Supporting Information

Insights into the Limitations of Parameter Transferability in Heteronuclear SAFT-type Equations of State

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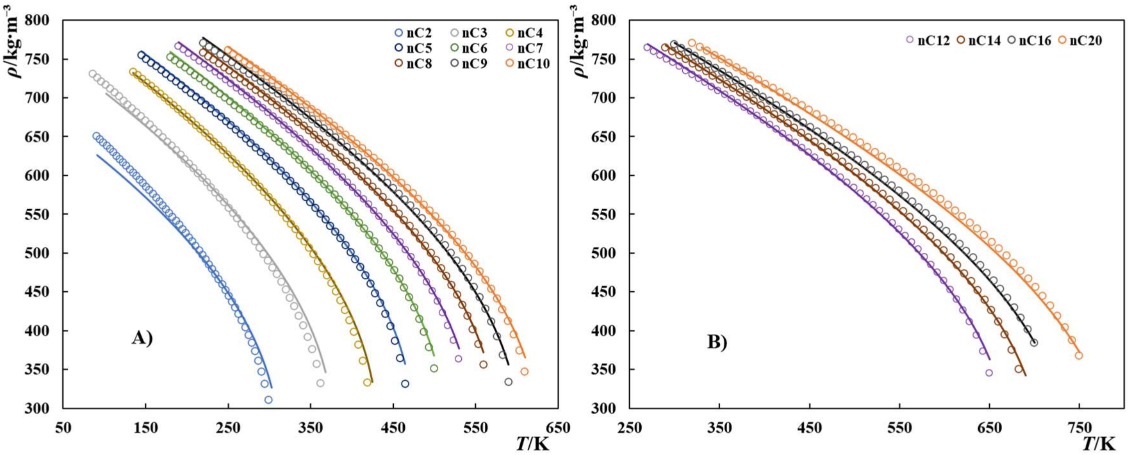


Figure S1. Saturated liquid density of linear alkanes. A) from ethane no n-decane (fitting) B) from n-dodecane to n-eicosane (predicted). Symbols represent experimental data from the DIPPR database[1] while the solid lines depict the SAFT-γ-Mie results.

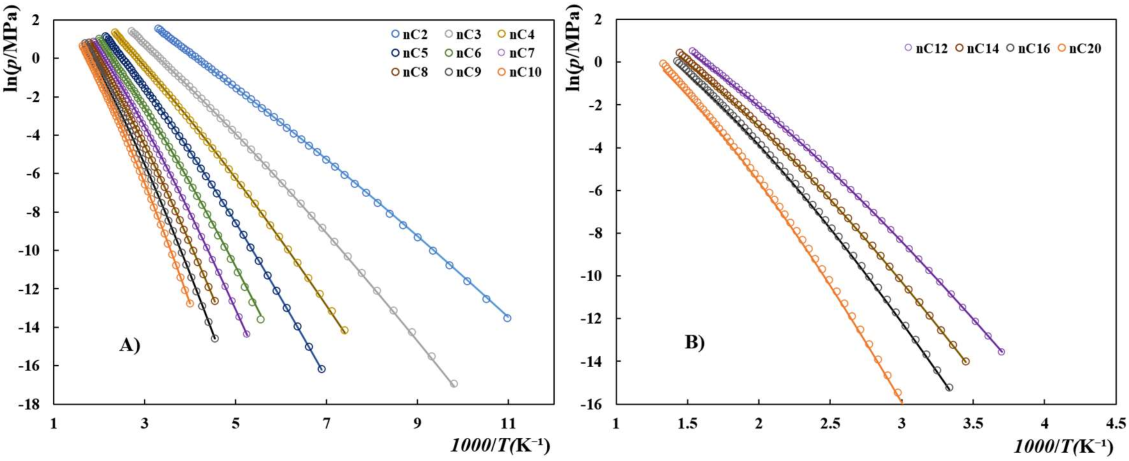


Figure S2. Vapor pressures of linear alkanes. A) from ethane to n-decane (fitting) B) from n-dodecane to n-eicosane (predicted). Symbols represent experimental data from the DIPPR database[1] while the solid lines depict the SAFT-γ-Mie results.

