DDBST
Dortmund Data Bank
Software & Separation
Technology

Predict Pure 2024

Estimation of Thermophysical Properties from Molecular Structure

Sophisticated estimation of pure component properties from molecular structure.

- Simple graphical structure entry.
- Large structure data base included.
- Large number of different group contribution methods.
- Wide variety of different properties.
- Implements “chemical know-how” via chemical neighborhood of structural groups, … .
- Topological indices and higher order corrections.

The tedious task of property estimation can be performed with a few clicks.

Predict Pure was verified during the development of the well-known UNIFAC and mod. UNIFAC methods and the test procedures of the Dortmund Data Bank (DDB).

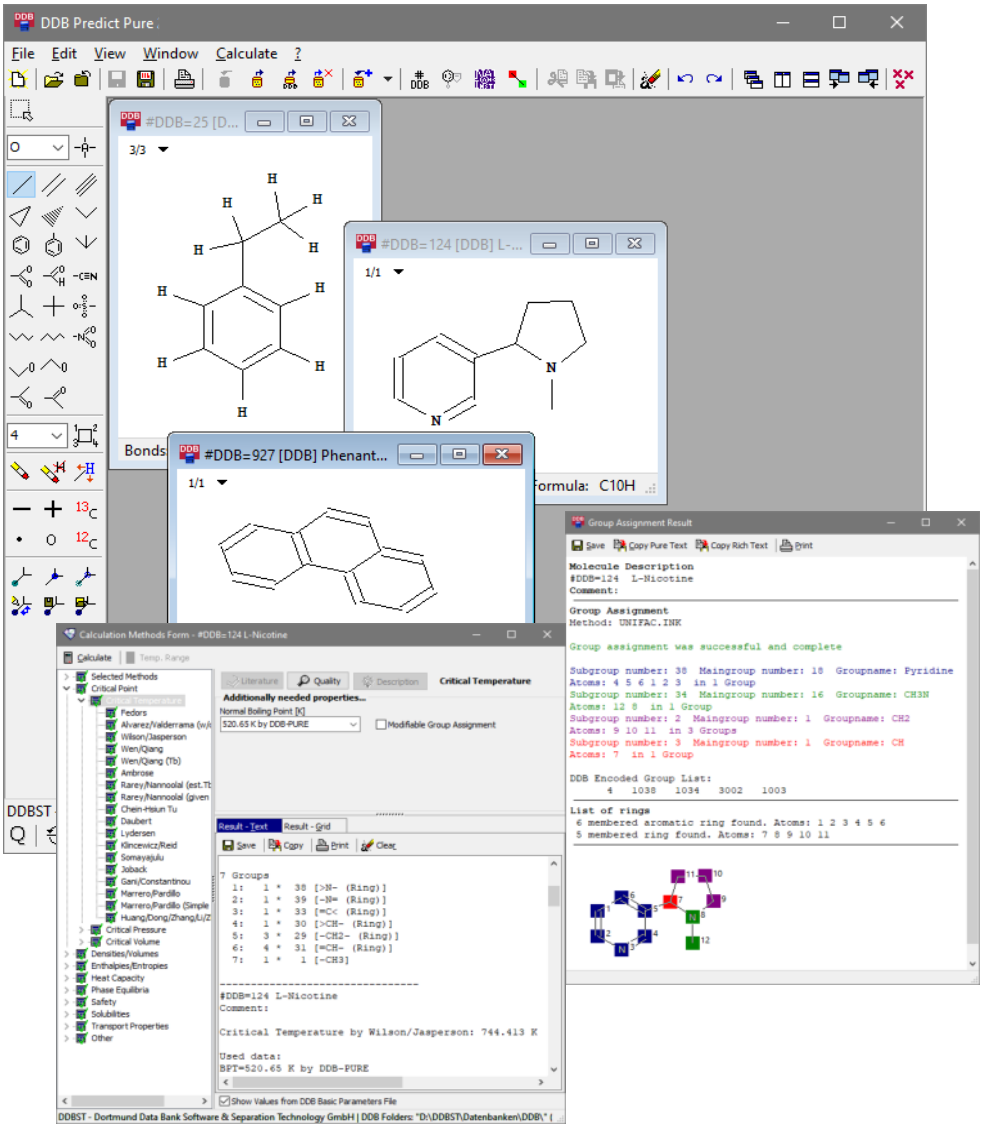
More than a million data points were automatically estimated and compared to experimental data from literature.

