.00</td>
<td>353.15 - 496.65</td>
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<td>( n )-Docosane</td>
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<td>353.05 - 510.65</td>
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<td>( n )-Tricosane</td>
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<td>( n )-Tetracosane</td>
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<td>156,158–161</td>
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<tr>
<td>( n )-Octacosane</td>
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<td>323.15 - 573.81</td>
<td>25,156,162</td>
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<tr>
<td>( n )-Triacanone</td>
<td>0.1000 - 0.10</td>
<td>343.15 - 363.15</td>
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<tr>
<td>( n )-Hexatriacanone</td>
<td>0.1000 - 0.10</td>
<td>340.55 - 363.15</td>
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<tr>
<td>( n )-Dotriacontane</td>
<td>0.3000 - 0.30</td>
<td>354.11 - 466.30</td>
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</tr>
<tr>
<td>( n )-Tetriacontane</td>
<td>0.1000 - 0.10</td>
<td>353.15 - 363.15</td>
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<tr>
<td>( n )-Pentatriacontane</td>
<td>0.1000 - 0.10</td>
<td>353.15 - 579.15</td>
<td>156,160</td>
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<td>( n )-Hexatriacontane</td>
<td>0.1000 - 0.10</td>
<td>348.15 - 573.54</td>
<td>25,156,162,164</td>
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<tr>
<td>Substance</td>
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<td>temperature range K</td>
<td>Reference</td>
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<td>15,111,169–171</td>
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<td>298.15 - 485.65</td>
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<td>303.15 - 351.15</td>
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<td>313.15 - 313.15</td>
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<td>3-Ethylpentane</td>
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<td>2,2,4-Trimethylpentane</td>
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<td>197.93 - 548.15</td>
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<td>158.15 - 473.15</td>
<td>169,190,197–199</td>
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<td>0.0980 - 245.16</td>
<td>298.15 - 473.70</td>
<td>198,200</td>
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<td>1-Octene</td>
<td>0.0980 - 245.16</td>
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<td>1-Nonene</td>
<td>0.1000 - 50.00</td>
<td>203.00 - 473.00</td>
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<td>1-Decene</td>
<td>0.0990 - 245.16</td>
<td>298.15 - 475.02</td>
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<td>Benzene</td>
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<td>283.15 - 673.15</td>
<td>108,120,147,169,171,174,196,203–237</td>
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<td>Ethylbenzene</td>
<td>0.1000 - 195.00</td>
<td>288.15 - 673.15</td>
<td>136,216,227,234,262–268</td>
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<td>1,3-Dimethylbenzene</td>
<td>0.0981 - 784.53</td>
<td>295.36 - 673.15</td>
<td>132,171,186,216,227,229,230,263,267–273</td>
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<td>1,4-Dimethylbenzene</td>
<td>0.0160 - 196.13</td>
<td>293.15 - 673.15</td>
<td>140,171,186,216,227,229,230,263,266–268,271–277</td>
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<td>p-Cymene</td>
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<td>293.15 - 348.15</td>
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<tr>
<td>n-Heptylbenzene</td>
<td>0.1000 - 100.00</td>
<td>293.15 - 353.15</td>
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<tr>
<td>n-Nonylbenzene</td>
<td>0.1000 - 40.00</td>
<td>731.15 - 353.15</td>
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<tr>
<td>n-Dodecylbenzene</td>
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<td>298.15 - 363.15</td>
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<td>Cycloalkanes</td>
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<tr>
<td>Cyclopentane</td>
<td>0.0093 - 400.00</td>
<td>218.74 - 449.10</td>
<td>169,176,247,281–286</td>
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<td>Cyclohexane</td>
<td>0.0027 - 210.00</td>
<td>279.85 - 673.15</td>
<td>108,118,120,151,152,171,171,210,212,220–222,225–228,232,243,247–297</td>
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<td>Ester</td>
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<tr>
<td>n-Propyl acetate</td>
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<td>297.46 - 494.16</td>
<td>298,300</td>
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<tr>
<td>n-Butyl acetate</td>
<td>0.0990 - 49.00</td>
<td>289.86 - 492.46</td>
<td>298,301–304</td>
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<td>Isopentyl acetate</td>
<td>0.1000 - 50.10</td>
<td>292.30 - 461.50</td>
<td>305,306</td>
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<td>Ethyl acetate</td>
<td>50.0000 - 195.00</td>
<td>298.15 - 373.15</td>
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<tr>
<td>n-Pentyl acetate</td>
<td>0.1000 - 50.10</td>
<td>300.20 - 502.90</td>
<td>305,306</td>
</tr>
<tr>
<td>n-Heptyl acetate</td>
<td>0.1000 - 50.10</td>
<td>300.50 - 491.30</td>
<td>305,306</td>
</tr>
</tbody>
</table>
Table 3: Overview of investigated non-\textit{n}-alkanes with their range of conditions and references, part 2

