EXAMPLE 13.11

$ORIGIN := 1$

$T := 500 \qquad P := 40 \qquad R := 8.314$

$$K_{a1} := \exp\left(\frac{5772.5}{T} - 4.81\cdot\ln(T) + 1.72\cdot10^{-3}\cdot T - 6.79\cdot10^{-7}\cdot T^2 + 19.1\right) = 4.233$$

$$K_{a2} := \exp\left(\frac{-5130}{T} + 3.16\cdot\ln(T) - 4.023\cdot10^{-3} + 1.55\cdot10^{-6}\cdot T^2 - 14.15\right) = 0.012$$

$$\Delta H_1 := R\cdot T^2\cdot\left(\frac{-5772.5}{T^2} - \frac{4.81}{T} + 1.72\cdot10^{-3} - 13.58\cdot10^{-7}\cdot T\right) = -6.582\times10^4$$

$$\Delta H_2 := R\cdot T^2\cdot\left(\frac{5130}{T^2} + \frac{3.16}{T} - 4.023\cdot10^{-3} + 3.1\cdot10^{-6}\cdot T\right) = 5.065\times10^4$$

$$T_c := \begin{pmatrix}487.2\\33.2\\513\end{pmatrix} \qquad P_c := \begin{pmatrix}60\\13\\81\end{pmatrix} \qquad \omega := \begin{pmatrix}0.257\\-0.216\\0.556\end{pmatrix} \qquad k := \begin{pmatrix}0&0&0\\0&0&0\\0&0&0\end{pmatrix}$$

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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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$$
\phi(\varepsilon) :=
\begin{array}{|l}
y_1 \leftarrow \dfrac{1-\varepsilon}{5-\varepsilon} \\
y_2 \leftarrow \dfrac{4-2\varepsilon}{5-\varepsilon} \\
y_3 \leftarrow \dfrac{2\varepsilon}{5-\varepsilon} \\
n \leftarrow 3 \\
\text{for } \; i \in 1 .. n \\
\quad \begin{array}{|l}
T_{r_i} \leftarrow \dfrac{T}{T_{c_i}} \\
P_{r_i} \leftarrow \dfrac{P}{P_{c_i}} \\
\alpha_i \leftarrow \left[1 + \left[0.37464 + 1.54226 \cdot \omega_i - 0.26992 \cdot (\omega_i)^2\right] \cdot \left(1 - \sqrt{T_{r_i}}\right)\right]^2 \\
A_{i,i} \leftarrow 0.45724 \cdot \left[\dfrac{P_{r_i}}{\left(T_{r_i}\right)^2}\right] \cdot \alpha_i \\
B_i \leftarrow 0.07780 \cdot \left(\dfrac{P_{r_i}}{T_{r_i}}\right)
\end{array} \\
\text{for } \; i \in 1 .. n \\
\quad \text{for } \; j \in 1 .. n \\
\quad\quad A_{i,j} \leftarrow \left(1 - k_{i,j}\right) \cdot \sqrt{A_{i,i} \cdot A_{j,j}} \\
A_{mix} \leftarrow \displaystyle\sum_{i=1}^{n} \sum_{j=1}^{n} \left(y_i \cdot y_j \cdot A_{i,j}\right) \\
B_{mix} \leftarrow \displaystyle\sum_{i=1}^{n} \left(y_i \cdot B_i\right) \\
p \leftarrow -1 + B_{mix} \\
q \leftarrow A_{mix} - 3 \cdot B_{mix}^{2} - 2 \cdot B_{mix} \\
r \leftarrow -A_{mix} \cdot B_{mix} + B_{mix}^{2} + B_{mix}^{3} \\
Z \leftarrow \text{root}(p, q, r)_1 \\
C \leftarrow \ln\left[\dfrac{Z + \left(1 + \sqrt{2}\right) \cdot B_{mix}}{Z + \left(1 - \sqrt{2}\right) \cdot B_{mix}}\right]
\end{array}
$$

$$\left|\begin{array}{l} \text{for} \quad i \in 1..n \\ \quad \phi_i \leftarrow \exp\left[\dfrac{B_i\cdot(Z-1)}{B_{mix}} - \ln(Z - B_{mix}) - \dfrac{A_{mix}\cdot C}{2\sqrt{2}\cdot B_{mix}}\cdot\left[\dfrac{2\cdot\sum_{j=1}^{n}(y_j\cdot A_{i,j})}{A_{mix}} - \dfrac{B_i}{B_{mix}}\right]\right] \\ \phi \end{array}\right.$$

$$K_\phi(\varepsilon) := \frac{(\phi(\varepsilon)_3)^2}{\phi(\varepsilon)_1\cdot(\phi(\varepsilon)_2)^2} \qquad K_y(\varepsilon) := \frac{4\varepsilon^2\cdot(5-\varepsilon)}{(1-\varepsilon)(4-2\varepsilon)^2}$$

$\varepsilon := 0.99$

Given

$$K_{a1} = \frac{K_\phi(\varepsilon)\cdot K_y(\varepsilon)}{P}$$

$\text{Find}(\varepsilon) = 0.983$