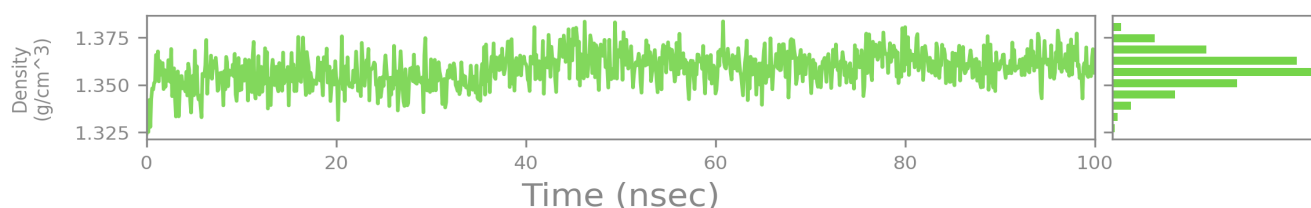


Bulk Properties

	Volume Angstrom^3	Density g/cm^3	Cohesive E kcal/mol	Solubility Parameter MPa^(1/2)	Solubility Parameter Vdw MPa^(1/2)	Solubility Parameter Ele MPa^(1/2)	Heat of Vap. kcal/mol	Specific Heat Capacity (Cp) J / (g * K)
Average:	27652.33	1.36	34.73	23.63	19.79	12.91	35.33	2.31
Stdev:	140.423	0.007	0.295	0.138	0.116	0.164	0.295	N/A

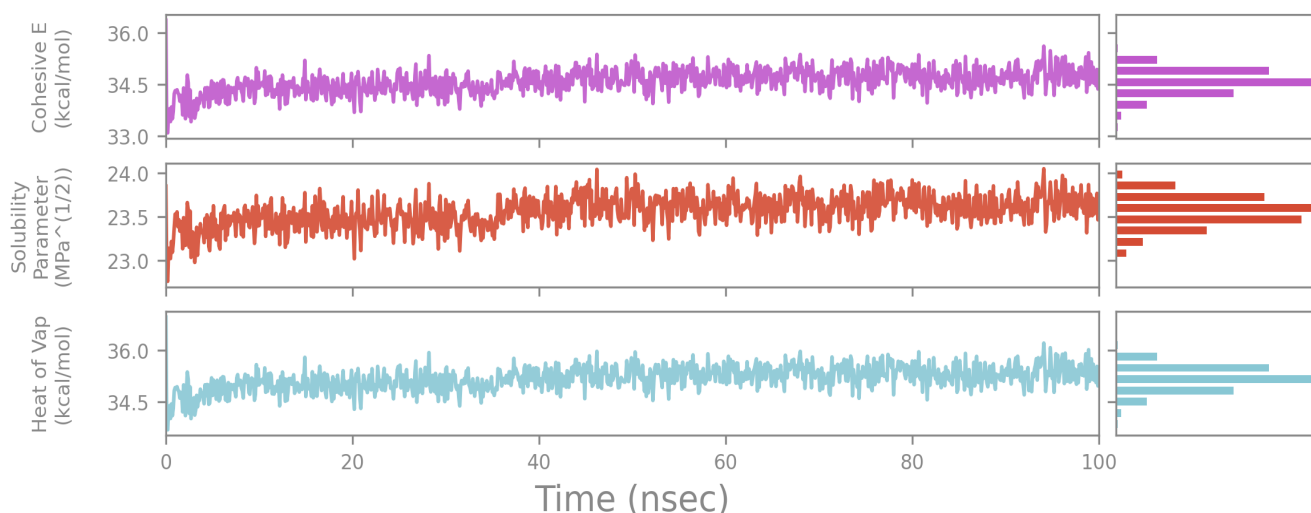
Note: Statistics reported are for the final 20% of the simulation.



Density is a fundamental structural parameter that can be compared directly to experiment. Density (ρ) is defined as mass, m , per unit volume:

$$\rho = m/V$$

Density is expressed in g/cm³, and is computed for each frame over the course of the trajectory. Inspection of the convergence of density gives important feedback on the degree of system convergence. With the OPLS force fields, the fully equilibrated density can be computed to within 3% of experimental values.



The heat of vaporization and Hildebrand solubility parameter are closely related properties. The solubility parameter is useful for estimating the miscibility of various components being considered for applications requiring multicomponent mixtures. The solubility parameter (δ) for a pure liquid is defined as

$$\delta = [(\Delta H_v - RT)/V_m]^{1/2}$$

where ΔH_v is the heat of vaporization and V_m is the molar volume. RT is the ideal gas PV term. The heat of vaporization, ΔH_v , is measured in kcal/mol and is calculated from the energy of periodic unit cell minus the sum of the N individual molecules, E_i , averaged over the MD trajectory.

$$\Delta H_{vap} = \langle |E_{cell} - \sum_{i=1}^N E_i| \rangle + RT$$