



Paramètres

Propriétés Couplage

type de couplage: α Poncutelle

Atome existant: B (Bore)

Valeur: 3.04199418  $m^3$

Première énergie d'ionisation: 800.6 kJ/mol

Distance: 0.28 nm

Énergie

$$U_{\mu_1^* \mu_2^*} = \frac{1}{r^6} * \frac{2}{3} * (\alpha_1') * (\alpha_2') * k_c^2 * \frac{I_1 * I_2}{I_1 + I_2}$$
$$U_{\mu_1^* \mu_2^*} = \frac{1}{(0.28 * 10^{-9} \text{ m})^6} * \frac{2}{3} * (0.819 * 10^{-30} \text{ m}^3) * (3.04199418 * 10^{-30} \text{ m}^3) * (9 * 10^9)^2$$
$$* \frac{1488 \text{ kJ/mol} * \frac{1000 \text{ J/kJ}}{6.022 * 10^{23} \text{ mol}} * 800.6 \text{ kJ/mol} * \frac{1000 \text{ J/kJ}}{6.022 * 10^{23} \text{ mol}}}{1488 \text{ kJ/mol} * \frac{1000 \text{ J/kJ}}{6.022 * 10^{23} \text{ mol}} + 800.6 \text{ kJ/mol} * \frac{1000 \text{ J/kJ}}{6.022 * 10^{23} \text{ mol}}}$$
$$U_{\mu_1^* \mu_2^*} = 2.413 * 10^{-1} \text{ J}$$