

Information for COSMOtherm academic trainings

The academic training is organized for customers or interested scientists from academic and non profit institutions. It is designed as an introduction for beginners level up to intermediate knowledge regarding COSMOtherm.

Time schedule:

- 10:00 – 10:15: Kick off and introduction
- 10:15 – 12:30: Basic theory, the graphical user interface, basic property calculation
- 12:30 – 13:15: Lunch
- 13:15 – 16:00: More properties, discussion (open end if you like)

Covered COSMOtherm aspects:

- The COSMO-RS method
- The graphical user interface COSMOthermX, σ -profiles, σ -surfaces, conformers
- Vapor pressure, gas solubility, activity coefficients, partition coefficients (logP), vapor liquid equilibria (VLE), liquid liquid equilibria (LLE), solubility of liquids in liquids, solubility of solids in liquids
- Short introduction into the calculation of the pK_a and how to use ionic liquids (no details)

Not covered COSMOtherm aspects (If you have detailed questions in this fields, we will cover them in the general discussion with our experts):

- Details and results on ionic liquids, pK_a and chemical reaction constants
- COSMOmic, COSMOfrag, COSMOSim, Flatsurf, COSMOtherm based QSAR

Preparations:

- Please bring your own laptop, preferably Windows XP or newer.
- You can also have your own installation of COSMOthermX. We will also provide USB-sticks with an installer for the training.
- Please bring some questions and an idea how you want to use the software. If you send us the questions we will take a look into the specific details.

Costs, location and traveling

- The training itself is free of charge
- Lunch and drinks (coffee, water, juice) are free.
- Traveling and accomodation have to be paid by the participants
- The training will take place in our office:
Burscheider Straße 515, 513841 Leverkusen, Germany
- Please see <http://www.cosmologic.de/journey> for traveling details