

## Transferable Molecular Models for the Calculation of Thermodynamic and Transport Properties of Common Hydrofluorocarbon Refrigerants and New Alternative Blends with the Soft-SAFT Equation

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Hydrofluorocarbons (HFCs) have become common refrigerants in the last decade, replacing the classical chlorinated compounds (CFCs and HCFCs), once it was shown that the latter were a major source of inorganic chlorine in the stratosphere and destroyers of the ozone layer. The characterization and optimization of the thermodynamic and transport properties of refrigerants represent a key part of both theoretical and experimental work before they are put into their final use. In this work, we present a thermophysical characterization of the most common HFCs using the statistical mechanics-based soft-SAFT equation of state (EoS), including phase equilibria, interfacial tensions and derivative properties. An appropriate molecular model is proposed for the different refrigerants, looking for the transferability of the molecular parameters. Several correlations with the molecular weight and the number of carbons are proposed, in order to be able to predict the properties of other HFCs. The interfacial tension of these compounds is obtained using the soft-SAFT EoS with the Density Gradient Theory approach (DGT). Prediction of derivative properties is also included, with good agreement with experimental data. Finally, the Free Volume Theory has been coupled into soft-SAFT for the calculation of the viscosities of the different refrigerants in the range of industrial interest. Once the pure compounds have been well characterized, the vapor-liquid equilibrium of several mixtures of refrigerants between them and with carbon dioxide and alkanes are revised. Finally, the thermodynamics of some new blends of refrigerants combining a hydrofluorocarbon and an ionic liquid for absorption processes are modeled and described in good agreement with the available data.

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