

COSMOtherm computes a broad variety of thermodynamic properties of pure compounds and mixtures and it covers a wide range of problems:

- Activity coefficients
- Henry's law coefficients
- Vapor pressure of pure compounds and mixtures
- Heat of vaporization
- Partition of a solute between two arbitrary solvents
- Distillation separation coefficients
- Heat of mixing
- Phase diagrams including azeotropes, miscibility gaps
- Vapor-liquid-equilibria (VLE)
- Liquid-liquid-equilibria (LLE)
- Solid-liquid-equilibria (SLE)
- Solubility of gases, liquids and solids
- Reaction thermodynamics in solution
- Solubility in polymers
- General adsorption phenomena
- Physiological and general partition coefficients

COSMOtherm is subject to active research and development, but further it is fully applicable just now.

Start with us into the future of thermodynamic property prediction!

COSMOlogic GmbH & Co. KG

Your Competent Partner for
Computational Chemistry and Fluid Thermodynamics

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COSMOlogic Products

- **COSMOtherm**: Software for Fluid Phase Thermodynamics
- **COSMObase**: Database of 1150 DFT/COSMO-files for common solvents and compounds
- **TURBOMOLE**: Fast Quantum Chemical Program (Prof. R. Ahlrichs, Univ. of Karlsruhe, Redistribution and Support by COSMOlogic)

COSMOlogic Services

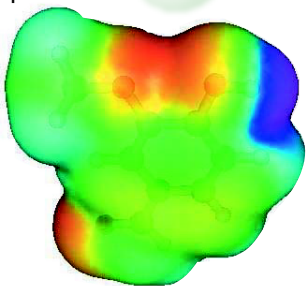
- Consulting in Computational Chemistry and Fluid Phase Thermodynamics
- Contract Calculations in the Context of COSMOtherm
- Contract Research, Development, and Programming in Computational Chemistry related Areas
- General Programming of Interfaces and Tools for Chemistry and Chemical Engineering

COSMOtherm

Reliable Thermodynamic Data of Liquids from Quantum Chemistry

Cosmotherm works where group contribution methods fail!

COSMOtherm (originally COSMO-RS) derives the thermophysical behavior of liquids from the information provided by unimolecular quantum chemical calculations (DFT) on the compounds of interest. In these calculations each molecule is handled as if it was embedded in a conductor (COSMO-approximation). As a result, the screening charge density σ is available on each part of the molecular surface, as it is illustrated by vanillin on the right.

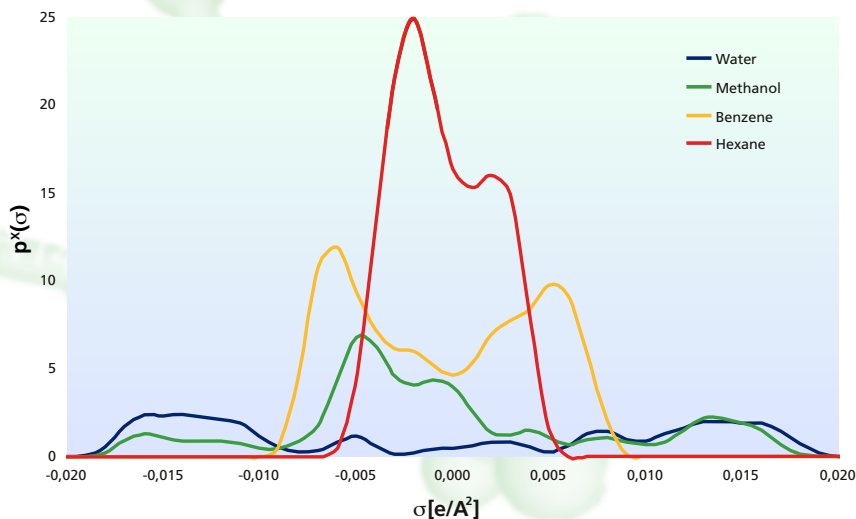


As a second step all interactions of molecules in liquids are described as contact interactions of molecular surfaces, and the interaction energies are quantified using the screening charge densities σ and σ' of the two interacting surface pieces. This results in the expressions

$$E_{hb}(\sigma, \sigma') = a_{eff} e_{hb}(\sigma, \sigma') = a_{eff} c_{hb} \min\{0, \sigma\sigma' + \sigma_{hb}^2\}$$

$$E_{misfit}(\sigma, \sigma') = a_{eff} e_{misfit}(\sigma, \sigma') = a_{eff} \frac{\alpha'}{2} (\sigma + \sigma')^2$$

for the electrostatic misfit and for the hydrogen bonding energy, respectively. The few parameters appearing in these formulae have been carefully adjusted to experimental data.

