

EXAMPLE 13.8

ORIGIN := 1

T := 500

Ethylene

$\Delta H_{f298} := 52340$

$\Delta G_{f298} := 68160$

a := 17.562

b := $0.692 \cdot 10^{-1}$

c := $0.936 \cdot 10^{-4}$

d := $-1.293 \cdot 10^{-7}$

e := $4.294 \cdot 10^{-11}$

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

$\Delta G = 8.07021 \times 10^4$

Water

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

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

$$a := 33.763$$

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

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

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

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

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

$$\Delta G = -2.19399 \times 10^5$$

Ethanol

$$\Delta H_{f298} := -235000$$

$$\Delta G_{f298} := -168400$$

$$a := 19.959$$

$$b := 1.428 \cdot 10^{-1}$$

$$c := 0.776 \cdot 10^{-4}$$

$$d := -1.513 \cdot 10^{-7}$$

$$e := 5.366 \cdot 10^{-11}$$

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

$$\Delta G = -1.20408 \times 10^5$$