

SMIRNOFF99Frosst ΔG (kcal/mol)

RMSE = 0.82 [0.61, 1.04]
 $R^2 = 0.53$ [0.32, 0.73]

$R^2 = 0.72$
 $R^2 = 0.40$
 $R^2 = 0.76$

Experimental ΔG (kcal/mol)

