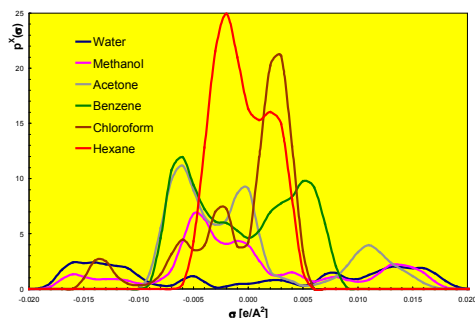


# Thermodynamic Property Prediction Tools from

# COSMOlogic GmbH & Co. KG

Your Competent Partner for  
Computational Chemistry and Fluid Thermodynamics

COSMOlogic's unique suite of tools\* for accurately predicting thermodynamic and physical properties from quantum chemistry, is distributed & supported in the Americas exclusively by CAChe Research LLC.



Sigma-profiles provide insight into miscibility, solubility & ADME properties

## Thermodynamic Property Prediction

**COSMOtherm** predicts a wide range of properties for both pure compounds and mixtures, such as boiling points, vapor pressures, solubilities, ADME properties, viscosities, partition coefficients, phase equilibria, phase diagrams, azeotropes, heat of mixing, reaction thermodynamics, activity coefficients, sigma profiles, and much more. **COSMOtherm** is based on quantum chemistry and the novel COSMORS methodology developed by Andreas Klamt, and so does not suffer from the same limitations as the group-contribution methods. **COSMOtherm** is widely used in chemical process engineering, environmental chemistry, and life sciences.

## Micelle & Biomembrane Modeling

**COSMOmic** models surfactant micelles or biomembranes as inhomogeneous, layered liquids, allowing the calculation of properties such as free energy profiles and membrane partition coefficients of solutes. **COSMOmic** can deal with neutral or ionic solutes in spherical, cylindrical or lamellar type membranes.

## High-throughput ADME Screening

**COSMOfrag** is a program for the rapid generation of sigma-profiles of novel compounds from a database of pre-computed DFT COSMO files of drug-like molecules. Combined with **COSMOtherm**, it can estimate thermodynamic properties of new compounds in a fraction of a second. **COSMOfrag** is designed for high-throughput applications such as pharmaceutical R&D, where full DFT calculations on every candidate molecule would not be practical. When searching large libraries of candidate molecules for ADME and other thermodynamic properties, **COSMOfrag** offers a huge gain in speed and throughput for only a slight loss in accuracy.

## Solvents & Chemicals Database

**COSMObase** is a database of over 3,500 DFT-optimized structures and COSMO files of common solvents and chemicals. As the database is ready to use with **COSMOtherm**, it can save a vast amount of computer time and resources.

## Ionic Liquids Database

**COSMObase-IL** is a pre-calculated database of commonly used and commercially available ionic liquid anions and cations. **COSMObase-IL** facilitates the fast screening of thermodynamic properties and activity coefficients of solutes in these ionic liquids. New anions and cations can be easily added using DFT/**COSMOtherm** calculations, or by request to **COSMOlogic**.

## Sigma-profile Similarity Screening

**COSMOsim** is an extension of **COSMOfrag**. It performs sigma-profile similarity searches on large libraries of molecules. Since sigma-profiles correlate closely with ADME properties and drug-receptor binding, **COSMOsim** can offer valuable new ideas for drug analogues that may be missed by other methods. A key advantage of **COSMOsim** is its scaffold-hopping capability, as it is based on similarity of properties rather than the underlying chemical structures.

## Fast, Accurate DFT & ab initio

**TURBOMOLE** is a powerful quantum chemistry program developed by Prof. Ahlrichs' group at the University of Karlsruhe. It is designed for speed and robustness to deal with practical applications including large molecules and condensed phase simulation. **TURBOMOLE** is one of the fastest DFT codes available and can be used to create accurate input files for **COSMOtherm**.

## Contract Services

Please contact us for more information.

\***COSMOlogic** SW is available for Windows® & LINUX

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