A set of complete thermodynamic models for hydrofluoro- and hydrochlorofluoroolefins

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The hydrofluoroolefins add-on in FluidProp contains a consistent set of complete thermodynamic models for four hydrofluoroolefins and one hydrochlorofluoroolefin. The thermodynamic models are based on both the iPRSV and the PCP-SAFT equation of state and can therefore be used in the (free)StanMix and PCP-SAFT libraries in FluidProp. Table 1 contains an overview of the available hydrofluoroolefins in FluidProp.

Table 1: Available fluids in the hydrofluoroolefins family of FluidProp

FluidProp name	**IUPAC name**	**CAS Nr.**	**Chemical formula**
HCFO-1233zd-E	trans-1-chloro-3,3,3-trifluoro-1-propene	102687-65-0	CF_3-CH=CHCl
HFO-1234yf	2,3,3,3-tetrafluoro-1-propene	754-12-1	CF_3-CF=CH_2
HFO-1234ze-E	trans-1,3,3,3-tetrafluoro-1-propene	29118-24-9	CF_3-CH=CHF
HFO-1243zf	3,3,3-trifluoropropene	677-21-4	CF_3-CH=CH_2
HFO-1336mzz-Z	cis-1,1,1,4,4,4-hexafluoro-2-butene	692-49-9	CF_3-CH=CH-CF_3

The PCP-SAFT based models were fitted to experimental, measured, saturated liquid density and vapor pressure data from literature listed in table 3. The iPRSV based models were just fitted to the same vapor pressure data as the PCP-SAFT based models. Data generated from molecularly simulations were employed where experimental data were not available, see table 3.

Table 2 lists deviations with experimental data for the PCP-SAFT based and iPRSV based models, respectively. Note that, as it is customary for cubic equations of state, the deviations of thermodynamic properties are much larger for the liquid state. Because freeStanMix is based on the PRSV equation of state and StanMix on the iPRSV equation of state, deviations between experimental data and freeStanMix can slightly differ from deviations between experimental data and StanMix.

*Table 2: Average (AAD%) and maximum (MAD%) absolute deviations between **PCP-SAFT/iPRSV** and experimental data*

FluidProp name	ΔP^{sat} AAD%	ΔP^{sat} MAD%	$\Delta \rho^{sat,liq}$ AAD%	$\Delta \rho^{sat,liq}$ MAD%
HCFO-1233zd-E	0.65/0.76	2.50/2.44	0.09/2.30	0.31/2.86
HFO-1234yf	0.15/0.36	2.24/2.64	0.45/8.43	1.17/19.8
HFO-1234ze-E	0.16/0.66	1.51/1.80	0.69/7.68	1.82/16.7
HFO-1243zf	0.48/0.72	3.22/3.63	0.31/2.79	2.10/10.2
HFO-1336mzz-Z	2.53/2.75	5.74/6.17	0.22/3.93	0.44/5.43

Table 3: Literature references

Fluid	**Literature references**
HCFO-1233zd-E	- R.J. Hulse, R.S. Basu, R.R. Singh, and R.H.P. Thomas, Physical Properties of HCFO-1233zd(E), J. Chem. Eng. Data 57 (2012) 3581−3586. - M.E. Mondéjar, M.O. McLinden, and E.W. Lemmon, Thermodynamic Properties of trans-1-Chloro-3,3,3-trifluoropropene (R1233zd(E))- Vapor Pressure, (p, ρ, T) Behavior, and Speed of Sound Measurements, and Equation of State, J. Chem. Eng. Data 60 (2015) 2477−2489. - G. Raabe, Molecular Simulation Studies on the Vapor−Liquid Equilibria of the cis- and trans-HCFO-1233zd and the cis- and trans-HFO-1336mzz, J. Chem. Eng. Data 60 (2015) 2412−2419.
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HFO-1234ze-E	- M.O. McLinden, M. Thol, E.W. Lemmon, Thermodynamic Properties of trans-1,3,3,3-tetrafluoropropene [R1234ze(E)]: Measurements of Density and Vapor Pressure and a Comprehensive Equation of State, International Refrigeration and Air Conditioning Conference at Purdue, July 12-15, 2010. - Y. Higashi and K. Tanaka, Critical parameters and saturated densities in the critical region for trans -1,3,3,3-Tetrafluoropropene (HFO-1234ze(E)), J. Chem. Eng. Data 55 (2010) 1594–1597. - K. Tanaka, G. Takahashi, and Y. Higashi,, Measurements of the Vapor Pressures and pρT Properties for trans-1,3,3,3-Tetrafluoropropene (HFO-1234ze(E)), J. Chem. Eng. Data 55 (2010) 2169–2172. - G. Di Nicola, J.S. Brown, L. Fedele, S. Bobbo, C. Zilio, Saturated Pressure Measurements of trans-1,3,3,3-Tetrafluoroprop-1-ene (R1234ze(E)) for Reduced Temperatures Ranging from 0.58 to 0.92, J. Chem. Eng. Data 57 (2012) 2197−2202.
HFO-1243zf	- T.E.Daubert, , Jalowka, J.W., Goren, V., "Vapor Pressure of 22 Pure Industrial Chemicals, " AIChE Symposium Series, 83, 256, 128 (1987) (DIPPR), - Material Safety data Sheet for 3,3,3-Trifluoropropene, Great Lakes Chemical Corporation (2002) (DIPPR) - J.S. Brown, G. Di Nicola, L. Fedele, S. Bobbo, C. Zilio, Saturated pressure measurements of 3,3,3-trifluoroprop-1-ene (R1243zf) for reduced temperatures ranging from 0.62 to 0.98, Fluid Phase Equilibria 351 (2013) 48–52. - N.A. Lai, Thermodynamic properties of HFO-1243zf and their application in study on a refrigeration cycle, Applied Thermal Engineering 70 (2014) 1-6 (where saturated liquid densities where retrieved by using an ancillary equation fitted to data in G. Di Nicola, J.S. Brown, L. Fedele, M. Securo, S. Bobbo, C. Zilio, Subcooled liquid density measurements and PvT measurements in the vapor phase for 3,3,3-trifluoroprop-1-ene (R1243zf), Int.J. Refrig. 36 (2013) 2209-2215). - C. Kondou, R. Nagata, N. Nii, S. Koyama, Y. Higashi, Surface tension of low GWP refrigerants R1243zf, R1234ze(Z), and R1233zd(E), Int.J. Refrig. 53 (2015) 80-89.
HFO-1336mzz-Z	- G. Raabe, Molecular Simulation Studies on the Vapor−Liquid Equilibria of the cis- and trans-HCFO-1233zd and the cis- and trans-HFO-1336mzz, J. Chem. Eng. Data 60 (2015) 2412−2419.