General Subroutine for Calculating

\[ \int_{T_{0}}^{T} \frac{\Delta C_{P}}{R} \, dT \]

MDCPS---Mean Differential Heat Capacity for Entropy Calculations
IDCPS----Integral Differential Heat Capacity for Entropy Calculations

\[ \Delta A = \sum_{i} v_{i} \cdot A_{i} \hspace{1cm} \Delta B = \sum_{i} v_{i} \cdot B_{i} \hspace{1cm} \Delta C = \sum_{i} v_{i} \cdot C_{i} \hspace{1cm} \Delta D = \sum_{i} v_{i} \cdot D_{i} \]

'\( i \)' refers to the total number of products and reactants in the chemical reaction under consideration

'\( v_{i} \)' refers to the stoichiometric coefficient of the \( i \)th component of the reaction

Use the following subroutine to your main worksheet for the differential heat capacity calculations to find the entropy:

\[ \tau(T_{0}, T) := \frac{T}{T_{0}} \]

\[ S_{2}(T_{0}, T, \Delta C, \Delta D) := \Delta C \cdot T_{0}^{2} + \frac{\Delta D}{\tau(T_{0}, T)^{2} \cdot T_{0}^{2}} \]

\[ S_{3}(T_{0}, T) := \frac{\tau(T_{0}, T) + 1}{2} \]

\[ S_{4}(T_{0}, T) := \frac{\tau(T_{0}, T) - 1}{\ln(\tau(T_{0}, T))} \]

\[ \text{MDCPS}(T_{0}, T, \Delta A, \Delta B, \Delta C, \Delta D) := \Delta A + (\Delta B \cdot T_{0} + S_{2}(T_{0}, T, \Delta C, \Delta D) \cdot S_{3}(T_{0}, T)) \cdot S_{4}(T_{0}, T) \]

\[ \text{IDCPS}(T_{0}, T, \Delta A, \Delta B, \Delta C, \Delta D) := \text{MDCPS}(T_{0}, T, \Delta A, \Delta B, \Delta C, \Delta D) \cdot \ln(\tau(T_{0}, T)) \]

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