A Correlation for Cp for Solid Hydrocarbons Based on Elemental Composition

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A correlation for the constant pressure heat capacity, C_p, valid from 0 K to the fusion temperature for pure solid hydrocarbons is presented. The predictive correlation includes 7 universal coefficients. The variables are temperature and the number of atoms per unit mass. The training data set comprises more than 90 compounds with a wide range of molecular structures and elemental compositions that include nitrogen, oxygen and sulfur substituted hydrocarbon compounds. Solid-solid transition enthalpies were excluded from the data set. The average absolute error for the training data set is less than 0.07 kJ/K·kg. The principal applications for the correlation are for the estimation of heat capacity of large organic molecules, where data are normally unavailable, and for poorly defined organic solids such as asphaltenes where elemental analysis but not molecular structure, are available. The correlation is described and key applications illustrated.