

COSMOtherm Version C2.1 Release 01.05 (November 2005)

New features of this distribution include:

1. Improved accuracy and applicability of COSMOtherm predictions:

- Greatly improved accuracy in the prediction of pure compound vapor pressure and heat of vaporization.
- Greater improvement in accuracy in the prediction of the properties of alkanes such as vapor pressure, heat of vaporization, activity coefficients, partition coefficients and solubility.
- New and 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 greatly enlarged test set of thermodynamic properties the new parameters results in higher overall accuracy and even broader applicability.
- Optimized COSMO-radii and COSMOtherm van der Waals interaction parameters for elements Arsenic (**As**), Selenium (**Se**), allow for the computation of arbitrary Arsenic- and Selenium- containing metal-organics with an accuracy comparable to the prediction of common organic compounds.

2. COSMOthermX graphical user interface (GUI):

- Improved stability and enhanced functionality of the COSMOthermX GUI allows for the simple and efficient setup of COSMOtherm calculations and the graphical postprocessing of the computed results.
- Improved and simpler choice of compounds from a compound database and new automatic search function for compound COSMO files.
- Rapid 'string' searching and the addition of many synonym names allow for greater ease in the selection of compounds from COSMObase.

3. Enhanced and improved COSMO*therm* functionality:

- **PK_A**: New pK_A computation for acids and bases in water and non-aqueous solvents: new and improved pK_A-LFER parameter sets for the prediction of the pK_A of aqueous acids, aqueous bases and acidic compounds in the dipolar-aprotic solvent, dimethyl sulfoxide (DMSO). All new pK_A-LFER parameter sets were determined for both high level (BP-TZVP-COSMO) and screening level (BP-SVP-AM1) quantum chemistry.
- **SOLGAS**: New automatic computation option for the iterative determination of a gas solutes solubility in a liquid solvent or solvent mixture at a given pressure.
- **FLATSURF**: New 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.
- **DENSITY**: A new and unique QSPR-based calculation method for the prediction of the molecular volume and liquid density of pure compounds. This feature is accessible from a new automatic option in COSMO*therm* for the calculation of density. The QSPR parameters for room temperature liquid density/volume predictions were optimized and are available for both high level (BP-TZVP-COSMO) and screening level (BP-SVP-AM1) quantum chemistry.
- **VISCOSITY**: A new and unique QSPR-based calculation method for the prediction of the liquid viscosity of pure compounds. This feature is accessible from a new option in COSMO*therm* for the automatic calculation of liquid density. The QSPR parameters for the prediction of liquid viscosity at room temperature were optimized and are available for both high level (BP-TZVP-COSMO) and screening level (BP-SVP-AM1) quantum chemistry.
- **PROPQSPR**: A new automatic calculation option for σ -moment QSPR properties. This option allows for the computation of several QSPR thermodynamic properties in one COSMO*therm* run.
- **PROPQSPR**: COSMO*therm* σ -moment QSPR coefficients have been correlated with the five parameters of **Abrahams general solvation equation**. Moreover, if the Abraham property coefficients are given, the Abraham thermodynamic property defined by these coefficients can be calculated automatically by COSMO*therm*. Within the new COSMO*therm* release, 25 different Abraham property coefficient files for the prediction of organic solvent and biological partition properties are provided for both high level (BP-TZVP-COSMO) and screening level (BP-SVP-AM1) quantum chemistry.

3. Enhanced and improved COSMO*therm* **functionality** (continued):

- **GAMMA:** A new reference state allowing for the simplified calculation of mean ionic activity coefficients γ^+ has been introduced into the automatic activity coefficient calculation option (GAMMA) of COSMO*therm*.
- **LLE:** A new iterative search option for liquid-liquid equilibria (LLE) of binary systems allows for the determination of LLE with significantly higher accuracy and with strongly improved stability and robustness of the search algorithm.
- **SOLUBILITY:** The algorithm for the iterative calculation of solubility in arbitrary solvents and solvent mixtures (SOLUB ITERATIVE option) has been improved and refined. As a result, the stability and robustness of the iterative prediction of solubility greatly has been enhanced.

4. Improved and simplified COSMO*therm* **input** and **output**:

- The Wagner equation coefficients for the calculating the temperature-dependency of vapor pressure from experimental data have been modified: now the calculations can be extrapolated smoothly beyond the given range of valid minimum and maximum temperatures.
- Improved detection and handling of DOS/UNIX special ASCII characters in COSMO*therm* input files and also in the auxiliary program ct_create.
- New error handling in the case of missing compounds. Now the error message is only produced after all compounds have been checked, not intermediately.

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

- Currently *COSMObase* holds over 4000 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 3400 chemical compounds.
- For release version C2.1 - 01.05 of *COSMObase*, all compound geometries have been critically reviewed for conformational effects and for over 500 compounds COSMO and/or gas phase geometries have been re-optimized and/or additional conformers have been added.
- Currently *COSMObase* holds over 1000 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.