

SMIRNOFF99Frosst - $T\Delta S$ (kcal/mol)

RMSE = 1.55 [1.25, 1.85]
 $R^2 = 0.70$ [0.54, 0.82]

$R^2 = 0.73$
 $R^2 = 0.61$
 $R^2 = 0.74$

GAFF v2.1 - $T\Delta S$ (kcal/mol)

