Enthalpy of Combustion of 1,4-Benzenedicarboxaldehyde

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Chemical process engineers need the fundamental thermodynamic properties of various reactants, intermediates, and products to efficiently design an industrial process. However, more often than naught, the necessary thermodynamic properties are not available for many of the industrial chemicals of interest. Results of a study on 1,4-benzenedicarboxaldehyde will be presented where techniques will be demonstrated for both the measurement and estimation of some desired thermodynamic properties. The specific energy of combustion of crystalline 1,4-benzenedicarboxaldehyde was determined in a PARR adiabatic bomb calorimeter. The standard molar enthalpy of combustion at T = 298.15 K and p° = 10^5 Pa is $\Delta_c H_m^\circ$ ($C_8H_6O_2$, cr, 298.15 K) = -(3765.70 ± 0.58) kJ·mol^{-1}. The derived standard molar enthalpy of formation is $\Delta_f H_m^\circ$ ($C_8H_6O_2$, cr, 298.15 K) = -(239.87 ± 1.20) kJ·mol^{-1}. The enthalpy of fusion $\Delta_{fus} H_m^\circ$ ($C_8H_6O_2$, cr, 387.36 K) = (24.10 ± 0.24) kJ·mol^{-1} was determined by differential scanning calorimetry. The Kirchhoff relationship, d(ΔH) = ΔC_p • dT, was used to convert this value to T=298.15 K and is $\Delta_{fus} H_m^\circ$ ($C_8H_6O_2$, cr, 298.15 K) = (20.96 ± 0.42) kJ·mol^{-1}. The enthalpy of fusion was used to calculate the enthalpy of formation for the liquid state of 1,4-benzenedicarboxaldehyde, $\Delta_f H_m^\circ$ ($C_8H_6O_2$, l, 298.15 K) = -(218.91 ± 1.27) kJ·mol^{-1}. An enthalpy of vaporization $\Delta_{vap} H_m^\circ$ ($C_8H_6O_2$, l, 298.15 K) = (48.45 ± 0.49) kJ·mol^{-1} was calculated using an estimation scheme of Lebedev and Miroshnichenko. The enthalpy of vaporization was used to calculate the enthalpy of formation for the gaseous state of 1,4-benzenedicarboxaldehyde, $\Delta_f H_m^\circ$ ($C_8H_6O_2$, g, 298.15 K) = -(170.46 ± 1.36) kJ•mol^{-1} from the enthalpy of formation of the liquid state.