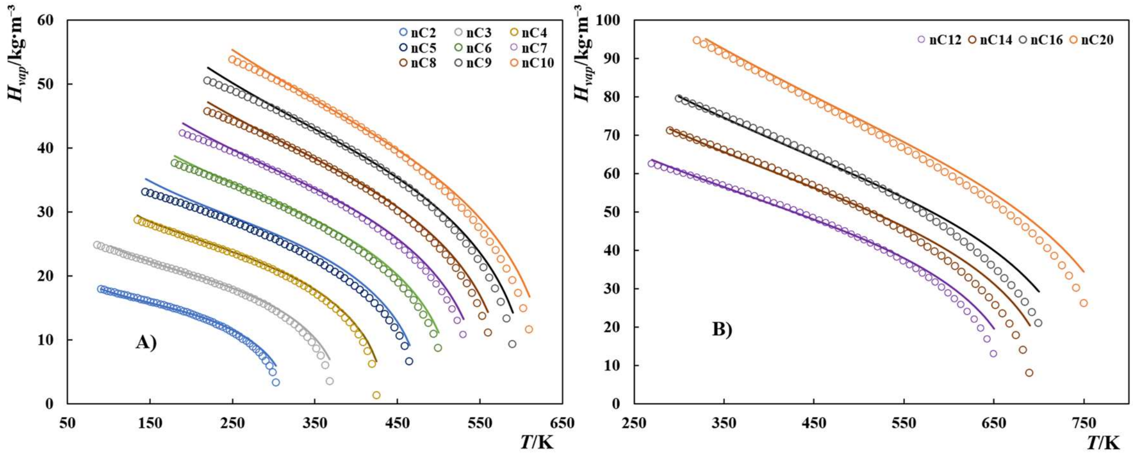


Figure S3. Enthalpies of vaporization of linear alkanes. A) from ethane to n-decane (fitting); B) from n-dodecane to n-eicosane (predicted). Symbols represent experimental data from the DIPPR database[1] while the solid lines depict the SAFT-γ-Mie results.

