

**DDBST**DORTMUND DATA BANK
SOFTWARE & SEPARATION
TECHNOLOGY**DDBSP 2011 – ARTIST**

Estimation of Thermophysical Properties from Molecular Structure

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The program package ARTIST was developed for the estimation of pure component properties using the most sophisticated methods. It incorporates a large number of different group contribution methods for a multitude of different properties. Using a special coding scheme for molecular structures, ARTIST is able to take into account the chemical neighborhood of the individual groups thus implementing chemical know-how. Special features of some group contribution methods like topological indices and second order group corrections are automatically taken into account. Thus after entering the structure or retrieving it from the large data base included, the tedious task of property estimation can be performed with a single click. To ensure the correctness of the algorithm, the program has already been tested for years during the development of the well known UNIFAC and mod. UNIFAC methods.

It has also proven very helpful for years during the compilation of the Dortmund Data Bank (DDB) pure component data bank. Thousands of data points were automatically estimated and compared to experimental data from literature thus eliminating errors in data input and/or the estimation routines.

Structures can be stored in 3D and rotated on the screen. To find components with a similar structural element, a powerful substructure search has been implemented. The whole package utilizes a user-friendly Windows graphical user interface. Results can be copied to the clipboard or automatically sent to Microsoft Excel™ for further processing.

Whether you are dealing with process simulation, risk assessment, environmental protection or combinatorial chemistry, this is the package of choice for automatic property estimation.

The screenshot displays the ARTIST software interface with several windows open:

- Artist - The Structure Editor:** Shows chemical structures for Ethylbenzene (#DDB=25), Nicotine (#DDB=124), and another Nicotine structure (#DDB=124).
- Group Assignment Result:** Displays the results of a UNIFAC.INK group assignment for Nicotine (#DDB=124). The assignment was successful and complete. The results are as follows:
Molecule Description: #DDB=124 Nicotine
Comment:
Group Assignment Method: UNIFAC.INK
Group assignment was successful and complete
Subgroup number: 38 Maingroup number: 18 Groupname: Pyridine
Atoms: 4 5 6 1 2 3 in 1 Group
Subgroup number: 35 Maingroup number: 16 Groupname: CH2N
Atoms: 7 11 in 1 Group
Subgroup number: 3 Maingroup number: 1 Groupname: CH
Atoms: 8 in 1 Group
Subgroup number: 2 Maingroup number: 1 Groupname: CH2
Atoms: 9 10 in 2 Groups
Subgroup number: 1 Maingroup number: 1 Groupname: CH3
Atoms: 12 in 1 Group
DDB Encoded Group List:
5 1038 1035 1003 2002 1001
List of rings
6 membered aromatic ring found. Atoms: 1 2 3 4 5 6
5 membered ring found. Atoms: 7 8 9 10 11
- Calculation Methods Form - #DDB=25 Ethylbenzene:** Shows a list of selected methods and a table of results for various properties.

| Property | Method | Value | Unit | Notes |
|----------|-------------------------------|---------|------|--------------------------------------|
| TC | Alvarez/Valderrama (w/o isome | 616.371 | K | <input type="checkbox"/> No BPT=409. |
| TC | Wilson/Jasperson | 626.286 | K | <input type="checkbox"/> No |
| TC | Wen/Qiang | | | |
| TC | Wen/Qiang (Tb) | | | |
| TC | Ambrose | | | |
| TC | Rarey/Nannolal (est.Tb) | | | |
| TC | Rarey/Nannolal (given Tb) | | | |
| TC | Chein-Hsiun Tu | | | |

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. 30670 structures of commonly used chemicals (ARTIST - Additional Structures)
- Basic data from the Dortmund Data Bank (DDB) (critical data, liquid density, dipole moment) already included for a large number of components (optional addition)
- 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(OI) and COSMO-SAC.
- Generate data tables by calculating properties over a given temperature range
- 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™ simulator and ProSim™ products.
- Seamless integration into the Dortmund Data Bank software systems

System Requirements: Windows 2000/XP/Vista/7-32,64

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, Tateviiskii, Thomas, Tsibanogiannis/ Kalospiros /Tassios, Tu/Liu, Tyn/Callus, van Velzen,

Licenses

ARTIST – Basic Version

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)

| | |
|-------------------------------------|--------|
| Basic price for a PC version* | € 2680 |
| Basic price for a 1-year PC version | € 670 |
| Yearly fee for 7-year license** | € 804 |

ARTIST – Additional Structures

Molecular structures for approximately 30,670 components

| | |
|-------------------------------------|--------|
| Basic price for a PC version* | € 1500 |
| Basic price for a 1-year PC version | € 375 |
| Yearly fee for 7-year license** | € 450 |

* For approx. 16 2/3 % of the price, a yearly update is available

** The license includes 6 yearly updates. After 7 years, regular updates are available for approx. 16 2/3 % of the basic price.

For more than one computer, special prices apply: 2 PCs add 50 %, 3 PCs add 80 %, 4 PCs add 100 %. A discount of 50 % is available for universities. Not available as site or world-wide license.

Contact Information

Visit our website

<http://www.ddbst.com>

<http://www.dortmunddatabank.com>

to view additional information or download the ARTIST documentation, the free DDB/DDBSP Explorer Version or view the software presentations.

The free “Explorer Edition” also includes a basic Artist version.