

dihedral angle  $\phi$

180°  
120°  
60°  
0°  
-60°  
-120°  
-180°

interaction = Coulomb

0.0 0.125 0.25 0.375 0.5 0.75 1.0

$\lambda$

interaction = VDW

0.0 0.05 0.1 0.2 0.3 0.4 0.5 0.6 0.65 0.7 0.75 0.8 0.85 0.9 0.95 1.0

$\lambda$

solvent

water

octanol