Predict Pure features a method ranking (quality) for several important properties based on performance in case of similar molecules.

Direct export to the most common process simulation programs avoids possible unit conversion errors.

To find components with similar structural elements, a powerful substructure search has been implemented.

Whether you are dealing with process simulation, risk assessment, environmental protection or combinatorial chemistry, this is the package of choice used by many companies world-wide.



Major Features

- Easy graphical molecular structure input. New structure storage in the integrated data base or on file.
- 3D structures can be moved, scaled and rotated.
- Approx. 86,800 structures of commonly used chemicals (Predict Pure - Additional Structures).
- Basic data from the Dortmund Data Bank (DDB) (critical data, liquid density, dipole moment) available for a large number of components (optional).
- Fast automatic property estimation by a large number of well-known group contribution methods.
- Quality estimation expert system for normal boiling point and critical data estimation.
- Interactive interface to MOPAC©, input file generation for Gaussian©, ... for the calculation of σ-profiles for COSMO-RS models.
- Group contribution estimation of σ-profiles for COSMO-RS(Ol) and COSMO-SAC.
- Generate data tables by calculating properties over a given temperature range and automatically regress equation parameters.
- Automatic fragmentation of molecules into structural groups for more than 60 group contribution methods incl. UNIFAC, mod. UNIFAC, ASOG, etc. .
- Automatic second order corrections, aromatic ring recognition, etc. .
- Automatic generation of topological indices (Balaban, Wiener, ...).
- User-definable set of preferred methods.
- Substructure search for molecules containing user defined structural elements.
- Re-usable user defined fragments.
- Windows graphical user interface.
- Exports data to Microsoft Excel™ and data to input files for the Aspen Plus™ simulator and ProSim™ products.
- Seamless integration into the Dortmund Data Bank software systems.

Estimated Properties

- Critical Data
- Normal Boiling Point, Vapor Pressure
- Acentric Factor
- Liquid Density
- Second Virial Coefficient
- Heat Capacity (Vapor/Gas, Liquid, Solid)
- Enthalpy, Entropy, Energy of Vaporization
- Gibbs Energy and Stand. Enthalpy of Formation
- Viscosity (Vapor/Gas, Liquid)
- Thermal Conductivity
- Surface Tension
- Water Solubility
- Flammability Limit
- Activity Coefficients and many more

Models Included

Ambrose, Basarova/Svoboda, Benson, Bondi, Brock, Campbell/Thodos, Chein-Hsiun Tu, Chueh /Swanson, Cordes/ Rarey, Daubert, Devotta/Rao, Gani/Constantinou, Gomez-Nieto/Thodos, Han /Peng, Hearing/Domalski, High, Horvath, Hoshino, Hoshino/Nagahama, Joback, Klincewicz/Reid, Kolbasov, Kuehne, Lakshmi, Le Bas, Luria/Benson, Lydersen, Ma/Zhao, Mavrovouniotis, Mc Cann/Danner, Meissner, Miller, Missenard, Motoc/Balaban, Nannoolal/Rarey, Nagvekar /Daubert, Orrick/Erbar, Reichenberg, Riedel, Ruzicka/Domalski, Sastri/Mohanty/Rao, Sastri/Rao, Schroeder, Seaton, Shaw, Shebeco, Skubla, Somayajulu, Souders, Stein/ Brown, Tassios, Tatevskii, Thomas, Tsibanogiannis/ Kalospiros /Tassios, Tu/Liu, Tyn/Callus, van Velzen, ...

Licenses

Predict Pure

Graphical editor for molecular structures, structure data base and basic data for approx. 300 components, automatic group fragmentation, property estimation from chemical structure (approx. 60 group contribution methods).

Predict Pure – Additional Structures

This add-on significantly enhances the ARTIST property estimation methods by providing molecular structures for more than 100,000 compounds.

Changes and errors are possible regarding all information and prices.