EXAMPLE 13.9

$ORIGIN := 1$

$$\Delta H_f := \begin{pmatrix} 82.98 \\ 0 \\ -123.2 \end{pmatrix} \qquad \Delta G_f := \begin{pmatrix} 129.7 \\ 0 \\ 31.78 \end{pmatrix} \qquad \alpha := \begin{pmatrix} -1 \\ -3 \\ 1 \end{pmatrix}$$

$$a := \begin{pmatrix} -60.711 \\ 27.004 \\ -63.733 \end{pmatrix} \qquad b := \begin{pmatrix} 6.267 \\ 0.119 \\ 6.444 \end{pmatrix} \cdot 10^{-1} \qquad c := \begin{pmatrix} -5.795 \\ -0.241 \\ -2.633 \end{pmatrix} \cdot 10^{-4}$$

$$d := \begin{pmatrix} 2.799 \\ 0.215 \\ -0.378 \end{pmatrix} \cdot 10^{-7} \qquad e := \begin{pmatrix} -5.493 \\ -0.615 \\ 3.796 \end{pmatrix} \cdot 10^{-11}$$

$i := 1 .. 3$

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

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

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

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

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

$R := 8.314 \qquad T := 550$

$$K_a := \exp\left[\frac{1}{R} \cdot \left(\Delta a \cdot \ln(T) + \frac{\Delta b}{2} \cdot T + \frac{\Delta c}{6} \cdot T^2 + \frac{\Delta d}{12} \cdot T^3 + \frac{\Delta e}{20} \cdot T^4 + \frac{\Lambda}{T} - \Omega\right)\right] = 1.47$$

$\varepsilon := 0.1$

Given

$$K_a = \frac{\varepsilon}{1-\varepsilon}\cdot\left(\frac{5.5 - 3\cdot\varepsilon}{4.5 - 3\varepsilon}\right)^3$$

$\text{Find}(\varepsilon) = 0.399$

Part (b)

$$T_c := \begin{pmatrix} 562.0 \\ 33.2 \\ 554.0 \end{pmatrix} \qquad P_c := \begin{pmatrix} 48.9 \\ 13 \\ 40.7 \end{pmatrix} \qquad \omega := \begin{pmatrix} 0.212 \\ -0.216 \\ 0.212 \end{pmatrix} \qquad P := 15$$

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root(p, q, r) := | v ← (r, q, p, 1)^T
                 | x ← polyroots(v)
                 | for  i ∈ 1 .. 3
                 |    x_i ← 0  if  Im(x_i) ≠ 0
                 | x1 ← max(x)
                 | y ← min(x)
                 | x2 ← | max(x)  if  y = 0
                 |      | y  otherwise
                 | (x1, x2)^T
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$$\phi := \left| \begin{array}{l} \text{for } i \in 1..3 \\ \quad \left| \begin{array}{l} T_{r_i} \leftarrow \dfrac{T}{T_{c_i}} \\ P_{r_i} \leftarrow \dfrac{P}{P_{c_i}} \\ \alpha_i \leftarrow \left[1 + \left[0.37464 + 1.54226\,\omega_i - 0.26992\left(\omega_i\right)^2\right]\cdot\left(1 - \sqrt{T_{r_i}}\right)\right]^2 \\ A_i \leftarrow 0.45724\cdot\dfrac{P_{r_i}\cdot\alpha_i}{\left(T_{r_i}\right)^2} \\ B_i \leftarrow 0.07780\cdot\dfrac{P_{r_i}}{T_{r_i}} \\ p_i \leftarrow -1 + B_i \\ q_i \leftarrow A_i - 2\,B_i - 3\left(B_i\right)^2 \\ r_i \leftarrow -A_i\cdot B_i + \left(B_i\right)^2 + \left(B_i\right)^3 \\ Z_i \leftarrow \text{root}\left(p_i , q_i , r_i\right)_1 \\ \Theta_i \leftarrow \dfrac{A_i}{\sqrt{8}\cdot B_i}\cdot\ln\left[\dfrac{Z_i + \left(1 + \sqrt{2}\right)\cdot B_i}{Z_i + \left(1 - \sqrt{2}\right)\cdot B_i}\right] \\ \phi_i \leftarrow \exp\left(Z_i - 1 - \ln\left(Z_i - B_i\right) - \Theta_i\right) \end{array}\right. \\ \phi \end{array}\right.$$

$$\phi = \begin{pmatrix} 0.879 \\ 1.004 \\ 0.862 \end{pmatrix}$$

$$K_f := \frac{\phi_3}{\phi_1\cdot\left(\phi_2\right)^3} = 0.969$$

$\varepsilon := 0.5$

Given

$$\frac{K_a\cdot P^3}{K_f} = \frac{\varepsilon}{1-\varepsilon}\cdot\left(\frac{5.5 - 3\cdot\varepsilon}{4.5 - 3\varepsilon}\right)^3$$

$\text{Find}\left(\varepsilon\right) = 0.999$