

**EXAMPLE 3.21**

ORIGIN := 1

$$T := 343 \quad P := 15$$

$$T_c := 369.9 \quad P_c := 42.5 \quad \omega := 0.153$$

$$T_r := \frac{T}{T_c} \quad P_r := \frac{P}{P_c}$$

$$b := \begin{pmatrix} 0.1181193 \\ 0.265728 \\ 0.154790 \\ 0.030323 \end{pmatrix} \quad c := \begin{pmatrix} 0.0236744 \\ 0.0186984 \\ 0 \\ 0.042724 \end{pmatrix} \quad d := \begin{pmatrix} 1.55488 \cdot 10^{-5} \\ 6.23689 \cdot 10^{-5} \end{pmatrix}$$

$$B := b_1 - \frac{b_2}{T_r} - \frac{b_3}{T_r^2} - \frac{b_4}{T_r^3} \quad C := c_1 - \frac{c_2}{T_r} + \frac{c_3}{T_r^3} \quad D := d_1 + \frac{d_2}{T_r}$$

$$\beta := 0.65392 \quad \gamma := 0.060167$$

$$x := 2.1$$

Given

$$\frac{P_r \cdot x}{T_r} = 1 + \frac{B}{x} + \frac{C}{x^2} + \frac{D}{x^5} + \frac{c_4}{T_r^3 \cdot x^2} \cdot \left( \beta + \frac{\gamma}{x^2} \right) \cdot \exp\left(\frac{-\gamma}{x^2}\right)$$

$$V0 := \text{Find}(x) = 2.184$$

$$Z0 := \frac{P_r \cdot V0}{T_r} = 0.831$$

$$bc := \begin{pmatrix} 0.2026579 \\ 0.331511 \\ 0.027655 \\ 0.203488 \end{pmatrix} \quad cc := \begin{pmatrix} 0.0313385 \\ 0.0503618 \\ 0.016901 \\ 0.041577 \end{pmatrix} \quad dc := \begin{pmatrix} 4.8736 \cdot 10^{-5} \\ 7.40336 \cdot 10^{-6} \end{pmatrix}$$

$$\beta_c := 1.226 \quad \gamma_c := 0.03754$$

$$Bc := bc_1 - \frac{bc_2}{T_r} - \frac{bc_3}{T_r^2} - \frac{bc_4}{T_r^3} \quad Cc := cc_1 - \frac{cc_2}{T_r} + \frac{cc_3}{T_r^3} \quad Dc := dc_1 + \frac{dc_2}{T_r}$$

$$xc := 2.1$$

Given

$$\frac{P_r \cdot xc}{T_r} = 1 + \frac{Bc}{xc} + \frac{Cc}{xc^2} + \frac{Dc}{xc^5} + \frac{cc_4}{T_r^3 \cdot xc^2} \cdot \left( \beta c + \frac{\gamma c}{xc^2} \right) \cdot \exp\left(\frac{-\gamma c}{xc^2}\right)$$

$$VR := \text{Find}(xc) = 2.114$$

$$ZR := \frac{P_r \cdot VR}{T_r} = 0.805$$

$$Z1 := \frac{ZR - Z0}{0.3978} = -0.066$$

$$Z := Z0 + \omega \cdot Z1 = 0.821$$

### Enthalpy Departure Function

$$E0 := \frac{c_4}{2 \cdot T_r^3 \cdot \gamma} \cdot \left[ \beta + 1 - \left( \beta + 1 + \frac{\gamma}{V0^2} \right) \cdot \exp\left(\frac{-\gamma}{V0^2}\right) \right] = 3.686 \times 10^{-3}$$

$$H0 := T_r \cdot \left[ Z0 - 1 - \frac{1}{T_r \cdot V0} \cdot \left( b_2 + \frac{2 \cdot b_3}{T_r} + \frac{3 \cdot b_4}{T_r^2} \right) - \frac{1}{2 \cdot T_r \cdot V0^2} \cdot \left( c_2 - \frac{3 \cdot c_3}{T_r^2} \right) + \frac{d_2}{5 \cdot T_r \cdot V0^5} + 3 \cdot E0 \right]$$

$$Ec := \frac{cc_4}{2 \cdot T_r^3 \cdot \gamma c} \cdot \left[ \beta c + 1 - \left( \beta c + 1 + \frac{\gamma c}{VR^2} \right) \cdot \exp\left(\frac{-\gamma c}{VR^2}\right) \right] = 7.146 \times 10^{-3}$$

$$HR := T_r \cdot \left[ ZR - 1 - \frac{1}{T_r \cdot VR} \cdot \left( bc_2 + \frac{2 \cdot bc_3}{T_r} + \frac{3 \cdot bc_4}{T_r^2} \right) - \frac{1}{2 \cdot T_r \cdot VR^2} \cdot \left( cc_2 - \frac{3 \cdot cc_3}{T_r^2} \right) + \frac{dc_2}{5 \cdot T_r \cdot VR^5} + 3 \cdot Ec \right]$$

$$\underline{H1} := \frac{HR - H0}{0.3978} = -0.527$$

$$\underline{H} := H0 + \omega \cdot H1 = -0.552$$

$$HDEPART := H \cdot 8.314 \cdot T_c = -1.698 \times 10^3$$