
Research Paper

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PII: S0939-6411(13)00152-5
DOI: http://dx.doi.org/10.1016/j.ejpb.2013.04.006
Reference: EJPB 11398

To appear in: *European Journal of Pharmaceutics and Biopharmaceutics*

Received Date: 24 October 2012
Accepted Date: 12 April 2013

Please cite this article as: S. Just, F. Sievert, M. Thommes, J. Breitkreutz, Improved group contribution parameter set for the application of solubility parameters to melt extrusion, *European Journal of Pharmaceutics and Biopharmaceutics* (2013), doi: http://dx.doi.org/10.1016/j.ejpb.2013.04.006

# Improved group contribution parameter set for the application of solubility parameters to melt extrusion

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## Abstract

Hot-melt extrusion is gaining importance for the production of amorphous solid solutions; in parallel, predictive tools for estimating drug solubility in polymers are increasingly demanded. The Hansen solubility parameter (SP) approach is well acknowledged for its predictive power of the miscibility of liquids as well as the solubility of some amorphous solids in liquid solvents. By solely using the molecular structure, group contribution (GC) methods allow the calculation of Hansen SPs. The GC parameter sets available were derived from liquids and polymers which conflicts with the object of prediction, the solubility of solid drugs. The present study takes a step from the liquid based SPs towards their application to solid solutes. On the basis of published experimental Hansen SPs of solid drugs and excipients only, a new GC parameter set was developed. In comparison to established parameter sets by van Krevelen/Hoftyzer, Beerbower/Hansen, Breitkreutz and Stefanis/Panayiotou, the new GC parameter set provides the highest overall predictive power for solubility experiments (correlation coefficient r=-0.87 to -0.91) as well as for literature data on melt extrudates and casted films (r=-0.78 to -0.96).

## Keywords

partial solubility parameters, group contribution method, hot-melt extrusion, solid drug solutions, polyethylene glycol