

COSMOtherm Version C2.1 Release 01.08 (November 2008)

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 a thorough reconsideration of conformers for all compounds involved in the fitting and validation procedure. In addition the fitting and validation procedures were further enhanced, now including temperature dependent pure compound and mixture thermodynamic data of organic, and inorganic neutral compounds, salts and ionic liquids.. The new fitting and validation procedure ensures an improved overall quality of COSMOtherm predictions and assures a widespread applicability over all areas of organic chemistry and some areas of inorganic chemistry.
- Two new quantum chemical COSMO calculation levels and according COSMOtherm parameterizations have been introduced: BP-TZVP-ISOCAV and DMOL3-PBE. The parameter sets for both of the new quantum chemistry levels have been optimized and validated with the same procedure as the standard levels BP-TZVP-COSMO and BP-SVP-AM1 and support the full COSMOtherm functionality:
 - o BP-TZVP-ISOCAV: scaled isodensity (ISOCAV) COSMO-files generated by Turbomole, based on optimized geometries on quantum chemical BP-TZVP-COSMO level (RI-DFT with BP-functional and TZVP basis set).
 - o DMOL3-PBE: DMOL3 quantum chemical COSMO calculations (full geometry optimization) using the PBE DFT-functional with numerical DNP basis set.

2. Enhanced and improved COSMOtherm **functionality**:

- **VLE/LLE/SLE**: In the computation of binary vapor-liquid, liquid-liquid, and solid-liquid phase diagrams it is now possible to define one phase of the phase diagram as a **salt** or **ionic liquid** and thus perform a pseudo-binary calculation of salts or ionic liquids with a second phase.
- **Solubility**: In addition to the computation of solubilities of neutral compounds it is now possible to perform solubility calculation for **ionic liquids** or solid **salts** (in the latter case the salts net free energy of fusion has to be provided).

- **Density:** In addition to the computation of densities of pure neutral compounds it is now possible to perform density calculations for **ionic liquids** and **zwitterions**. A new density QSPR model has been developed to achieve a similar quality with the ionic compounds compared to neutral compounds.
- **Similarity:** A new alternative similarity definition, the sigma-match-similarity (**SMS**, see Thormann, et al. J. Chem. Inf. Model. 46, (2006) 1040) has been added to the automatic similarity computation option.
- **Solvation Energy:** A suboption of the automatic Henry law constant computation option now allows the direct automatic computation of a compounds **free energy of solvation** in a given solvent.
- **Periodic Boundary Conditions:** It is now possible to use COSMO-files with periodic boundary condition (i.e. crystal cell or crystal surface COSMO-files) as computed by the DMOL3 program.
- **Henry:** The output of the automatic Henry law constant computation now can be switched between regular (pressure units) and logarithmic output.
- **Vapor Pressure:** The output of the automatic vapor pressure computation now can be switched between regular (pressure units) and logarithmic output.
- **Conformer Treatment:** COSMO*therm* provides the automatic recognition and usage of conformers, if conformer COSMO-files present are following COSMO*logic's* conformer COSMO-file naming convention.
- **VLE/LLE/SLE:** In the computation of binary vapor-liquid, liquid-liquid, and solid-liquid phase diagrams it is now possible to print and visualize the conformer weights of all compounds along the phase diagram concentrations.
- **COSMO-metafiles:** COSMO*therm* now allows the conformer treatment of COSMO-metafiles (mcos-files). In addition charged COSMO-metafiles can be used.
- **Solubility:** For the output of mass based solubilities now three different definitions can be used: unnormalized mass based solubility, mass based solubility and normalized mass fraction solubility.
- **Contact:** In the visualization of computed contact maps, now all contact maps given in one contact-file can be visualized.
- **Flatsurf:** The flatsurf (surface interaction) computation option has been reviewed and now performs considerably faster than before.
- **Atomic Weights:** In the input of atomic weight strings in the COSMO*therm* input or in a COSMO-metafile, it is now possible to set a default atomic weight different from one .

3. *COSMOthermX* graphical user interface (GUI):

- Significantly improved and extended graphical user interface with newly written graphics routines that are significantly faster and more reliable. Overall new look and feel of the GUI, with lesser clicks required to obtain a result. In addition numerous new usage features have been implemented into the GUI:
 - Strongly enhanced functionality: The (nearly) complete functionality of *COSMOtherm* as available in the command line version, now can be toggled and controlled from within the *COSMOthermX* GUI. New control features include handling of salts and ionic liquid calculations, simplified database handling (including the new BP-TZVP-ISOCAV and DMOL3-PBE methods) and the simplified processing of compound lists.
 - Graphical post-processing of computed thermodynamics has been extended to ternary and n-dimensional "multinary" isobar and isothermal VLE/LLE phase diagrams, the visualization of conformer distribution along a VLE/LLE phase diagram as well as vapor pressure curves.
 - Rapid 'string' searching, smiles code identifiers, atomic weights, and the addition of many synonyms allow for greater ease in the selection of compounds from *COSMObase*.
 - Improved and simplified weight-string and COSMO-meta-file editor for the easier set up of advanced polymer, surface and micelle applications.
 - Simplified *COSMObase* (database of COSMO-files) installation and new editing function for database entries. Several COSMO-file databases can be used from within one compound selection and search window.
 - Improved stability and easier usability plus a simplified installation procedure of the *COSMOthermX* GUI allows for the simple and efficient setup of *COSMOtherm* calculations and the graphical postprocessing of the computed results.
 - In the graphics window, new tool tips allow for easier understanding and creation of plots.
 - All computed tables (graphics tables as well as text files) can be exported to Microsoft-Excel.

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

- All of COSMObase's compounds have been re-optimized with the latest Turbomole version TM5.10 and some database entries and/or cosmo-files have been bug-fixed.
- To ensure an optimum prediction quality in COSMOtherm, COSMObase compound geometries have been critically reviewed for conformational effects and for more than one third of the compounds already present in COSMObase, additional conformers have been added and/or existing conformers have been replaced by better (lower energy) conformers.
- Currently COSMObase holds over 10000 molecular COSMO-files, gas phase energy-files and geometry xyz-files for high level (BP-TZVP-COSMO, BP-TZVP-ISOCAP, and DMOL3-PBE) quantum chemistry and over 15000 molecular COSMO-files, gas phase energy-files and geometry xyz-files for screening level (BP-SVP-AM1) quantum chemistry. This corresponds to over 4700 chemical compounds. Geometry xyz-files are provided for both COSMO and gas phase energy files.
- 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. A unique smiles code (USMI) of the compound geometry has been added to the synonyma of all nonionic compounds in COSMObase. Moreover, if available, the Beilstein-, RTECS-, EC-, and Merck-Index code of the compounds has been added to the synonyma. Solvent compounds are marked by special solvent identifier.
- Every compound COSMO-file now is accompanied by a vapor pressure and property (`name.vap`) file, holding the compounds CAS registry number, a unique code identifier, and compound experimental data information:
 - Pure compound vapor pressure Wagner or Antoine coefficients, which can be used to obtain the pure compound measured/validated vapor pressure, are available in over 1100 vapor pressure / experimental data property compound vap-files.
 - For more than 3000 of the COSMObase compounds experimental boiling points and/or melting points are available in the database index file and the compound vap-files.
 - For over 250 COSMObase compounds experimental heat of fusion data (enthalpy of fusion and melting point) and critical point data are available in the compound vap-files.
 - For over 100 COSMObase compounds UNIQUAC volume and area coefficients are available. This data can be used in the fitting of activity coefficients to the UNIQUAC equation.