Modeling the Phase Behavior in Mixture of Pharmaceuticals with Liquid or Supercritical Solvents - DTU Orbit (24/12/2018)

Modeling the Phase Behavior in Mixtures of Pharmaceuticals with Liquid or Supercritical Solvents

The concept of solubility parameter, which is widely used for the screening of solvents in pharmaceutical applications, is combined with a thermodynamic theory that is able to model systems with large deviations from ideal behavior. The nonrandom hydrogen-bonding (NRHB) theory is applied to model the phase behavior of mixtures of six pharmaceuticals (i.e., ibuprofen, ketoprofen, naproxen, benzoic acid, methyl paraben, and ethyl paraben). The pure fluid parameters of the studied pharmaceuticals were estimated using limited available experimental (or predicted) data on sublimation pressures, liquid densities, and Hansen’s solubility parameters. The complex hydrogen-bonding behavior was explicitly accounted for, while the corresponding parameters were adopted from simpler molecules of similar chemical structure or/she explicitly fitted to the aforementioned pure fluid properties. In this way, the solubility of the studied pharmaceuticals in liquid solvents was calculated. The average root-mean-square deviation between experimental and calculated solubilities is 0.190 and 0.037 in log10 units for prediction (calculations without a binary interaction parameter adjustment) and for correlation (calculations using one binary interaction parameter fitted to experimental data), respectively. In addition, using one temperature-independent binary interaction parameter the phase behavior of pharmaceuticals in supercritical CO2 and ethane was satisfactorily correlated. Finally, preliminary encouraging results are shown concerning two ternary mixtures where the model is able to predict accurately the solubility of pharmaceuticals in mixed solvents based on interaction parameters fitted to corresponding single solvent data.

General information
State: Published
Organisations: Center for Phase Equilibria and Separation Processes, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering
Contributors: Tsivintzelis, I., Economou, I., Kontogeorgis, G.
Pages: 6446-6458
Publication date: 2009
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry Part B: Condensed Matter, Materials, Surfaces, Interfaces & Biophysical
Volume: 113
Issue number: 18
ISSN (Print): 1520-6106
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.13 SJR 1.331 SNIP 1.015
Web of Science (2017): Impact factor 3.146
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.03 SJR 1.345 SNIP 1.012
Web of Science (2016): Impact factor 3.177
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.25 SJR 1.335 SNIP 1.076
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.28 SJR 1.449 SNIP 1.138
Web of Science (2014): Impact factor 3.302
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 3.53 SJR 1.504 SNIP 1.202
Web of Science (2013): Impact factor 3.377
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.66 SJR 1.943 SNIP 1.256
Web of Science (2012): Impact factor 3.607
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 3.62 SJR 1.801 SNIP 1.223
Web of Science (2011): Impact factor 3.696
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.881 SNIP 1.22
Web of Science (2010): Impact factor 3.603
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.266 SNIP 1.353
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.58 SNIP 1.383
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.422 SNIP 1.426
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.335 SNIP 1.484
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.199 SNIP 1.542
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.163 SNIP 1.513
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.178 SNIP 1.54
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.177 SNIP 1.524
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.114 SNIP 1.532
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.658 SNIP 1.8
Original language: English
DOIs:
10.1021/jp807952v
Source: orbit
Source-ID: 220955
Research output: Research - peer-review › Journal article – Annual report year: 2009