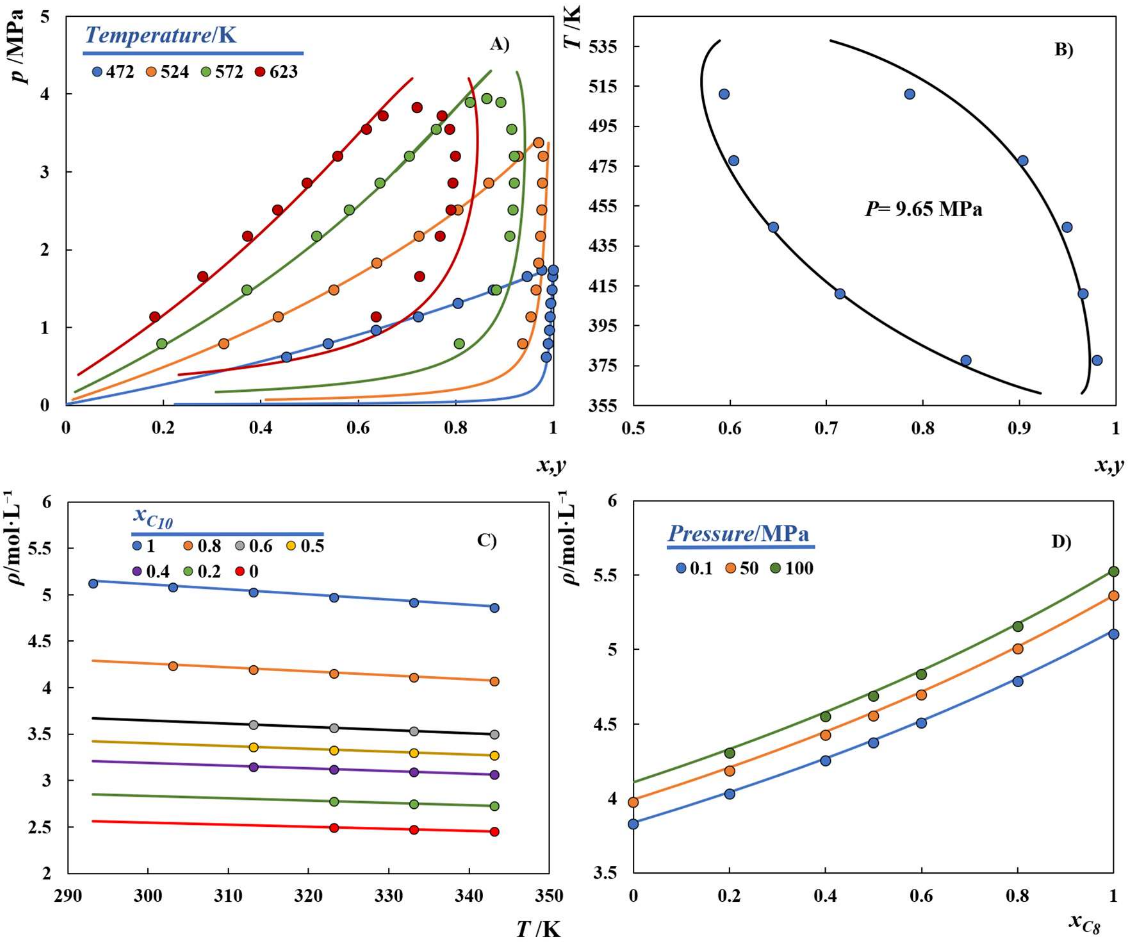


Figure S4. A) Isobaric VLE of n-hexane + n-hexadecane; B) Isothermal VLE of ethane + n-decane; C) Atmospheric liquid densities of n-decane + n-C22; D) High-pressure liquid densities of n-octane + n-dodecane.

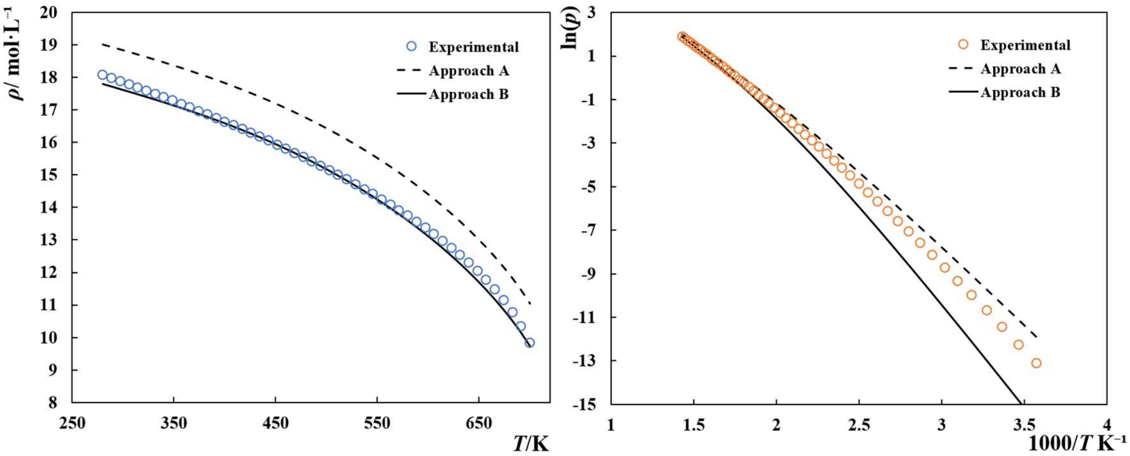


Figure S5. Saturation liquid densities and vapor pressures of pure ethylene glycol. Symbols represent experimental data[1] while the dashed and solid lines represent the SAFT-γ-Mie results following approach A and approach B, respectively.

