Furfuryl Alcohol

$$F_{val} := \begin{pmatrix} \text{"OH"} & 1 & 0.0741 & 0.0112 & 28 \\ \text{"CH2"} & 1 & 0.0189 & 0 & 56 \\ \text{"Oring"} & 1 & 0.0098 & 0.0048 & 13 \\ \text{">C="} & 1 & 0.0143 & 0.0008 & 32 \\ \text{"CH="} & 3 & 0.0082 & 0.0011 & 41 \end{pmatrix}$$

$T_b := 443.2K$

$n := 4 \qquad n_a := 13$

$dm := 0.1m$

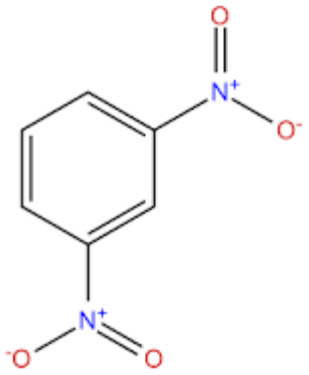
$kmol := 1000mol$

$$T_c := \frac{T_b}{0.584 + 0.965 \cdot \left[\sum_{i=0}^{n} \left(F_{val_{i,1}} F_{val_{i,2}}\right)\right] - \left[\sum_{i=0}^{n} \left(F_{val_{i,1}} \cdot F_{val_{i,2}}\right)\right]^2} = 632.545\,K$$

$$P_c := \frac{1bar}{\left[0.113 + 0.0032 \cdot n_a - \left[\sum_{i=0}^{n} \left(F_{val_{i,1}} \cdot F_{val_{i,3}}\right)\right]\right]^2} = 5.528 \times 10^6\,Pa$$

$$V_c := \left[17.5 + \sum_{i=0}^{n} \left(F_{val_{i,1}} \cdot F_{val_{i,4}}\right)\right] \frac{dm^3}{kmol} = 2.695 \times 10^{-4} \frac{m^3}{mol}$$

m-dinitrobenzene



$$F_{val} := \begin{pmatrix} \text{"OH"} & 1 & 0.0741 & 0.0112 & 28 \\ \text{"CH2"} & 1 & 0.0189 & 0 & 56 \\ \text{"Oring"} & 1 & 0.0098 & 0.0048 & 13 \\ \text{">C="} & 1 & 0.0143 & 0.0008 & 32 \\ \text{"CH="} & 4 & 0.0082 & 0.0011 & 41 \end{pmatrix}$$

$T_b := 443.2K$

$n := 4 \qquad n_a := 13$

$dm := 0.1m$

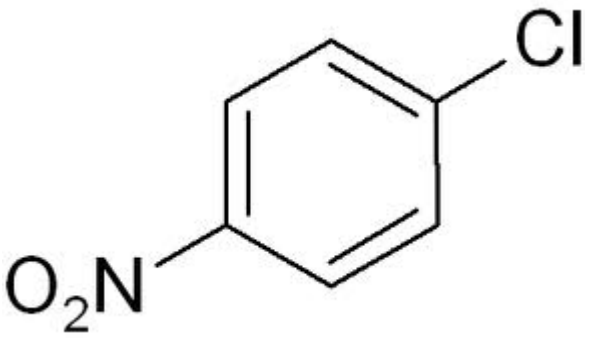
$kmol := 1000mol$

$kJ := 1000J$

$$T_c := \frac{T_b}{0.584 + 0.965 \cdot \left[\sum_{i=0}^{n} \left(F_{val_{i,1}} F_{val_{i,2}}\right)\right] - \left[\sum_{i=0}^{n} \left(F_{val_{i,1}} \cdot F_{val_{i,2}}\right)\right]^2} = 627.599\ K$$

$$P_c := \frac{1bar}{\left[0.113 + 0.0032 \cdot n_a - \left[\sum_{i=0}^{n} \left(F_{val_{i,1}} \cdot F_{val_{i,3}}\right)\right]\right]^2} = 5.619 \times 10^6\ Pa$$

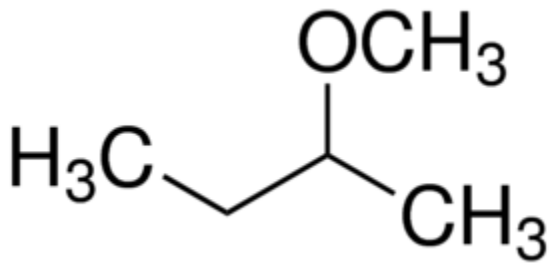
$$V_c := \left[17.5 + \sum_{i=0}^{n} \left(F_{val_{i,1}} \cdot F_{val_{i,4}}\right)\right] \frac{dm^3}{kmol} = 3.105 \times 10^{-4}\ \frac{m^3}{mol}$$



$$DH := \begin{pmatrix} \text{"Cb-H-2Cb"} & 4 & 6.53 \\ \text{"Cb-NO2-2Cb"} & 1 & -32.5 \\ \text{"Cb-Cl-2Cb"} & 1 & -32 \end{pmatrix}$$

$$\Delta H_f := \frac{kJ}{mol}\left[\sum_{i=0}^{2} \left(DH_{i,1} \cdot DH_{i,2}\right)\right] = -38.38\ \frac{kJ}{mol}$$

$$\Delta H_{fDippr} := -40.056\ \frac{kJ}{mol} \qquad \frac{\Delta H_f - \Delta H_{fDippr}}{\Delta H_{fDippr}} = -4.184\ \%$$



