



## 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.

ARTIST 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.

ARTIST 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.

The screenshot displays the 'Artist - The Structure Editor' software interface. It features a main window with a toolbar and a central area showing three molecular structures: Ethylbenzene (#DDB=25), Nicotine (#DDB=124), and Phenanthrene (#DDB=927). A 'Group Assignment Result' dialog box is open, showing the following information for Nicotine:

```
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: 34 Maingroup number: 16 Groupname: CH3N
Atoms: 12 8 in 1 Group
Subgroup number: 3 Maingroup number: 1 Groupname: CH
Atoms: 7 in 1 Group
Subgroup number: 2 Maingroup number: 1 Groupname: CH2
Atoms: 9 10 11 in 3 Groups

DDB Encoded Group List:
4 1038 1034 1003 3002

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
```

Below the dialog box, a 'Calculation Methods Form - #DDB=124 Nicotine' is visible, showing a list of methods and a table of results:

Selected Methods	Quality
Critical Point	
Critical Temperature	
Alvarez/Valderrama (w/o Wilson/Jasperson)	Normal Boiling Point [K]
Wilson/Jasperson	520.65 K by DDB PURE
Wen/Qiang	
Wen/Qiang (Tb)	
Ambrose	
Rarey/Nannoolal (est. Tb)	
Rarey/Nannoolal (given)	
Chen-Hsuan Tu	
Daubert	
Lydersen	
Klincewicz/Reid	
Somayajulu	
Joback	
Gani/Constantinou	
Marrero/Pardillo	
Marrero/Pardillo (Simple)	
Huang/Dong/Zhang/Liu	
Critical Pressure	
Critical Volume	
Densities/Volumes	
Enthalpies/Entropies	
Heat Capacity	
Phase Equilibria	
Safety	
Solubilities	
Transport Properties	
Other	

The 'Result - Text' tab shows the following data:

7 Groups	1	2	3	4	5	6	7
1:	1	*	38	[>N-			
2:	1	*	39	[-N]			
3:	1	*	33	[<C			
4:	1	*	30	[>CH-			
5:	3	*	29	[-CH2-			
6:	4	*	31	[-CH-			
7:	1	*	1	[-CH3]			

The 'DDB Encoded Group List' is: 4 1038 1034 1003 3002. The 'List of rings' shows a 6 membered aromatic ring (atoms 1-6) and a 5 membered ring (atoms 7-11). The 'Critical Temperature by Wilson/Jasperson' is 744.413 K.

## 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. 44,300 structures of commonly used chemicals (ARTIST - 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<sup>©</sup>, input file generation for Gaussian<sup>©</sup>, ... for the calculation of  $\sigma$ -profiles for COSMO-RS models.
- Group contribution estimation of  $\sigma$ -profiles for COSMO-RS(OI) 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<sup>™</sup> and data to input files for the Aspen Plus<sup>™</sup> simulator and ProSim<sup>™</sup> 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

### 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 an indefinite PC version*	€ 3000
Basic price for a 1-year PC version	€ 750
Yearly fee for 7-year license**	€ 900

### ARTIST – Additional Structures

Molecular structures for nearly 44,300 components

Basic price for a PC version*	€ 1700
Basic price for a 1-year PC version	€ 425
Yearly fee for 7-year license**	€ 510

\* 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 or 1 concurrent add 50 %
- 3 PCs or 2 concurrent add 80 %
- 4 PCs or 3 concurrent add 100 %.

A discount of 75 % is available for universities. Not available as site or world-wide license.