

EXAMPLE 3.19

ORIGIN := 1

T_c := 461

P_c := 33.8

ω := 0.227

R := 8.314

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root(p, q, r) :=  
v ←  $\begin{pmatrix} r \\ q \\ p \\ 1 \end{pmatrix}$   
x ← polyroots(v)  
for i ∈ 1 .. 3  
  xi ← 0 if Im(xi) ≠ 0  
x1 ← max(x)  
y ← min(x)  
x2 ←  $\begin{cases} \max(x) & \text{if } y = 0 \\ y & \text{otherwise} \end{cases}$   
 $\begin{pmatrix} x1 \\ x2 \end{pmatrix}$ 
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$$\begin{aligned}
 \text{Dep}(T, P) := & \left[\begin{array}{l}
 T_r \leftarrow \frac{T}{T_c} \\
 P_r \leftarrow \frac{P}{P_c} \\
 \alpha \leftarrow \left[1 + \left(0.37464 + 1.54226\omega - 0.26992\omega^2 \right) \cdot \left(1 - \sqrt{T_r} \right) \right]^2 \\
 A \leftarrow 0.45724 \cdot \frac{P_r \cdot \alpha}{T_r^2} \\
 B \leftarrow 0.07780 \cdot \frac{P_r}{T_r} \\
 p \leftarrow -1 + B \\
 q \leftarrow A - 2B - 3B^2 \\
 r \leftarrow -A \cdot B + B^2 + B^3 \\
 Z \leftarrow \text{root}(p, q, r)_1 \\
 \Gamma \leftarrow \left(0.37464 + 1.54226\omega - 0.26992\omega^2 \right) \cdot \sqrt{\frac{T_r}{\alpha}} \\
 H \leftarrow R \cdot T \cdot \left[Z - 1 - \frac{A \cdot (1 + \Gamma)}{\sqrt{8} B} \cdot \ln \left[\frac{Z + (1 + \sqrt{2}) \cdot B}{Z + (1 - \sqrt{2}) \cdot B} \right] \right] \\
 S \leftarrow R \cdot \left[\ln(Z - B) - \frac{A \cdot \Gamma}{\sqrt{8} B} \cdot \ln \left[\frac{Z + (1 + \sqrt{2}) \cdot B}{Z + (1 - \sqrt{2}) \cdot B} \right] \right] \\
 \left(\begin{array}{l} H \\ S \end{array} \right)
 \end{array} \right.
 \end{aligned}$$

$$\underline{H}(T, P) := \text{Dep}(T, P)_1$$

$$\underline{S}(T, P) := \text{Dep}(T, P)_2$$

This is Eq. (3.6-3)

$$\Delta H := -H(500, 3) + H(500, 20) = -2.282 \times 10^3$$

This is Eq. (3.6-4)

$$\Delta S := -S(500, 3) - R \cdot \ln\left(\frac{20}{3}\right) + S(500, 20) = -19.058$$