T.b

$$Nan := \begin{pmatrix} \text{"CH3-(e)"} & 1 & 251.8338 \\ \text{"CH3-(ne)"} & 2 & 177.3066 \\ \text{"C(c)H2"} & 1 & 239.4531 \\ \text{"C(c)H"} & 1 & 240.6785 \\ \text{"C-O-C"} & 1 & 146.4836 \end{pmatrix} \qquad n := 6$$

$$T_b := \left[\frac{\sum_{i=0}^{rows(Nan)-1} \left(Nan_{i,1} \cdot Nan_{i,2} \right)}{n^{0.6583} + 1.6868} + 84.3395 \right] K = 333.968\,K$$

$$T_{b.DIPPR} := 332.15K$$

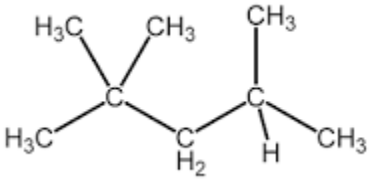
$$\frac{T_b - T_{b.DIPPR}}{T_{b.DIPPR}} = 0.547\,\%$$

$$Nan := \begin{pmatrix} \text{"CH3-(e)"} & 1 & 251.8338 \\ \text{"CH3-(ne)"} & 2 & 177.3066 \\ \text{"C(c)H2"} & 1 & 239.4531 \\ \text{"C(c)H"} & 1 & 240.6785 \\ \text{"C-O-C"} & 1 & 146.4836 \end{pmatrix} \qquad n := 6$$

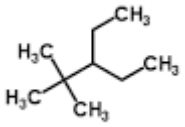
$$T_b := \left[\frac{\sum_{i=0}^{rows(Nan)-1} \left(Nan_{i,1} \cdot Nan_{i,2} \right)}{n^{0.6583} + 1.6868} + 84.3395 \right] K = 333.968\,K$$

$$T_{b.DIPPR} := 332.15K$$

$$\frac{T_b - T_{b.DIPPR}}{T_{b.DIPPR}} = 0.547\,\%$$



$$W_{mat} := \begin{pmatrix} 0 & 1 & 2 & 2 & 2 & 3 & 4 & 4 \\ 1 & 0 & 1 & 1 & 1 & 2 & 3 & 3 \\ 2 & 1 & 0 & 2 & 2 & 3 & 4 & 4 \\ 2 & 1 & 2 & 0 & 2 & 3 & 4 & 4 \\ 2 & 1 & 2 & 2 & 0 & 1 & 2 & 2 \\ 3 & 2 & 3 & 3 & 1 & 0 & 1 & 1 \\ 4 & 3 & 4 & 4 & 2 & 1 & 0 & 2 \\ 4 & 3 & 4 & 4 & 2 & 1 & 2 & 0 \end{pmatrix}$$



$$W_{mat} := \begin{pmatrix} 0 & 1 & 2 & 2 & 2 & 3 & 3 & 4 & 4 \\ 1 & 0 & 1 & 1 & 1 & 2 & 2 & 3 & 3 \\ 2 & 1 & 0 & 2 & 2 & 3 & 3 & 4 & 4 \\ 2 & 1 & 2 & 0 & 2 & 3 & 3 & 4 & 4 \\ 2 & 1 & 2 & 2 & 0 & 1 & 1 & 2 & 2 \\ 3 & 2 & 3 & 3 & 1 & 0 & 2 & 1 & 3 \\ 3 & 2 & 3 & 3 & 1 & 2 & 0 & 3 & 1 \\ 4 & 3 & 4 & 4 & 2 & 1 & 3 & 0 & 4 \\ 4 & 3 & 4 & 4 & 2 & 3 & 1 & 4 & 0 \end{pmatrix}$$

$n_c := 9$

$$w_b := \frac{1}{2} \cdot \sum_{i=0}^{rows(W_{mat})-1} \sum_{j=0}^{rows(W_{mat})-1} W_{mat_{i,j}} = 88$$

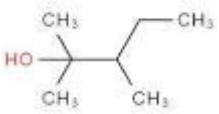
$Pb_2 := match(3, W_{mat})$ $\quad p_b := \frac{rows(Pb_2)}{2} = 10$

$w_n := 120$ $\quad p_n := 6$

$$T_{b.w} := \left[1209.59 - \frac{1162.91}{1 + 0.074189 \cdot n_c^{0.85}} - 96.52 \cdot \left(\frac{w_n - w_b}{n_c^{2}} \right) - 5.45 \cdot (p_n - p_b) \right] K = 407.629\,K$$

$T_{b.DIPPR} := 406.99K$

$$\frac{T_{b.w} - T_{b.DIPPR}}{T_{b.DIPPR}} = 0.157\,\%$$



$$\delta := \begin{pmatrix} 1 \\ 3 \\ 3 \\ 2 \\ 2 \\ 5 \\ 1 \\ 1 \end{pmatrix}$$

$$X_{1v} := \frac{1}{\sqrt{\delta_0 \delta_1}} + \frac{1}{\sqrt{\delta_1 \delta_2}} + \frac{1}{\sqrt{\delta_1 \delta_6}} + \frac{1}{\sqrt{\delta_2 \delta_3}} + \frac{1}{\sqrt{\delta_2 \delta_7}} + \frac{1}{\sqrt{\delta_3 \delta_4}} + \frac{1}{\sqrt{\delta_4 \delta_5}} = 3.29$$

$$S := 10^{6.52-(2.61)\cdot X_{1v}} \frac{mol}{dm^3} = 8.58 \frac{mol}{m^3}$$

$$MW := 0.116 \frac{kg}{mol}$$

$$S \cdot MW = 0.995 \frac{gm}{L}$$