

ORIGIN := 1

T := 800

Methane

$$\Delta H_{f298} := -74900$$

$$\Delta G_{f298} := -50870$$

$$a := 36.155$$

$$b := -0.511 \cdot 10^{-1}$$

$$c := 2.215 \cdot 10^{-4}$$

$$d := -1.824 \cdot 10^{-7}$$

$$e := 4.899 \cdot 10^{-11}$$

$$\Delta G := \left| \begin{array}{l} n_H \leftarrow 2 \\ n_O \leftarrow 0 \\ n_C \leftarrow 1 \\ A \leftarrow a - 27.004n_H - 29.705n_O - 17.152n_C \\ B \leftarrow b - \left(0.119n_H - 0.099n_O + 4.273 \cdot 10^{-2}n_C \right) \cdot 10^{-1} \\ C \leftarrow c - \left(-0.241n_H + 0.399n_O \right) \cdot 10^{-4} \\ D \leftarrow d - \left(0.215n_H - 0.339n_O \right) \cdot 10^{-7} \\ E \leftarrow e - \left(-0.615n_H + 0.918n_O \right) \cdot 10^{-11} \\ F \leftarrow 8.7879 \cdot 10^5 \cdot n_C \\ f(z) \leftarrow A + B \cdot z + C \cdot z^2 + D \cdot z^3 + E \cdot z^4 + F \cdot z^{-2} \\ I(y) \leftarrow \Delta H_{f298} + \int_{298}^y f(z) dz \\ Y \leftarrow \int_{298}^T \frac{I(y)}{y^2} dy \\ \Delta G \leftarrow T \cdot \left(\frac{\Delta G_{f298}}{298} - Y \right) \\ \Delta G \end{array} \right.$$

$$\Delta G = -2.093 \times 10^3$$

Carbon Monoxide

$$\Delta H_{f298} := -110600$$

$$\Delta G_{f298} := -137400$$

$$a := 29.651$$

$$b := -0.007 \cdot 10^{-1}$$

$$c := 0.183 \cdot 10^{-4}$$

$$d := -0.094 \cdot 10^{-7}$$

$$e := 0.108 \cdot 10^{-11}$$

$$\Delta G := \left| \begin{array}{l} n_H \leftarrow 0 \\ n_O \leftarrow \frac{1}{2} \\ n_C \leftarrow 1 \\ A \leftarrow a - 27.004n_H - 29.705n_O - 17.152n_C \\ B \leftarrow b - \left(0.119n_H - 0.099n_O + 4.273 \cdot 10^{-2}n_C \right) \cdot 10^{-1} \\ C \leftarrow c - \left(-0.241n_H + 0.399n_O \right) \cdot 10^{-4} \\ D \leftarrow d - \left(0.215n_H - 0.339n_O \right) \cdot 10^{-7} \\ E \leftarrow e - \left(-0.615n_H + 0.918n_O \right) \cdot 10^{-11} \\ F \leftarrow 8.7879 \cdot 10^5 \cdot n_C \\ f(z) \leftarrow A + B \cdot z + C \cdot z^2 + D \cdot z^3 + E \cdot z^4 + F \cdot z^{-2} \\ l(y) \leftarrow \Delta H_{f298} + \int_{298}^y f(z) dz \\ Y \leftarrow \int_{298}^T \frac{l(y)}{y^2} dy \\ \Delta G \leftarrow T \cdot \left(\frac{\Delta G_{f298}}{298} - Y \right) \\ \Delta G \end{array} \right.$$

$$\Delta G = -1.835 \times 10^5$$

Water

$$\Delta H_{f298} := -242000$$

$$\Delta G_{f298} := -228800$$

$$a := 33.763$$

$$b := -0.006 \cdot 10^{-1}$$

$$c := 0.224 \cdot 10^{-4}$$

$$d := -0.1 \cdot 10^{-7}$$

$$e := 0.11 \cdot 10^{-11}$$

$$\Delta G := \left| \begin{array}{l} n_H \leftarrow 1 \\ n_O \leftarrow \frac{1}{2} \\ n_C \leftarrow 0 \\ A \leftarrow a - 27.004n_H - 29.705n_O - 17.152n_C \\ B \leftarrow b - \left(0.119n_H - 0.099n_O + 4.273 \cdot 10^{-2}n_C \right) \cdot 10^{-1} \\ C \leftarrow c - \left(-0.241n_H + 0.399n_O \right) \cdot 10^{-4} \\ D \leftarrow d - \left(0.215n_H - 0.339n_O \right) \cdot 10^{-7} \\ E \leftarrow e - \left(-0.615n_H + 0.918n_O \right) \cdot 10^{-11} \\ F \leftarrow 8.7879 \cdot 10^5 \cdot n_C \\ f(z) \leftarrow A + B \cdot z + C \cdot z^2 + D \cdot z^3 + E \cdot z^4 + F \cdot z^{-2} \\ I(y) \leftarrow \Delta H_{f298} + \int_{298}^y f(z) \, dz \\ Y \leftarrow \int_{298}^T \frac{I(y)}{y^2} \, dy \\ \Delta G \leftarrow T \cdot \left(\frac{\Delta G_{f298}}{298} - Y \right) \\ \Delta G \end{array} \right.$$

