

**COSMOtherm Version C2.1 Release 01.06 (November 2006)**

New features of this distribution include:

**1. Improved accuracy and applicability of COSMOtherm predictions:**

- Further improved sets of COSMOtherm parameters for both high level (BP-TZVP-COSMO) and screening level (BP-SVP-AM1) sigma-profiles were obtained from an enhanced fitting procedure, which includes pure compound and mixture thermodynamic data which is not limited to room temperature. In combination with a further enlarged test set of thermodynamic properties the new parameters results in higher overall accuracy and even broader applicability.
- Rapidly improved sets of COSMOtherm combinatorial contribution adjustable parameters for all quantum chemical levels (BP-TZVP-COSMO and BP-SVP-AM1) were obtained from an enhanced fitting procedure, which includes "simple chemistry" alkane-alkane activity coefficients that result from combinatorial effects (size and shape difference of molecules) only. This further improves the overall accuracy and stability of the method..
- Further improvement in accuracy in the prediction of the properties of alkanes such as vapor pressure, heat of vaporization, activity coefficients, partition coefficients and solubility.
- Optimized COSMO-radii and COSMOtherm van der Waals interaction parameters for elements Silicon (Si) and Germanium (Ge), allow for the computation of arbitrary Silicon- and Germanium- containing metal-organics with an accuracy comparable to the prediction of common organic compounds. The accuracy of the prediction of Silicon compound properties, especially vapor pressure and heat of vaporization, improved rapidly.
- COSMOtherm now is able to handle a "vacuum" molecule without any interactions, which may be used as model compound for special non-interacting phases or surfaces like air or noble gases,

## 2. COSMOthermX graphical user interface (GUI):

- Improved stability and easier usability plus a simplified installation procedure of the COSMOthermX GUI allows for the simple and efficient setup of COSMO $therm$  calculations and the graphical postprocessing of the computed results.
- COSMOthermX now includes a tool for the automatic usage and simple modification and application of external experimental compound data via vapor-pressure/property (name.vap) file usage.
- Strongly enhanced functionality: New automatic "Solgas" gas solubility, "SLE" solid liquid equilibrium, "Flatsurf" surface interaction energy, density, viscosity and  $\sigma$ -moment-QSPR calculation options.
- Graphical display of compound geometries and compound charge surfaces has been enhanced to process multi-compounds and conformers.
- Graphical display of VLE/LLE phase diagrams now is also possible on mass fraction basis.
- Rapid 'string' searching and the addition of many synonym names allow for greater ease in the selection of compounds from COSMO $base$ .

### 3. Enhanced and improved COSMO $therm$ functionality:

- **FLATSURF:** A new algorithm with a significantly improved accuracy has been introduced into the automatic computation option for the iterative determination of the surface activity of solute, i.e. of the free energy gain of a given molecule at a surface or interface between two different liquid phases. It is also possible now to use mixed multi-component solvent phases in the Flatsurf option.
- **CONTACT:** The contact statistics option now allows for the creation of molecular geometry files of binary molecule complexes that have show the highest probability of having a surface-segment contact. This allows the automatic creation of complexes and explicitly solvated molecules.
- **VLE-ISOBAR:** The iterative refinement of the isobar computation of constant-pressure vapor liquid equilibria (binary, ternary and multinary) has been improved strongly. Now the iterative procedure converges faster and significantly safer.

### 4. Improved and simplified COSMO $therm$ input and output:

- Optional output of all numbers in the COSMO $therm$  output file with the full numerical accuracy (i.e. 13 digits).
- Compound molecular weights now are written to the table file for several automatic calculation options, allowing for a mass-fraction based display of VLE curves in the graphical user interface COSMO $therm$ X.

5. Further extension of **COSMObase**, the database of COSMO-files:

- Currently **COSMObase** holds over 4600 molecular COSMO-files, gas phase energy-files and geometry car-files for both high level (BP-TZVP-COSMO) and screening level (BP-SVP-AM1) quantum chemistry. This corresponds to over 3800 chemical compounds.
- **COSMObase**, compound geometries have been critically reviewed for conformational effects and for over 250 compounds COSMO and/or gas phase geometries have been re-optimized and/or additional conformers have been added.
- Currently **COSMObase** holds over 1100 vapor pressure / experimental data property compound.vap-files with pure compound vapor pressure Wagner or Antoine coefficients that can be used to compute the pure compound measured/validated vapor pressure, as well as UNIQUAC volume and area coefficients that can be used in the fitting of activity coefficients to the UNIQUAC equation.
- A large number of compound synonyma and alternative and trivial names has been added to the **COSMObase** database index file, allowing for a simpler identification of a given compound in the database.
- Experimental boiling points and melting points have been added to the database index file for more than 2/3 of the **COSMObase** compounds.
- Experimental heat of fusion data (enthalpy of fusion and melting point) and critical point data for over 250 **COSMObase** compounds.
- All **COSMObase** molecules are identified with a novel unique code.