There is considerable interest in prediction of reactive hazards based on chemical structure. Calorimetric measurements to determine reactivity can be resource consuming, so computational methods to predict reactivity hazards present an attractive option. This paper reviews some of the commonly employed theoretical hazard evaluation techniques, including the oxygen balance method, ASTM CHETAH, and Calculated Adiabatic Reaction Temperature (CART). It also discusses the development of a study table to correlate and predict calorimetric properties of pure compounds. Quantitative structure-property relationships (QSPR) based on quantum calculations can be employed to correlate calorimetrically measured onset temperatures and heats of reaction with molecular properties. The QSPR technique is applied to DSC data for nineteen nitro compounds to test the feasibility of this approach.