

MSE = $9.56e+01$ $^{1.1e+02}_{8.4e+01}$ kcal/mol

RMSE = $9.78e+00$ $^{1.0e+01}_{9.2e+00}$ kcal/mol

$R = 9.26e-01$, $R_S = 0.92$, $n = 500$

