

EXAMPLE 3.13

ORIGIN := 1

 $T_c := 369.9$ $P_c := 42.5$ $\omega := 0.153$ $R := 8.314$

$$C_p(T) := 29.595 + 0.838 \cdot 10^{-1} T + 3.256 \cdot 10^{-4} T^2 - 3.958 \cdot 10^{-7} T^3 + 13.129 \cdot 10^{-11} T^4$$

$$\text{root}(p, q, r) := \left(\begin{array}{l} r \\ q \\ p \\ 1 \end{array} \right)$$

$$x \leftarrow \text{polyroots}(v)$$

$$\text{for } i \in 1 \dots 3$$

$$x_i \leftarrow 0 \text{ if } \text{Im}(x_i) \neq 0$$

$$x1 \leftarrow \max(x)$$

$$y \leftarrow \min(x)$$

$$x2 \leftarrow \begin{cases} \max(x) & \text{if } y = 0 \\ y & \text{otherwise} \end{cases}$$

$$\left(\begin{array}{l} x1 \\ x2 \end{array} \right)$$

a) Redlich-Kwong Equation of State

$$X(T, P) := \left(\begin{array}{l} T_r \leftarrow \frac{T}{T_c} \\ P_r \leftarrow \frac{P}{P_c} \\ A \leftarrow 0.42748 \cdot \frac{P_r}{T_r^{2.5}} \\ B \leftarrow 0.08664 \cdot \frac{P_r}{T_r} \\ p \leftarrow -1 \\ q \leftarrow A - B - B^2 \\ r \leftarrow -A \cdot B \\ Z \leftarrow \text{root}(p, q, r)_1 \\ X \leftarrow R \cdot T \cdot \left(Z - 1 - \frac{3A}{2B} \cdot \ln \left(1 + \frac{B}{Z} \right) \right) \\ X \end{array} \right)$$

$$T := \begin{pmatrix} 323 \\ 343 \end{pmatrix} \quad P := \begin{pmatrix} 5 \\ 15 \end{pmatrix}$$

This is Eq. (3.3-22)

$$\Delta H := X(T_2, P_2) - X(T_1, P_1) + \int_{T_1}^{T_2} C_p(T) dT = 674.335$$

b) Peng-Robinson Equation of State

$$\begin{array}{l} X(T, P) := \\ \left. \begin{array}{l} T_r \leftarrow \frac{T}{T_c} \\ P_r \leftarrow \frac{P}{P_c} \\ \alpha \leftarrow \left[1 + (0.37464 + 1.54226\omega - 0.26992\omega^2) \cdot (1 - \sqrt{T_r}) \right]^2 \\ A \leftarrow 0.45724 \cdot \frac{P_r \cdot \alpha}{T_r^2} \\ B \leftarrow 0.07780 \cdot \frac{P_r}{T_r} \\ p \leftarrow -1 + B \\ q \leftarrow A - 2B - 3B^2 \\ r \leftarrow -A \cdot B + B^2 + B^3 \\ Z \leftarrow \text{root}(p, q, r)_1 \\ \Gamma \leftarrow (0.37464 + 1.54226\omega - 0.26992\omega^2) \cdot \sqrt{\frac{T_r}{\alpha}} \\ X \leftarrow R \cdot T \cdot \left[Z - 1 - \frac{A \cdot (1 + \Gamma)}{\sqrt{8} B} \cdot \ln \left[\frac{Z + (1 + \sqrt{2}) \cdot B}{Z + (1 - \sqrt{2}) \cdot B} \right] \right] \\ X \end{array} \right\} \end{array}$$

This is Eq. (3.3-24)

$$\Delta H := X(T_2, P_2) - X(T_1, P_1) + \int_{T_1}^{T_2} C_p(T) dT = 554.088$$