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Thermochemistry of dihalogen-substituted benzenes: Data evaluation using experimental and quantum chemical methods

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Abstract

© 2014 American Chemical Society. Temperature dependence of vapor pressures for 12 dihalogen-substituted benzenes (halogen = F, Cl, Br, I) was studied by the transpiration method, and molar vaporization or sublimation enthalpies were derived. These data together with results available in the literature were collected and checked for internal consistency using structure-property correlations. Gas-phase enthalpies of formation of dihalogen-substituted benzenes were calculated by using quantum-chemical methods. Evaluated vaporization enthalpies in combination with gas-phase enthalpies of formation were used for estimation liquid-phase enthalpies of formation of dihalogen-substituted benzenes. Pairwise interactions of halogens on the benzene ring were derived and used for development of simple group additivity procedures for estimation of vaporization enthalpies, gas-phase, and liquid-phase enthalpies of formation of dihalogen-substituted benzenes.

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