

ORIGIN := 1

### Departure Function for Carbon dioxide

$T_C := 304.2$

$P_C := 73.8$

$R := 8.314$

$\text{root}(p, q, r) :=$

$$\left| \begin{array}{l} v \leftarrow \begin{pmatrix} r \\ q \\ p \\ 1 \end{pmatrix} \\ x \leftarrow \text{polyroots}(v) \\ \text{for } i \in 1..3 \\ \quad x_i \leftarrow 0 \text{ if } \text{Im}(x_i) \neq 0 \\ x1 \leftarrow \max(x) \\ y \leftarrow \min(x) \\ x2 \leftarrow \begin{cases} \max(x) & \text{if } y = 0 \\ y & \text{otherwise} \end{cases} \\ \begin{pmatrix} x1 \\ x2 \end{pmatrix} \end{array} \right.$$

$\text{HCO}_2(T, P) :=$

$$\left| \begin{array}{l} T_r \leftarrow \frac{T}{T_C} \\ P_r \leftarrow \frac{P}{P_C} \\ A \leftarrow 0.42748 \left[ \frac{P_r}{(T_r)^{2.5}} \right] \\ B \leftarrow 0.08664 \cdot \frac{P_r}{T_r} \\ p \leftarrow -1 \\ q \leftarrow A - B - B^2 \\ r \leftarrow -A \cdot B \\ Z \leftarrow \text{root}(p, q, r)_1 \\ H \leftarrow R \cdot T \cdot \left( Z - 1 - \frac{3}{2} \cdot \frac{A}{B} \cdot \ln \left( 1 + \frac{B}{Z} \right) \right) \\ H \end{array} \right.$$

$$\text{HCO}_2(350, 10) = -273.054$$

### Departure Function for Methane

$$T_{\text{ref}} := 190.6 \quad P_{\text{ref}} := 46.1$$

$$\text{HCH}_4(T, P) := \left. \begin{array}{l} T_r \leftarrow \frac{T}{T_c} \\ P_r \leftarrow \frac{P}{P_c} \\ A \leftarrow 0.42748 \left[ \frac{P_r}{(T_r)^{2.5}} \right] \\ B \leftarrow 0.08664 \cdot \frac{P_r}{T_r} \\ p \leftarrow -1 \\ q \leftarrow A - B - B^2 \\ r \leftarrow -A \cdot B \\ Z \leftarrow \text{root}(p, q, r)_1 \\ H \leftarrow R \cdot T \cdot \left( Z - 1 - \frac{3}{2} \cdot \frac{A}{B} \cdot \ln \left( 1 + \frac{B}{Z} \right) \right) \\ H \end{array} \right\}$$

$$\text{HCH}_4(270, 5) = -94.65$$

### Departure Function for the Mixture

$$T_{\text{ref}} := \begin{pmatrix} 304.2 \\ 190.6 \end{pmatrix} \quad P_{\text{ref}} := \begin{pmatrix} 73.8 \\ 46.1 \end{pmatrix} \quad y := \begin{pmatrix} 0.25 \\ 0.75 \end{pmatrix} \quad k := \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

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Hmix(T, P) :=
  for i ∈ 1..2
    Tr_i ← T / Tc_i
    Pr_i ← P / Pc_i
    Ai_i ← 0.42748 * [ Pr_i / (Tr_i)^2.5 ]
    Bi ← 0.08664 * Pr_i / Tr_i
  for i ∈ 1..2
    for j ∈ 1..2
      Ai_j ← (1 - ki_j) * sqrt(Ai_i * Aj_j)
    Amix ← sum_{i=1}^2 sum_{j=1}^2 (yi * yj * Ai_j)
    Bmix ← sum_{i=1}^2 (yi * Bi)
    p ← -1
    q ← Amix - Bmix - Bmix^2
    r ← -Amix * Bmix
    Z ← root(p, q, r)_1
    H ← 8.314 * T * ( Z - 1 - (3/2) * (Amix / Bmix) * ln(1 + (Bmix / Z)) )
  H

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$$C_1(T) := 29.268 - 0.224 \cdot 10^{-1} \cdot T + 2.653 \cdot 10^{-4} \cdot T^2 - 4.153 \cdot 10^{-7} \cdot T^3 + 20.057 \cdot 10^{-11} \cdot T^4$$

$$C_2(T) := (36.155 - 0.511 \cdot 10^{-1} \cdot T + 2.215 \cdot 10^{-4} \cdot T^2 - 1.824 \cdot 10^{-7} \cdot T^3 + 4.899 \cdot 10^{-11} \cdot T^4)$$

$$T := 250$$

Given

$$-\text{HCO}_2(350, 10) - 3 \text{HCH}_4(270, 5) + \int_{350}^T C_1(T) dT + 3 \int_{270}^T C_2(T) dT + 4 \text{Hmix}(T, 3) = 0$$

$$T := \text{Find}(T) = 288.829$$