$ORIGIN := 1$

$T := 332.4 \qquad x := \begin{pmatrix} 0.73 \\ 0.27 \end{pmatrix}$

i represents components, Acetone = 1, Benzene = 2

$i := 1 .. 2$

j represents functional groups, CH3 = 1, CH3CO = 2, ACH = 3

$j := 1 .. 3$

R and Q values for the functional groups

$R := \begin{pmatrix} 0.9011 \\ 1.6724 \\ 0.5313 \end{pmatrix} \qquad Q := \begin{pmatrix} 0.848 \\ 1.488 \\ 0.400 \end{pmatrix}$

vij is the number of functional group j present in component i

$v := \begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 6 \end{pmatrix}$

$r_i := \sum_j \left(v_{i,j} \cdot R_j\right) \qquad q_i := \sum_j \left(v_{i,j} \cdot Q_j\right)$

$\Phi_i := \frac{r_i \cdot x_i}{\sum_i \left(r_i \cdot x_i\right)} \qquad \theta_i := \frac{q_i \cdot x_i}{\sum_i \left(q_i \cdot x_i\right)} \qquad l_i := 1 - r_i + 5\left(r_i - q_i\right)$

Combinatorial Activity Coefficient

$$\ln\gamma C_i := \ln\left(\frac{\Phi_i}{x_i}\right) + 5\, q_i \cdot \ln\left(\frac{\theta_i}{\Phi_i}\right) + l_i - \frac{\Phi_i}{x_i} \cdot \left[\sum_i \left(x_i \cdot l_i\right)\right]$$

Interaction Parameters

$$a := \begin{pmatrix} 0 & 476.4 & 61.13 \\ 26.76 & 0 & 140.1 \\ -11.12 & 25.77 & 0 \end{pmatrix}$$

$m := 1 .. 3 \qquad n := 1 .. 3$

$$\Psi_{m,n} := \exp\left(\frac{-a_{m,n}}{T}\right)$$

Calculation of total Γ

$$X_j := \frac{\left[\sum_i \left(v_{i,j} \cdot x_i\right)\right]}{\left[\sum_j \left[\sum_i \left(v_{i,j} \cdot x_i\right)\right]\right]}$$

$$\Theta_j := \frac{Q_j \cdot X_j}{\sum_j \left(Q_j \cdot X_j\right)}$$

$$\ln\Gamma_j := Q_j \cdot \left[1 - \ln\left[\sum_m \left(\Theta_m \cdot \Psi_{m,j}\right)\right] - \sum_m \frac{\Theta_m \cdot \Psi_{j,m}}{\sum_n \left(\Theta_n \cdot \Psi_{n,m}\right)}\right]$$

Calculation of Γ for individual groups

$$X1_j := \frac{v_{1,j}}{\left(\sum_j v_{1,j}\right)}$$

$$\Theta1_j := \frac{Q_j \cdot X1_j}{\sum_j \left(Q_j \cdot X1_j\right)}$$

$k := 1 .. 2$

$$\ln\Gamma1_k := Q_k \cdot \left[1 - \ln\left[\sum_m \left(\Theta1_m \cdot \Psi_{m,k}\right)\right] - \sum_m \frac{\Theta1_m \cdot \Psi_{k,m}}{\sum_n \left(\Theta1_n \cdot \Psi_{n,m}\right)}\right]$$

$\ln\Gamma2 := 0$

Residual Activity Coefficient

$$\ln\gamma R_1 := \sum_k \left[v_{1,k} \cdot \left(\ln\Gamma_k - \ln\Gamma 1_k \right) \right]$$

$$\ln\gamma R_2 := \sum_m \left[v_{2,m} \cdot \left(\ln\Gamma_m - \ln\Gamma 2 \right) \right]$$

Activity Coefficient of Species

$$\gamma_i := \exp\left(\ln\gamma C_i + \ln\gamma R_i \right)$$

$$\gamma = \begin{pmatrix} 1.0395 \\ 1.2538 \end{pmatrix}$$