

Enthalpy of Fusion of Uranium Dioxide

Recommendation

The recommended value for the enthalpy of fusion of UO_{2,00} is:

$$\Delta H_f = 70 \pm 4 \text{ kJ} \cdot \text{mol}^{-1}$$

or $259.3 \pm 14.8 \text{ kJ} \cdot \text{kg}^{-1}$. The enthalpy of fusion was calculated from the following equations for the enthalpy of solid and of liquid UO₂ at the melting point of 3120 K:

Solid UO₂; $298.15 \text{ K} \leq T \leq 3120 \text{ K}$,

$$\begin{aligned} H(T) - H(298.15 \text{ K}) &= C_1 \theta \left[(e^{\theta/T} - 1)^{-1} - (e^{\theta/298.15} - 1)^{-1} \right] \\ &\quad + C_2 [T^2 - (298.15)^2] \\ &\quad + C_3 e^{-E_a/T} \end{aligned} \tag{1}$$

where $C_1 = 81.613$,

$$\theta = 548.68,$$

$$C_2 = 2.285 \times 10^{-3},$$

$$C_3 = 2.360 \times 10^7,$$

$$E_a = 18531.7,$$

T is the temperature in K and the enthalpy increment, $H(T) - H(298.15 \text{ K})$, is in J·mol⁻¹.

Liquid UO₂; $3120 \text{ K} \leq T \leq 4500 \text{ K}$,

$$H(l, T) - H(s, 298.15 \text{ K}) = 8.0383 \times 10^5 + 0.25136T - \frac{1.3288 \times 10^9}{T} \tag{2}$$

where T is the temperature in K and the enthalpy increment $H(l, T) - H(s, 298.15 \text{ K})$, is in J·mol⁻¹.

Discussion of Recommendation

Equation (1) for the enthalpy of solid UO₂ is a weighted least squares analysis of the enthalpy data of Leibowitz et al. [1], Fredrickson and Chasanov [2], Hein and Flagella [3,4], Ogard and Leary [5], and Moore and Kelly [6] and the heat capacity data from 293 to 1006 K of Huntzicker and Westrum [7] and Gronvold et al. [8] and the heat capacity data from 1997-2873 K from recent measurements by Ronchi et al.[9]. Equation (2) for the enthalpy of liquid UO₂, is a combined fit of the liquid UO₂ heat capacity data of Ronchi et al. [10] and the enthalpy data of Leibowitz et al. [11] and of Hein and Flagella [3,4]. No constraint on the value of the liquid enthalpy at the melting point has been included in this analysis of the liquid data.

The recommended value for the enthalpy of fusion is less than the previously recommended value, 74.8 kJ · mol⁻¹ [12,13]. The enthalpy of fusion given in MATPRO [14] is: 274.0 kJ · kg⁻¹ which is 74.0 kJ · mol⁻¹.

Uncertainty

The uncertainty in the recommended enthalpy of fusion of UO₂ is $\pm 6\%$

References

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