

EXAMPLE 13.6

ORIGIN := 1

$$\Delta H_f := \begin{pmatrix} 52.34 \\ -242 \\ -235 \end{pmatrix} \quad \Delta G_f := \begin{pmatrix} 68.16 \\ -228.8 \\ -168.4 \end{pmatrix} \quad \alpha := \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix}$$

$$a := \begin{pmatrix} 17.562 \\ 33.763 \\ 19.959 \end{pmatrix} \quad b := \begin{pmatrix} 0.692 \\ -0.006 \\ 1.428 \end{pmatrix} \cdot 10^{-1} \quad c := \begin{pmatrix} 0.936 \\ 0.224 \\ 0.776 \end{pmatrix} \cdot 10^{-4}$$

$$d := \begin{pmatrix} -1.293 \\ -0.100 \\ -1.513 \end{pmatrix} \cdot 10^{-7} \quad e := \begin{pmatrix} 4.294 \\ 0.110 \\ 5.366 \end{pmatrix} \cdot 10^{-11}$$

i := 1 .. 3

$$\Delta G_{298} := \left[\sum_i (\alpha_i \cdot \Delta G_{f_i}) \right] \cdot 1000 \quad \Delta H_{298} := \left[\sum_i (\alpha_i \cdot \Delta H_{f_i}) \right] \cdot 1000$$

$$\Delta a := \sum_i (a_i \cdot \alpha_i) \quad \Delta b := \left[\sum_i (b_i \cdot \alpha_i) \right] \quad \Delta c := \left[\sum_i (c_i \cdot \alpha_i) \right]$$

$$\Delta d := \left[\sum_i (d_i \cdot \alpha_i) \right] \quad \Delta e := \left[\sum_i (e_i \cdot \alpha_i) \right]$$

$$\Lambda := \Delta a \cdot 298 + \frac{298^2 \cdot \Delta b}{2} + \frac{298^3 \cdot \Delta c}{3} + \frac{298^4 \cdot \Delta d}{4} + \frac{298^5 \cdot \Delta e}{5} - \Delta H_{298}$$

$$\Omega := (1 + \ln(298)) \cdot \Delta a + 298 \cdot \Delta b + \frac{298^2 \cdot \Delta c}{2} + \frac{298^3 \cdot \Delta d}{3} + \frac{298^4 \cdot \Delta e}{4} - \frac{\Delta H_{298} - \Delta G_{298}}{298}$$

R := 8.314

$$K_a(T) := \exp \left[\frac{1}{R} \cdot \left(\Delta a \cdot \ln(T) + \frac{\Delta b}{2} \cdot T + \frac{\Delta c}{6} \cdot T^2 + \frac{\Delta d}{12} \cdot T^3 + \frac{\Delta e}{20} \cdot T^4 + \frac{\Lambda}{T} - \Omega \right) \right]$$

$$K_a(500) = 0.012$$