BIOVIA

3DEXPERIENCE®

BIOVIA COSMOtherm
PROPERTY PREDICTION FOR MOLECULES IN LIQUIDS

Datasheet

DASSAULT SYSTEMES

PREDICTION OF THERMODYNAMIC PROPERTIES

BIOVIA COSMOtherm is a software to predict thermodynamic properties such as solubilities, activity coefficients or vapor pressures in liquid mixtures.

WORKS WITHOUT EXPERIMENTAL DATA

BIOVIA COSMOtherm applies the fully predictive COSMO-RS model and requires no experimental data. All information is taken from COSMO files for each compound, which can be generated with quantum chemistry programs (e.g. TURBOMOLE) and stored for later use.

YOUR BENEFIT

- Guide your experiments to save lab time and improve your results
- Find new or unexpected solutions by screening large databases of possible solvents, co-solvents, entrainers, and other additives
- Investigate new areas of chemistry without further adjustments

Application Areas

- Chemical engineering
- Drug design & development
- Chemistry
- Environmental science
- Formulation
- Quantum chemistry

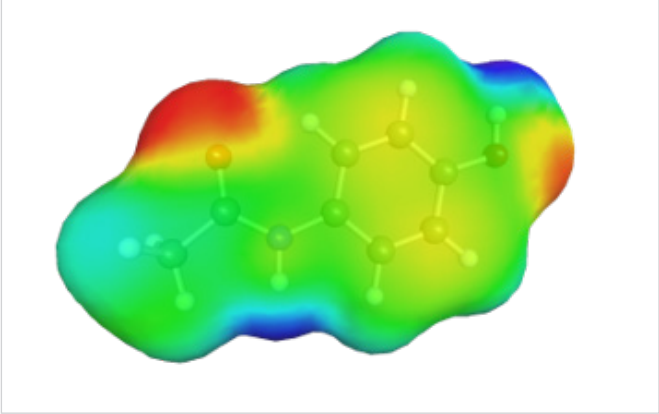
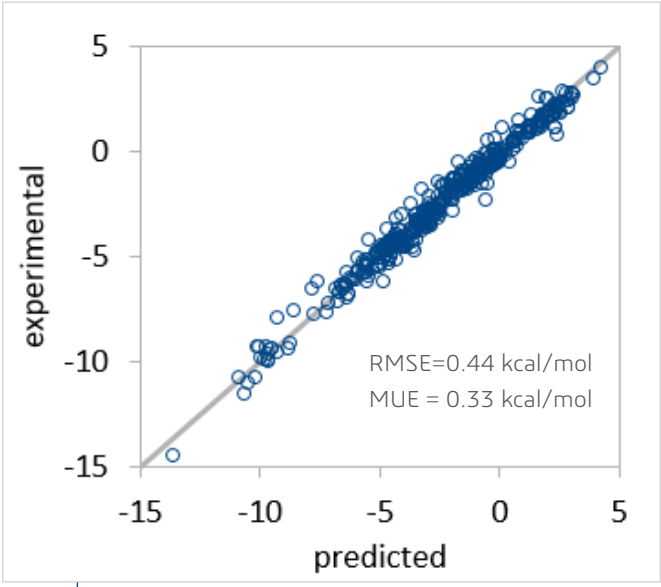


Figure 1: COSMO surface of paracetamol

PROPERTY OVERVIEW

A large number of liquid phase equilibrium properties can be predicted with consistent accuracy for pure compounds as well as complex mixtures and formulations. All equilibrium properties can be predicted with temperature dependence, i.e. also providing a split into enthalpy and entropy.

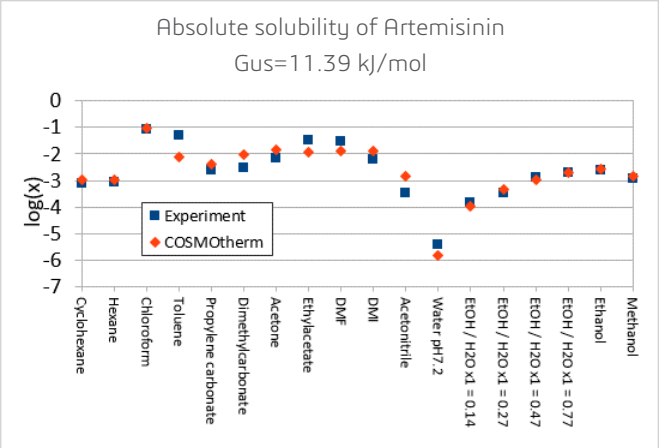
- Solubility of liquids, solids and gases
- Free energy of solvation and vapor pressure
- General activity and partition coefficents
- Multiphase-multicomponent liquid partitioning (extraction)
- pKa and chemical reaction equilibria in different solvents
- Conformer population in different mixtures
- VLE, LLE, and SLE phase diagrams
- Free energy of transfer to a liquid-liquid interface
- Soil adsorption and many other environmental properties
- Interfacial tension, critical micelle concentrations
- Micelles, microemulsions and biomembranes (BIOVIA COSMOplex)



