MM: openff-1.0.0

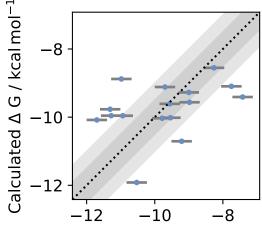
(N = 16)

RMSE: 1.20 [95%: 0.91, 1.53]

MUE: 1.02 [95%: 0.72, 1.38]

R2: 0.14 [95%: 0.00, 0.51]

rho: 0.37 [95%: -0.02, 0.68]



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