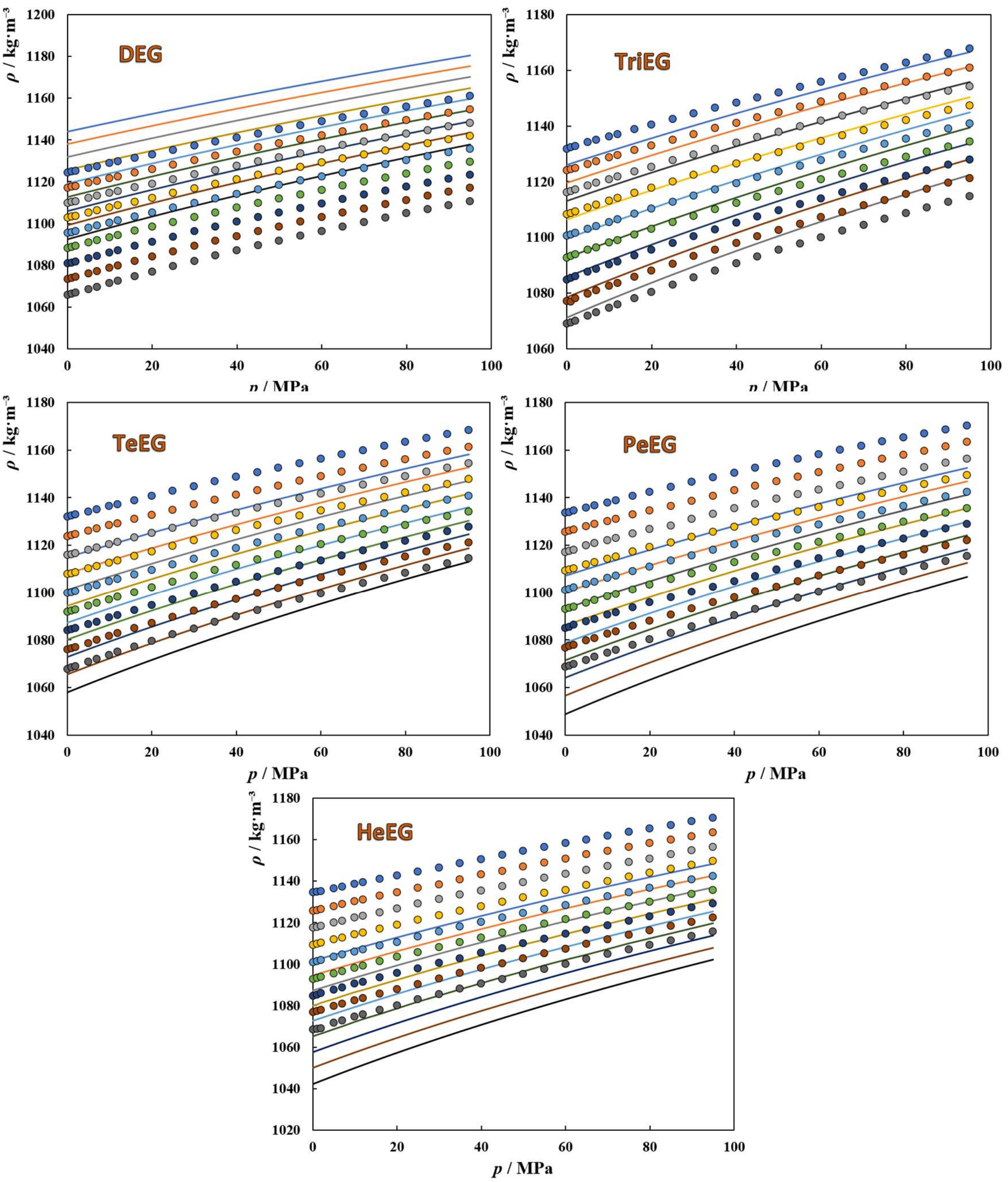
