# Condensed Data Sheet

**DDBSP** - Dortmund Data Bank Software Package


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# 1 Introduction

The Condensed Data Sheet program was originally designed to get access to equation parameters needed to calculate with equations published by DIPPR. Now it also integrates temperature independent data for properties that are stored in the DDB or DIPPR database. Of course it is still possible to calculate temperature dependent properties (like liquid density) by using DIPPR equations.

There are two versions of DIPPR database files supported: The Microsoft® Access® database delivered in 1998 and the database containing DIPPR data constructed by K. Schraner in 1994-97. As long as table structures are not changing all following versions are supported, too.

Remark: This documentation does not describe all features of Condensed Data Sheet in detail. It can be seen as possibility to get a little lead to the program functionality.

# 2 Setting up Condensed Data Sheet

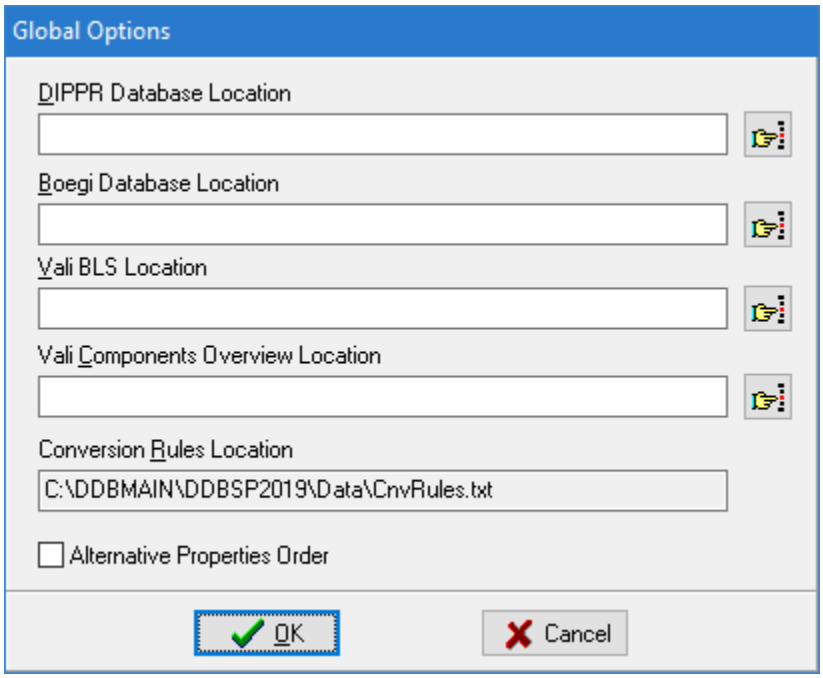
As nearly any DDB program the Condensed Data Sheet program relies on the DDB configuration which can be looked up and modified using the DDB configuration program. The DBB configuration is used to retrieve the public and private pure component information like name, CAS number as well as stored constant properties and equation parameters. A file called STOFF containing company specific component information is distributed with the program and has to be copied into the private folder.

In order to convert values from one unit into another Condensed Data Sheet uses conversion rules. These rules are read in from an external file, so extensions and corrections can easily be made by the user.

In addition, there are up to two external databases which can be integrated in Condensed Data Sheet:

- the Microsoft® Access® database where the DIPPR data is stored
- the Microsoft® Access® database file containing company specific data

The location of these files can be customized by the user. In the main window Options|Global Options will bring up a dialog to change (or check) the location of the mentioned files.