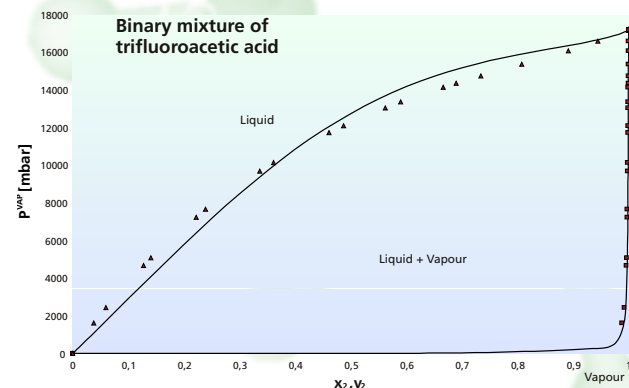


For an efficient statistical thermodynamics calculation the molecular surfaces are virtually split into small pieces of size a_{eff} , and contacts of such pieces are considered as independent. This approach (which is similar to the assumption of interacting surfaces in group contribution methods) corresponds to a reduction of the spatial screening charge distribution to a one-dimensional histogram, which we call σ -profile. As illustrated below σ -profiles $p^X(\sigma)$ are characteristic for each compound X.

It is important to note, that the σ -profile $p_S(\sigma)$ of a mixture S is simply given by the weighted sum of the σ -profiles of the components. Now the statistical thermodynamics of the system S of interacting surface pieces is calculated by an efficient and exact algorithm, ending up with a chemical potential of each component X. At this point, activity coefficients and many other thermophysical properties of the system (e.g. excess enthalpy and entropy and even vapor pressure) are readily available. This novel statistical thermodynamics is more exact than the algorithm used in group contribution methods, avoiding any mean-field assumption and hence being as reliable in the limit of infinite dilution as it is with finite concentrations.

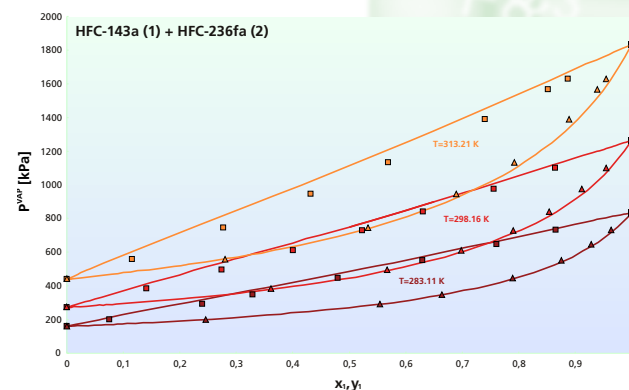
Applications

COSMOtherm can be used for the reliable calculation of activity coefficients and a broad variety of other thermophysical data of binary and multi-component mixtures.



Scope of COSMOtherm

The primary scope of COSMOtherm is not the calculation of relatively simple systems, which can be satisfactorily handled by group-contribution methods. The great advantage of the a priori method COSMOtherm compared to structure-interpolating group contribution methods is its almost **general applicability** to organic compounds, since all relevant elements of organic chemistry are parameterized. Thus there is no problem of missing interaction parameters any more. In contrast to group contribution methods, COSMOtherm is able to resolve molecular details like isomer differences, and it very well handles intramolecular interactions like electronic push-pull effects of polar substituents and intramolecular hydrogen bonds.



Finally, COSMOtherm is even able to handle exotic states like metastable compounds or transition states, which may be useful in reaction simulations. Thus, COSMOtherm is a tool for your hard problems, where other methods fail to predict properties. Even more, by its physically based interaction model COSMOtherm helps you to understand the interactions in liquid systems instead of just correlating them.

Efficiency Aspects

The quantum chemical density functional (DFT) COSMO calculations can nowadays be run over night for compounds up to about 20 atoms and over weekend for compounds up to about 35 atoms, even on powerful PC-processors.

It is important to note that the DFT-COSMO calculation is required only once per compound. The COSMO-files can be stored in a database and re-used in later COSMOtherm calculations. A database (COSMObase) with more than thousand solvents and other common compounds is available from COSMOlogic.

COSMOtherm only takes milliseconds for a calculation and is able to run on any PC or UNIX computer. Thus COSMOtherm is a very efficient tool for routine use in chemical engineering.

References:

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- A. Klamt, V. Jonas, T. Buerger, J.C.W. Lohrenz, J. Phys. Chem. A, **102** (1998) 5074
- A. Klamt, F. Eckert, Fluid Phase Equilibria **172** (2000) 43.