MM: openff-1.0.0

(N = 37)RMSE: 1.50 [95%: 1.23, 1.81] MUE: 1.19 [95%: 0.94, 1.54] Calculated  $\Delta \Delta$  G / kcal mol $^{-1}$ 2 0 -2.50.0 2.5

Experimental  $\Delta\Delta$  G / kcal mol<sup>-1</sup>