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Thermochemistry of halogen-substituted methylbenzenes

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Abstract

© 2014 American Chemical Society. Experimental vapor pressures, vaporization, fusion, and sublimation enthalpies of a number of bromo- and iodo-substituted methylbenzenes have been studied by transpiration method in order to evaluate a series of experimental measurements that appear to be internally self-consistent. The compounds studied in this regard include bromobenzene, iodobenzene, 1-bromo-2-methylbenzene, 1-bromo-3-methylbenzene, 1-brom--4-methylbenzene, 1-iodo-2-methylbenzene, 1-iodo-3-methylbenzene, 1-iodo-4-methylbenzene, 1-bromo-2,6-dimethylbenzene, 1-iodo-2,6-dimethylbenzene, and 1-iodo-2,4-dimethylbenzene. Gas-phase enthalpies of formation of halogen-substituted methylbenzenes were calculated by using quantum-chemical methods. Simple group-additivity procedures were developed for estimation of vaporization enthalpies and gas-phase and liquid-phase enthalpies of formation of halogen-substituted methylbenzenes. (Figure Presented).

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