Supporting Information

Purely Predictive Vapor-Liquid-Equilibrium Properties of 3,3,4,4,4-pentafluoro-1-butene (HFO-1345fz), 2,3,3,4,4,4-hexafluoro-1-butene (HFO-1336yf) and trans-1-chloro-2,3,3,3-tetrafluoropropene (HCFO-1224yd(E)) from Molecular Simulation

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Supplementary material – Force Field parameters

Table 1 Intramolecular Force field parameters for HFO-1345fz, HFO-1336yf, and HCFO-1224yd(E)

Force	force constant		
Bond	k_r (kJ mol^{-1} Å^{-2})	r_0 (Å)	
CM=CM	2831.69	1.331	
CM-CT	1328.84	1.511	
CT-CT	1328.84	1.545	
CT-F	1544.61	1.353	
CM-HC, CM-H1	1627.07	1.086	
CM-F	1864.73	1.330	
CM-Cl	953.8	1.734	
Angle	k_θ (kJ mol^{-1} rad^{-2})	θ_0 (deg)	
HC-CM=CM H1-CM=CM	152.09	120.6	
F-CT-F	367.61	107.5	
CM-CT-F	313.17	111.3	
HC-CM-CT	135.27	115.1	
HC-CM-HC	122.63	118.7	

CM=CM-F	211.38	122.6	
F-CM-CT	319.57	112.5	
CM=CM-CT	209.70	124.1	
Cl-CM=CM	280.8	122.9	
Cl-CM-H1	152.6	113.8	
CM-CT-CT	311.15	114.2	
F-CT-CT	313.17	109.5	
Dihedral	k_χ	n	δ (deg)
X-CM=CM-X	27.84	1/2	0/180
HC-CM-CT-F	0.745	3	0
F^-CM-CT-F	1.0445	3	0
CM=CM-CT-F	0.5951	3	180
F-CT-CT-F	1.0445	3	0

Table 2 Additional dihedral parameters for HFO-1345fz, HFO-1336yf

Dihedral	A_0 /kJ mol^{-1}	A_1 /kJ mol^{-1}	A_2/kJ mol^{-1}	A_3/kJ mol^{-1}
CM=CM-CT-CT	3.330	-2.878	-0.933	0.060
F-CM-CT-CT	6.124	-6.228	1.438	-0.005
CM-CT-CT-F	0.046	-0.013	0.052	-2.063
HC-CM-CT-CT	6.406	-3.376	-1.112	1.055

Table 3 Lennard Jones Parameters for the atom types in HFO-1345fz, HFO-1336yf, and HCFO-1224yd(E)

atom types	ε (kJ mol^{-1})	σ (Å)
CM	0.41000	3.40
CT	0.31091	3.40
F (HFO-1234fz)	0.22526	2.92
F (HFO-1336yf)	0.22215	2.92
F (HCFO-1224yd(E/Z))	0.22475	2.93
Cl	1.09086	3.525
HC	0.06570	2.65
H1	0.06570	2.47