

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

RMSE = 1.97 [1.67, 2.29]  
 $R^2 = 0.53$  [0.38, 0.66]

$R^2 = 0.64$   
 $R^2 = 0.54$   
 $R^2 = 0.38$

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

