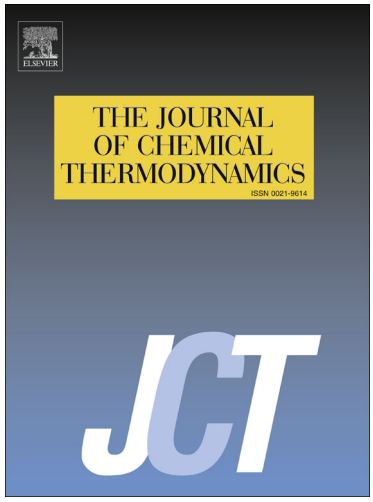

Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: evaluation of thermochemical data with complementary experimental and computational methods

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Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: evaluation of thermochemical data with complementary experimental and computational methods

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A B S T R A C T

The standard molar enthalpies of vaporization of alkyl-pyrazoles were derived from their vapor pressure - temperature dependence measured by the transpiration method as well as indirectly using solution calorimetry. Thermodynamic data on vaporization processes available in the literature were collected, evaluated, and combined with our own experimental results. Additional combustion experiments on the highly pure 1-methyl-pyrazoles helped to resolve ambiguity in the enthalpy of formation for this compound. We have evaluated and recommended a set of vaporization and formation enthalpies for the alkyl-pyrazoles at 298.15 K as the reliable benchmark properties for further thermochemical calculations. Gas phase molar enthalpies of formation of alkyl-pyrazoles calculated by the high-level quantum-chemical G4 and G3MP2 methods were in an excellent agreement with the recommended experimental data. The hydrogenation/dehydrogenation reaction enthalpies of alkyl-pyrazoles were calculated and compared with the data for other potential liquid organic hydrogen carriers.

Keywords: pyrazole derivatives; LOHC; vapor pressure measurements; solution calorimetry; enthalpy of vaporization; enthalpy of formation; quantum-chemical calculations

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