



## Structure–property relationships in halogenbenzoic acids: Thermodynamics of sublimation, fusion, vaporization and solubility



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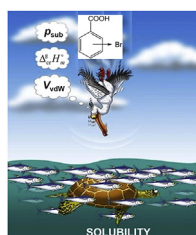
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### HIGHLIGHTS

- Vapor pressures for isomeric bromobenzoic acid measured by the transpiration method.
- Molar enthalpies of sublimation/vaporization were derived and tested for consistency.
- Hydrogen bonding in the condensed phase of the halogenbenzoic acids were quantified.
- Solubilities were correlated with sublimation pressures and sublimation enthalpies.
- New results resolve the ambiguity in available thermochemical and solubility data.

### GRAPHICAL ABSTRACT



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### ABSTRACT

Temperature dependences of vapor pressures for 2-, 3-, and 4-bromobenzoic acid, as well as for five isomeric bromo-methylbenzoic acids were studied by the transpiration method. Melting temperatures and enthalpies of fusion for all isomeric bromo-methylbenzoic acids and 4-bromobenzoic acid were measured with a DSC. The molar enthalpies of sublimation and vaporization were derived. These data together with results available in the literature were collected and checked for internal consistency using a group-additivity procedure and results from X-ray structural diffraction studies. Specific (hydrogen bonding) interactions in the liquid and in the crystal phase of halogenbenzoic acids were quantified based on experimental values of vaporization and sublimation enthalpies. Structure-property correlations of solubilities of halogenbenzoic acids with sublimation pressures and sublimation enthalpies were developed and solubilities of bromo-benzoic acids were estimated. These new results resolve much of the ambiguity in the available thermochemical and solubility data on bromobenzoic acids. The approach based on structure property correlations can be applied for the assessment of water solubility of sparingly soluble drugs.

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