

EXAMPLE 6.4

ORIGIN := 1

$$T_c := \begin{pmatrix} 369.9 \\ 425 \\ 469.8 \end{pmatrix}$$

$$P_c := \begin{pmatrix} 42.5 \\ 38 \\ 33.6 \end{pmatrix}$$

$$\omega := \begin{pmatrix} 0.153 \\ 0.199 \\ 0.251 \end{pmatrix}$$

$$y := \begin{pmatrix} 0.5 \\ 0.2 \\ 0.3 \end{pmatrix}$$

R := 8.314

$$k := \begin{pmatrix} 0 & 0.003 & 0.027 \\ 0.003 & 0 & 0.017 \\ 0.027 & 0.017 & 0 \end{pmatrix}$$

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root(p, q, r) :=  $\left. \begin{array}{l} v \leftarrow \begin{pmatrix} r \\ q \\ p \\ 1 \end{pmatrix} \\ x \leftarrow \text{polyroots}(v) \\ \text{for } i \in 1..3 \\ \quad x_i \leftarrow 0 \text{ if } \text{Im}(x_i) \neq 0 \\ x1 \leftarrow \max(x) \\ y \leftarrow \min(x) \\ x2 \leftarrow \begin{cases} \max(x) & \text{if } y = 0 \\ y & \text{otherwise} \end{cases} \\ \begin{pmatrix} x1 \\ x2 \end{pmatrix} \end{array} \right|$ 
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x(T,P) := for i ∈ 1..3
|
|   Tr_i ← T / Tc_i
|
|   Pr_i ← P / Pc_i
|
|   α_i ← [1 + [0.37464 + 1.54226 ω_i - 0.26992 (ω_i)^2] · (1 - √Tr_i)]^2
|
|   Ai,i ← 0.45724 [ Pr_i · α_i / (Tr_i)^2 ]
|
|   Bi ← 0.07780 · Pr_i / Tr_i
|
for i ∈ 1..3
  for j ∈ 1..3
    Ai,j ← (1 - ki,j) · √Ai,i · Aj,j
  Amix ← ∑_{i=1}^3 ∑_{j=1}^3 (yi · yj · Ai,j)
  Bmix ← ∑_{i=1}^3 (yi · Bi)
  p ← -1 + Bmix
  q ← Amix - 2Bmix - 3Bmix^2
  r ← -Amix · Bmix + Bmix^2 + Bmix^3
  Z ← root(p, q, r)_1
  for i ∈ 1..3
    Γ_i ← [0.37464 + 1.54226 ω_i - 0.26992 (ω_i)^2] · √(Tr_i / α_i)
  Ωmix ← -1/2 · ∑_{i=1}^3 ∑_{j=1}^3 [yi · yj · Ai,j · (Γ_i + Γ_j)] - Amix
  X ← R · T · [ Z - 1 + Ωmix / √(8 · Bmix) · ln [ (Z + (1 + √2) · Bmix) / (Z + (1 - √2) · Bmix) ] ]
..

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I X

$$T := \begin{pmatrix} 300 \\ 500 \end{pmatrix} \quad P := \begin{pmatrix} 1 \\ 40 \end{pmatrix}$$

$$C := \begin{pmatrix} 29.595 & 24.258 & 33.780 \\ 0.838 & 2.335 & 2.485 \\ 3.256 & 1.279 & 2.535 \\ -3.958 & -2.437 & -3.838 \\ 13.129 & 8.552 & 12.977 \end{pmatrix} \quad i := 1 .. 3$$

$$D_1 := \sum_i (y_i \cdot C_{1,i}) \quad D_2 := \sum_i (y_i \cdot C_{2,i}) \quad D_3 := \sum_i (y_i \cdot C_{3,i})$$

$$D_4 := \sum_i (y_i \cdot C_{4,i}) \quad D_5 := \sum_i (y_i \cdot C_{5,i})$$

This is Eq. (6.1-23)

$$I := \int_{T_1}^{T_2} \left(D_1 + D_2 \cdot 10^{-1} \cdot T + D_3 \cdot 10^{-4} \cdot T^2 + D_4 \cdot 10^{-7} \cdot T^3 + D_5 \cdot 10^{-11} \cdot T^4 \right) dT = 2.343 \times 10^4$$

$$\Delta H := X(T_2, P_2) - X(T_1, P_1) + I = 2.026 \times 10^4$$