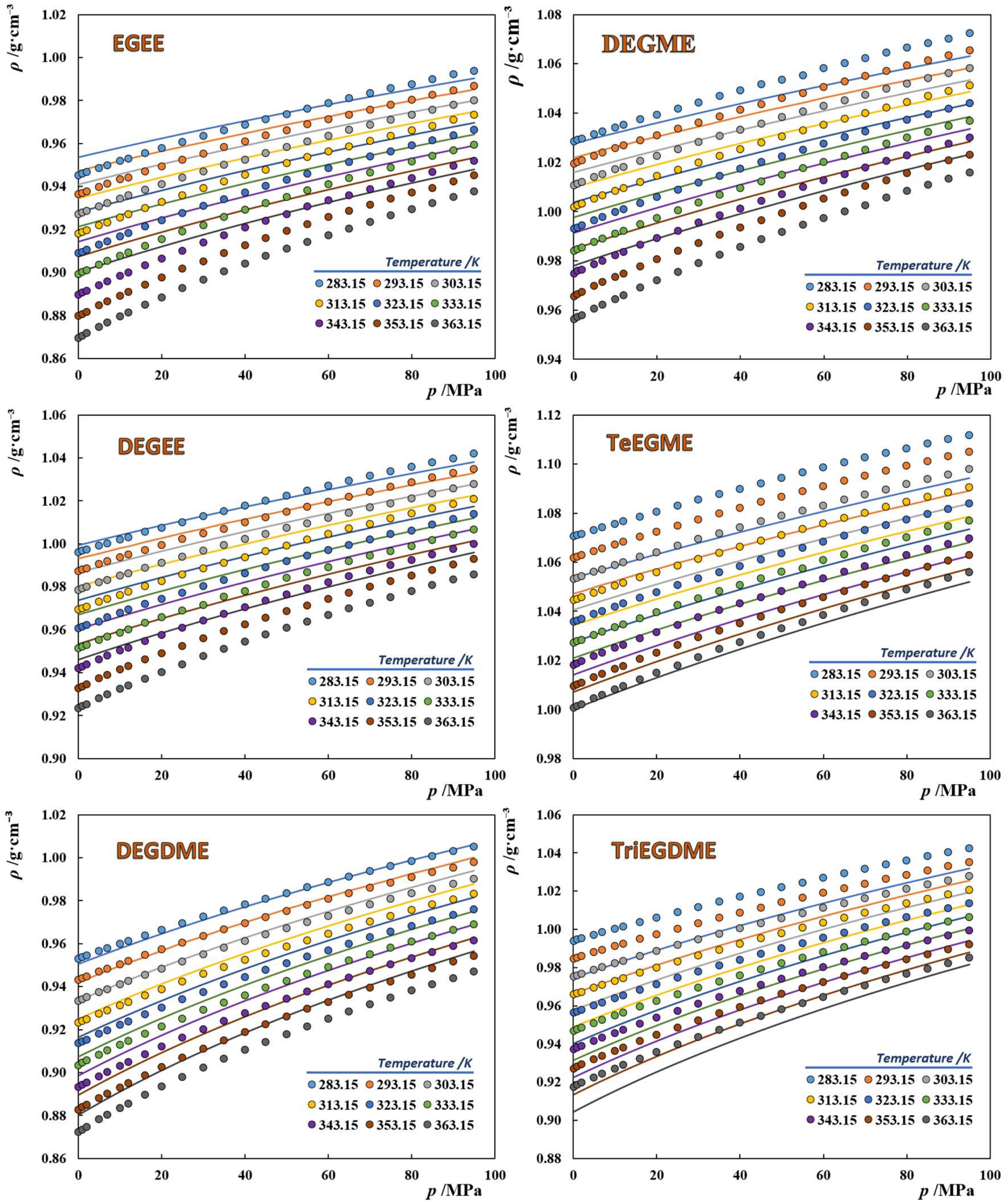