<table>
<thead>
<tr>
<th>Substance</th>
<th>Pressure range (MPa)</th>
<th>Temperature range (K)</th>
<th>Reference</th>
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<tbody>
<tr>
<td>Ether</td>
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<td>Dimethyl ether</td>
<td>0.1010 - 30.00</td>
<td>253.15 - 423.15</td>
<td>308,309</td>
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<tr>
<td>Dibutyl ether</td>
<td>0.1000 - 21.12</td>
<td>243.15 - 373.15</td>
<td>310 - 313</td>
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<tr>
<td>Methyl-tert-butyl ether</td>
<td>0.1000 - 0.10</td>
<td>293.15 - 308.15</td>
<td>173,314,315</td>
</tr>
<tr>
<td>Dipentyl ether</td>
<td>0.0981 - 1176.80</td>
<td>303.15 - 348.15</td>
<td>171</td>
</tr>
<tr>
<td>Diisopropyl ether</td>
<td>0.1010 - 58.86</td>
<td>293.00 - 513.00</td>
<td>316</td>
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<tr>
<td>Acetone</td>
<td>0.00027 - 0.10</td>
<td>273.25 - 350.95</td>
<td>221,317</td>
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<tr>
<td>3-Pentanone</td>
<td>0.1000 - 0.160.00</td>
<td>293.00 - 473.15</td>
<td>332</td>
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<tr>
<td>Methyl-Isobutyl-ketone</td>
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<td>273.15 - 473.15</td>
<td>332</td>
</tr>
<tr>
<td>2-Hexanone</td>
<td>0.0980 - 0.156.80</td>
<td>293.15 - 473.15</td>
<td>334</td>
</tr>
<tr>
<td>2-Octanone</td>
<td>0.0981 - 0.160.00</td>
<td>293.15 - 473.15</td>
<td>324,335</td>
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<td>202.45 - 673.00</td>
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<td>278.15 - 382.05</td>
<td>317,341 - 346</td>
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<td>317,341,347 - 363</td>
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<td>Propylamine</td>
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<td>283.15 - 318.15</td>
<td>341 - 346,355,362 - 373</td>
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<td>Butylamine</td>
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<td>291,341,343 - 346,355,362,363,366 - 406</td>
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<td>Pentylamine</td>
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<td>278.15 - 353.15</td>
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<td>341,388,408</td>
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<td>278.15 - 423.15</td>
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<td>341,367,368,383,388</td>
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<td>341,367,368,383,388</td>
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<td>1-Alcohols</td>
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<td>1-Propanol</td>
<td>0.0981 - 1176.80</td>
<td>273.15 - 423.00</td>
<td>116,171,228,283,287,302,303,311,315,364,376,463,473,554,578,595,615,623,629,686,701,702,706,707,730 - 738</td>
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<td>1-Butanone</td>
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<td>203.15 - 473.15</td>
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<td>1-Octanole</td>
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<td>343.15 - 423.15</td>
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References


   **1939**, 9, 1078 – 1080.


105. Grigorev, B.; Keramidi, A.; Prisyazhnyuk, S.


142. Naziev, Y.; Guseinov, S.


150. Arkhipov, V.


190. Naziev, Y.; Gusejnov, S.; Akhmedov, A. Untersuchung der Viskosität von einigen


198. Fomina, M.; Sagdeev, D.; Mukhamedzyanov, G.


202. Fomina, M.; Sagdeev, D.; Mukhamedzyanova, G.


30


251. Kandil, M.; Marsh, K.; Goodwin, A. Vibrating Wire Viscometer with Wire Diameters of (0.05 and 0.15) mm: Results for Methylbenzene and Two Fluids with Nominal Viscosities at T = 298 K and p = 0.01 MPa of (14 and 232) mPas at Temperatures


321. Mamedov, I. A.


351. Lutskii, A. E.; Obukhova, E. M.; Sidorov, I. A. Properties of Binary Mixtures of Organic


357. Guseinov, S. O.; Movsumov, T. G.; Naziev, Y. M.


of Propylene Carbonate with Tetrahydrofuran and Methanol at Different Temperatures. 


462. Pal, A.; Dass, G. Excess Molar Volumes and Viscosities for Binary Liquid Mixtures of


478. Pikkarainen, L. Thermodynamic and Physicochemical Properties of Binary Solvent


525. Gill, D. Evaluation of Single-Ion Conductances in Nonaqueous Solvents at 25C by the


569. Rodriguez, A.; Canosa, J.; Tojo, J. Dynamic Viscosities of the Ternary Liquid Mixture Involving CH\textsubscript{3}COOCH\textsubscript{3}, CH\textsubscript{3}OH, and CH\textsubscript{3}CH\textsubscript{2}CH\textsubscript{2}OH at T = 298.15 K. *J.Chem.Thermodyn.* **1998**, *30*, 1307 – 1318.


572. Hughes, O.; Hartley, H. The Effect of Small Water Additions Upon the Conductivity


578. Mamedov, I. A.; Aliev, A. A.


607. Rao, K.; Rao, S. Viscosities of Binary Liquid Mixtures of Formic Acid with Water,


615. Gonzalez, E. J.; Anlonso, L.; Domnguez, A. Physical Properties of Binary Mixtures of the Ionic Liquid 1-Methyl-3-octylimidazolium Chloride with Methanol, Ethanol, and
1-Propanol at $T = (298.15, 313.15, \text{and } 328.15) \, \text{K}$ and at $P = 0.1 \, \text{MPa}$. *J. Chem. Eng. Data* **2006**, *51*, 1446–1452.


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689. Brahman, D.; Sinha, B. Partial Molar Volumes and Viscosity B-Coefficients of N,N’-Ethylene-bis(salicylideneiminato)cobalt(II) in Binary Mixtures of 1,4-Dioxane +


736. Maximino, R. B. Viscosity and density of binary mixtures of alcohols and polyols with