$$\Delta G = -2.045 \times 10^5$$

Carbon Dioxide

$$\Delta H_{f298} := -393800$$

$$\Delta G_{f298} := -394600$$

$$a := 29.268$$

$$b := -0.224 \cdot 10^{-1}$$

$$c := 2.653 \cdot 10^{-4}$$

$$d := -4.153 \cdot 10^{-7}$$

$$e := 20.057 \cdot 10^{-11}$$

$$\Delta G := \left| \begin{array}{l} n_H \leftarrow 0 \\ n_O \leftarrow 1 \\ n_C \leftarrow 1 \\ A \leftarrow a - 27.004n_H - 29.705n_O - 17.152n_C \\ B \leftarrow b - \left(0.119n_H - 0.099n_O + 4.273 \cdot 10^{-2}n_C \right) \cdot 10^{-1} \\ C \leftarrow c - \left(-0.241n_H + 0.399n_O \right) \cdot 10^{-4} \\ D \leftarrow d - \left(0.215n_H - 0.339n_O \right) \cdot 10^{-7} \\ E \leftarrow e - \left(-0.615n_H + 0.918n_O \right) \cdot 10^{-11} \\ F \leftarrow 8.7879 \cdot 10^5 \cdot n_C \\ f(z) \leftarrow A + B \cdot z + C \cdot z^2 + D \cdot z^3 + E \cdot z^4 + F \cdot z^{-2} \\ I(y) \leftarrow \Delta H_{f298} + \int_{298}^y f(z) \, dz \\ Y \leftarrow \int_{298}^T \frac{I(y)}{y^2} \, dy \\ \Delta G \leftarrow T \cdot \left(\frac{\Delta G_{f298}}{298} - Y \right) \\ \Delta G \end{array} \right.$$

$$\Delta G = -3.954 \times 10^5$$

$$y_{CH_4} := 0.06$$

$$y_{H_2O} := 0.3$$

$$y_{CO} := 0.01$$

$$y_{CO_2} := 0.01$$

$$y_{H_2} := 0.4$$

$$\lambda_C := 1 \quad \lambda_H := 4 \quad \lambda_O := 20 \quad n := 8$$

Given

$$\ln(y_{\text{CH}_4}) + \lambda_C + 4\lambda_H = \frac{2093}{8.314 \cdot 800}$$

$$\ln(y_{\text{H}_2\text{O}}) + 2\lambda_H + \lambda_O = \frac{204500}{8.314 \cdot 800}$$

$$\ln(y_{\text{CO}}) + \lambda_C + \lambda_O = \frac{183500}{8.314 \cdot 800}$$

$$\ln(y_{\text{CO}_2}) + \lambda_C + 2\lambda_O = \frac{395400}{8.314 \cdot 800}$$

$$\ln(y_{\text{H}_2}) + 2\lambda_H = 0$$

$$y_{\text{CH}_4} + y_{\text{CO}} + y_{\text{CO}_2} = \frac{1}{n}$$

$$4y_{\text{CH}_4} + 2y_{\text{H}_2\text{O}} + 2y_{\text{H}_2} = \frac{12}{n}$$

$$y_{\text{H}_2\text{O}} + y_{\text{CO}} + 2y_{\text{CO}_2} = \frac{4}{n}$$

$$y_{\text{CH}_4} + y_{\text{H}_2\text{O}} + y_{\text{CO}} + y_{\text{CO}_2} + y_{\text{H}_2} = 1$$

$$\text{Find}(y_{\text{CH}_4}, y_{\text{H}_2\text{O}}, y_{\text{CO}}, y_{\text{CO}_2}, y_{\text{H}_2}, \lambda_C, \lambda_H, \lambda_O, n) = \begin{pmatrix} 0.065 \\ 0.473 \\ 0.02 \\ 0.077 \\ 0.366 \\ 1.035 \\ 0.503 \\ 30.49 \\ 6.193 \end{pmatrix}$$