Figure S6. High-pressure liquid densities of pure glycols. Symbols represent experimental data[2] while the solid lines represent the SAFT-γ-Mie results following approach A.


EGEE
DEGME
DEGEE
TeEGME
DEGDME
TriEGDME
Temperature /K
283.15
293.15
303.15
313.15
323.15
333.15
343.15
353.15
363.15
ρ /g·cm^{-3}
p /MPa

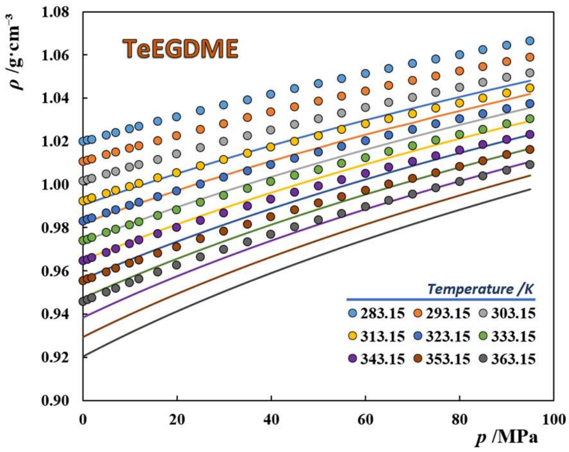
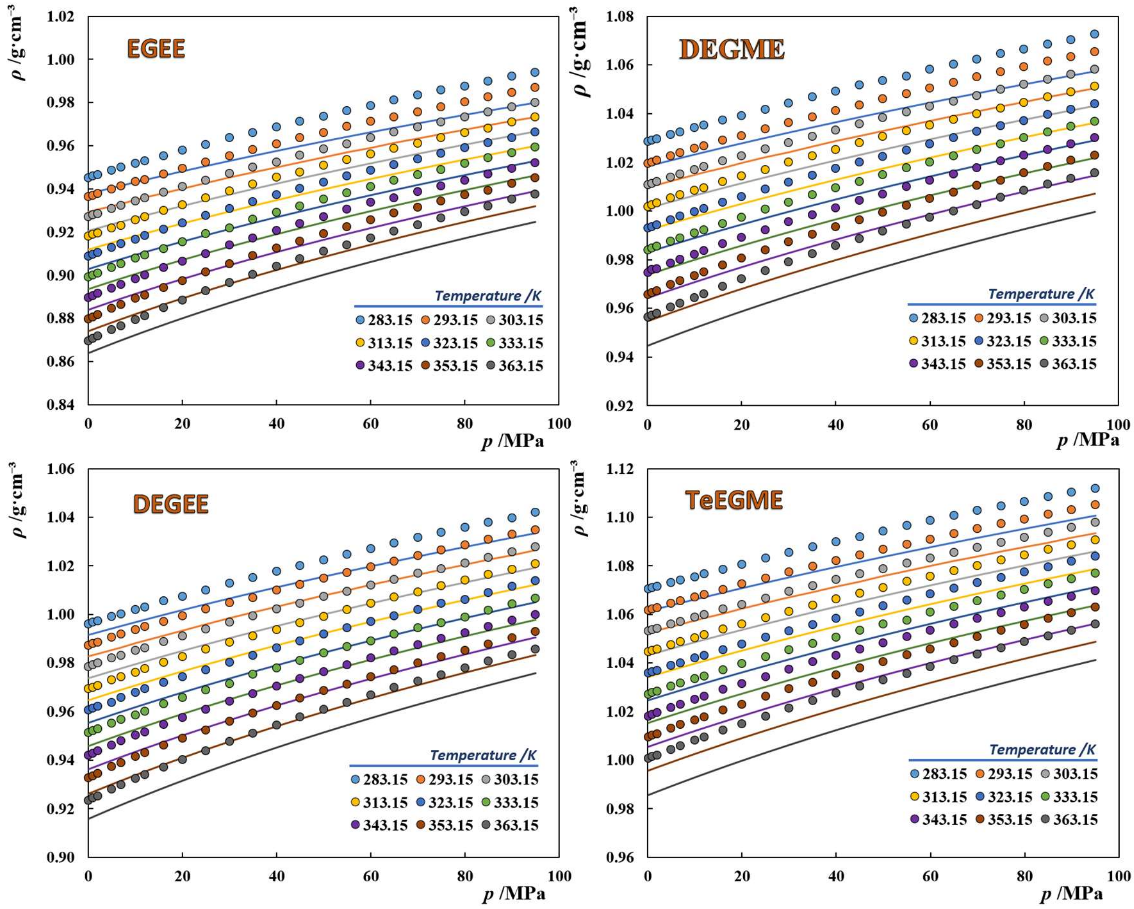


Figure S7. High-pressure liquid densities of pure glymes. Symbols represent experimental data[3] while the solid lines depict the SAFT-γ-Mie results, following approach A.