Example: ΔG_{hydr} prediction for 313 organic compounds

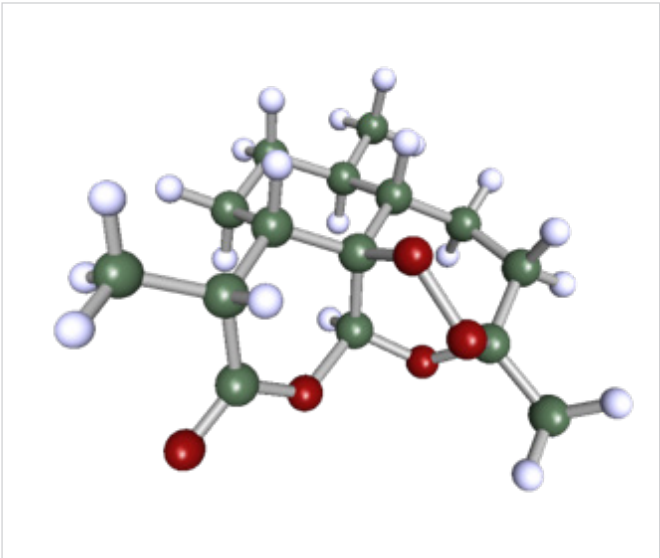
SOLUBILITY AND PARTITIONING

It is a frequent challenge to find an appropriate solvent, cosolvent or antisolvent. BIOVIA COSMOtherm enables you to screen large numbers of candidates and mixtures prior to your lab measurements. Relative solubilities and partition coefficients can be screened without any need for experimental data.



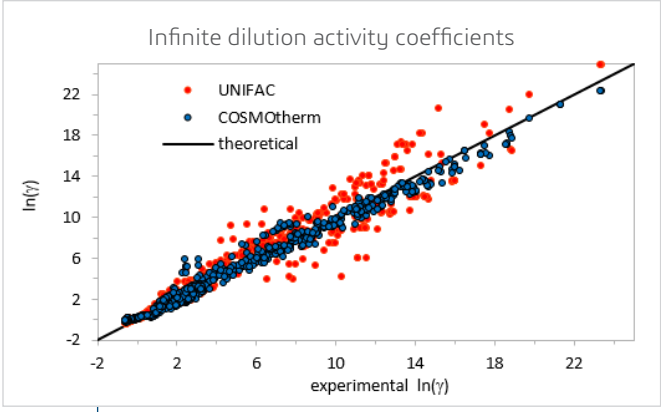
Use BIOVIA COSMOtherm to

- Screen for the optimal solvent or solvent mixture
- Optimize the partitioning behavior, e.g. for liquid extraction purposes
- Find entrainers or cosolvents

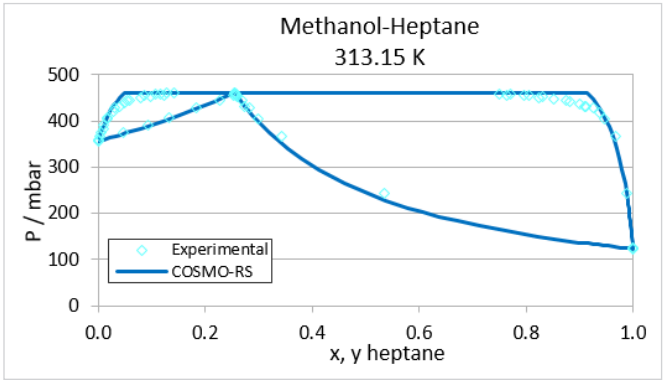


ACTIVITY COEFFICIENTS AND PHASE DIAGRAMS

Chemical engineers often depend on predictions if no experimental data is available. BIOVIA COSMOtherm can predict activity coefficients of solutes in arbitrary mixtures as function of temperature and concentration. Together with experimental or predicted vapor pressures complete phase diagrams can be calculated. Due to its generic, physical approach BIOVIA COSMOtherm robustly predicts even complex molecules.

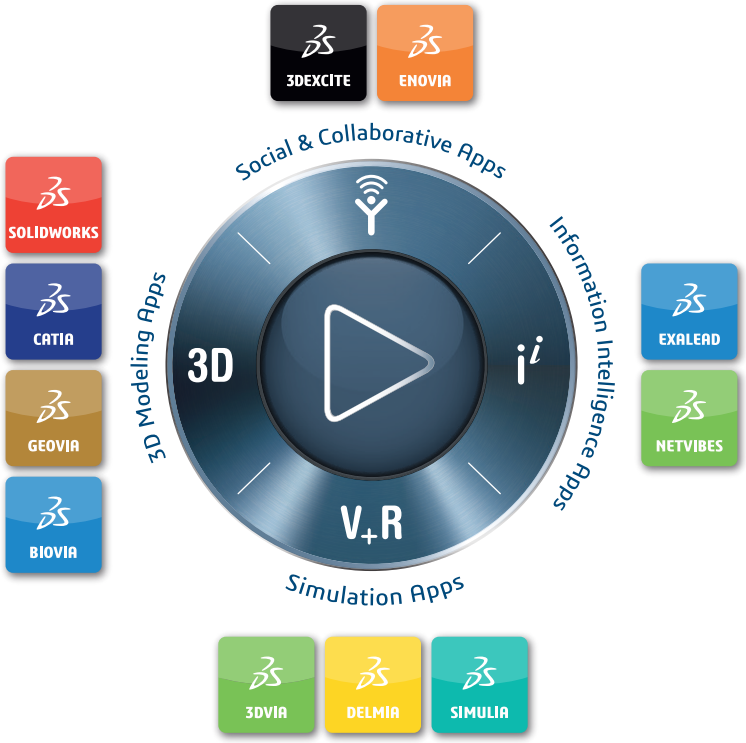


Renan P. Gerber and Rafael de P. Soares, Ind. Eng. Chem. Res. DOI: 10.1021/ie901947m with COSMOtherm1501 predictions



BIOVIA COSMOtherm Strengths

- Robust accuracy for systems containing water or complex molecules (e.g. drugs or drug candidates)
- No system specific adjustments or parameters required
- Widely applicable and predictive to new areas of chemistry
- Native vapor pressure prediction



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