

SMIRNOFF99Frosst ΔG (kcal/mol)

RMSE = 1.90 [1.69, 2.11]
 $R^2 = 0.46$ [0.28, 0.64]

$R^2 = 0.78$
 $R^2 = 0.43$
 $R^2 = 0.35$

GAFF v2.1 ΔG (kcal/mol)