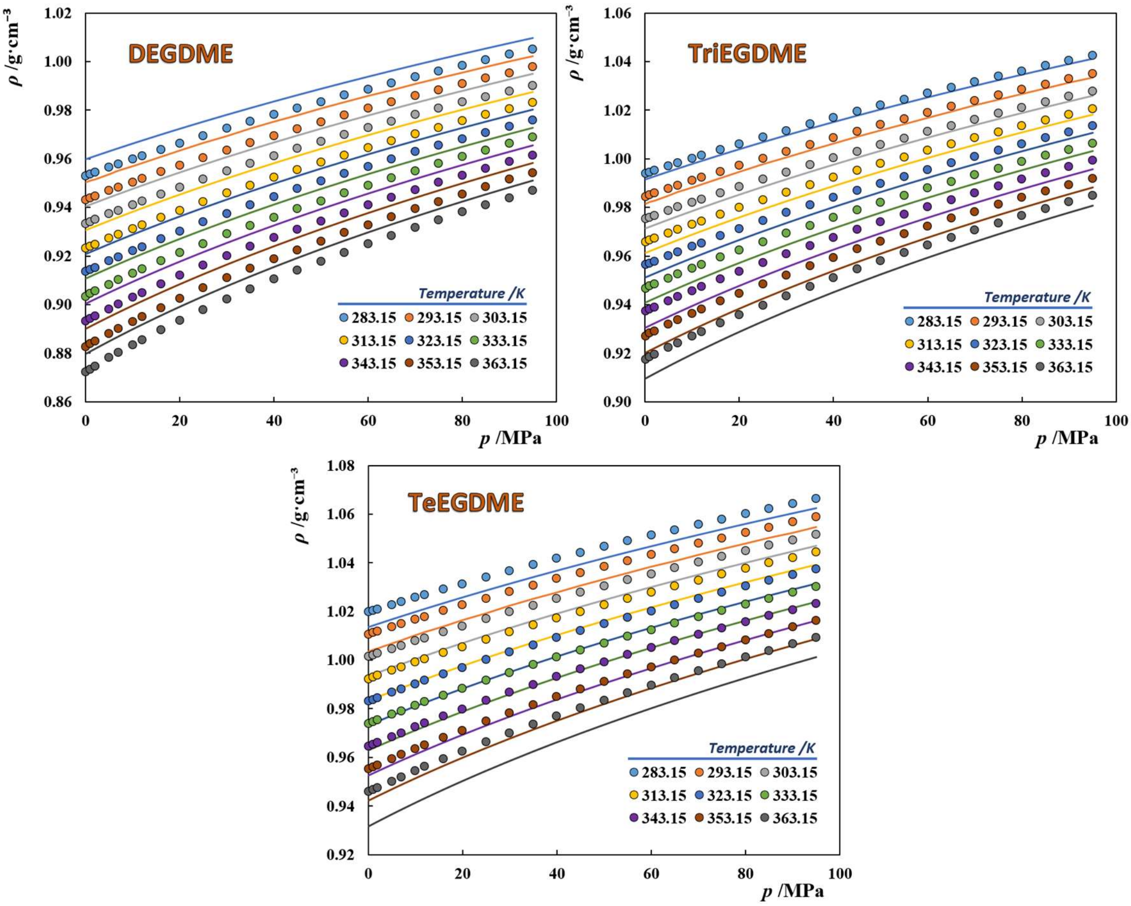


Figure S8. High-pressure liquid densities of pure glymes. Symbols represent experimental data[3] while the solid lines depict the SAFT-γ-Mie results following approach G.

References

(1) Daubert, T. E.; Sibul, H. M.; Stebbins, C. C.; Danner, R. P.; Rowley, R. L.; Adams, M. E.; Wilding, W. V; Marshall, T. L. *Physical and Thermodynamic Properties of Pure Chemicals: DIPPR: Data Compilation: Core + Supplements 1-10*; Taylor & Francis, 2000.

(2) Crespo, E. A.; Silva, L. P.; Martins, M. A. R.; Fernandez, L.; Ortega, J.; Ferreira, O.; Sadowski, G.; Held, C.; Pinho, S. P.; Coutinho, J. A. P. Characterization and Modeling of the Liquid Phase of Deep Eutectic Solvents Based on Fatty Acids/Alcohols and Choline Chloride. *Ind. Eng. Chem. Res.* **2017**, *56*, 12192–12202.

(3) Navarro, P.; Crespo, E.; Costa, J. J. M. L.; Llovell, F.; Garcia, J.; Rodríguez, F.; Carvalho, P. P. J.; Vega, L. L. F.; Coutinho, J. J. A. P.; García, J.; et al. New Experimental Data and Modeling of Glymes: Toward the Development of a Predictive Model for Polyethers. *Ind. Eng. Chem. Res.* **2017**, *56*, 7830–7844.