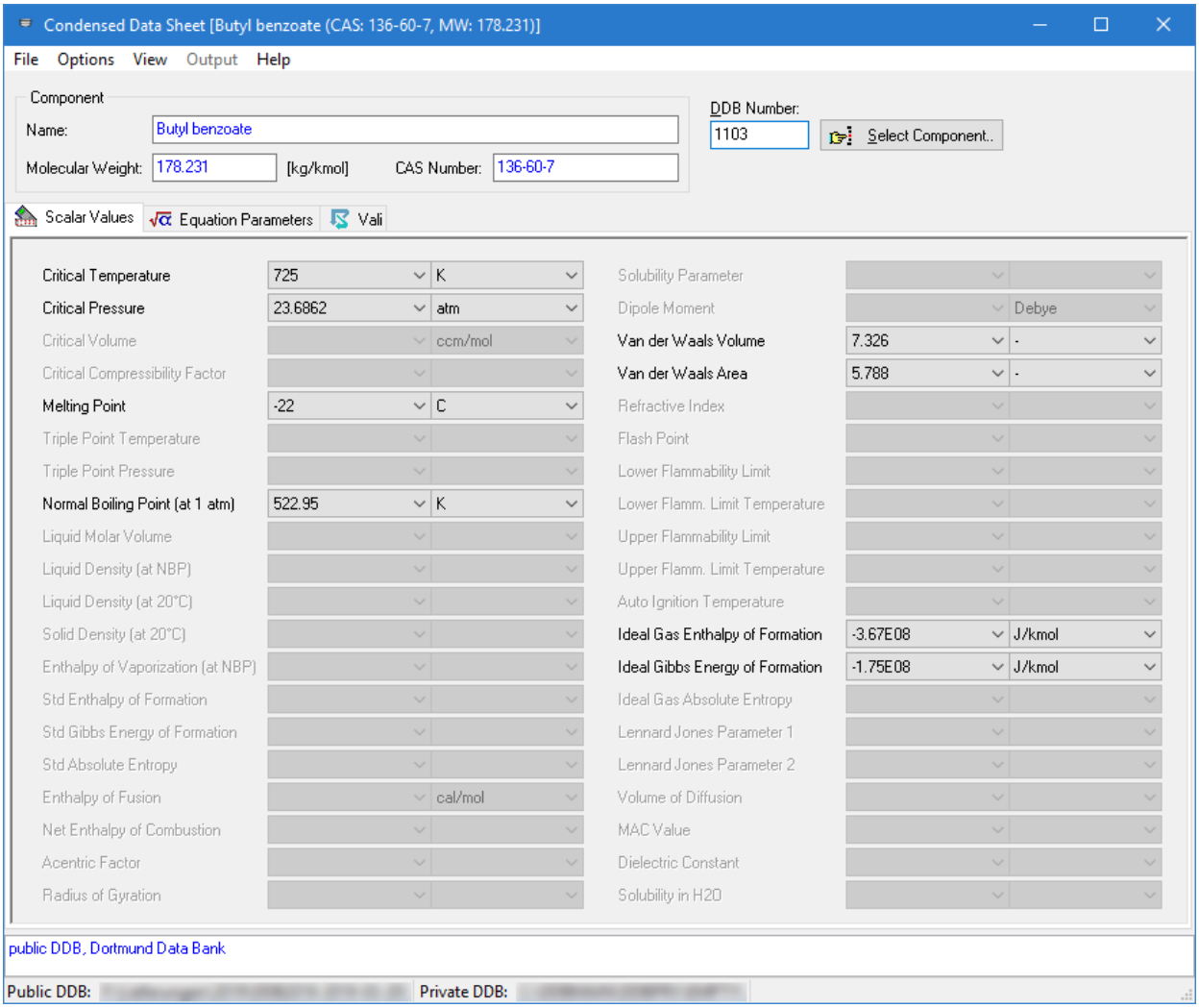


The default location of all files is in the *Data* subdirectory of the program itself. The default name of the rules file is *CnvRules.txt*, the default name of the DIPPR database file is *Dippr801.mdb* and of the company database file is *Lonza-Stoffdaten.mdb*.

If none of the database files is found, only data stored in DDB is available.

# 3 Retrieval of temperature independent information

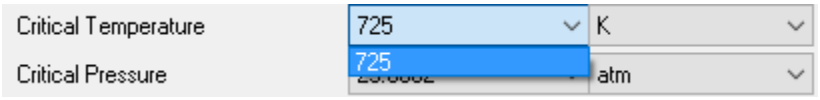
As long as no component is selected, the main window only shows the known temperature independent property names grayed out. A component can be selected either by entering its DDB number in the corresponding edit field or using the *Select Component* button which starts a comfortable component selection. Private component numbers are entered as negative numbers.



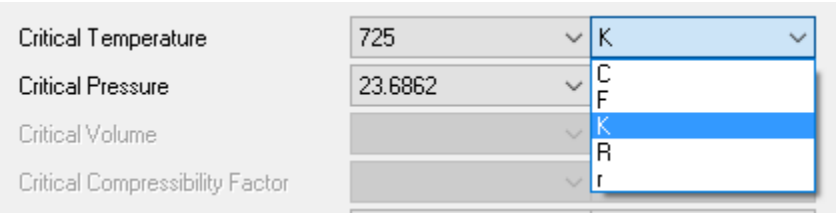

As there are more component names stored in DDB than there is information available in the DIPPR database not every selection will lead to success. A list of all components that are known in DIPPR is available as STL file.

If the component has been found in the database, all available information will be displayed in the main window. If there is no information given for a specific property, then the entry will be grayed out.

If there's more than one value stored in the database or there's information stored in more than one database all values can be looked up by using the push-down button next to a property value.




The first value is always the recommended one. Furthermore, the values can be displayed in different units by selection the push-down button next to the currently used unit.




If and which units are available depend on the entries of the conversion rules file.

The temperature dependent parameters can be looked up by switching to the *View Equation Parameters* page. All available equations parameters will be shown in the calculation page.

Scalar Values | Equation Parameters | Vali

| | Tmin [C] | Tmax [C] | Equation | Source | Error | A | B | C | D | E | SI-Unit | Target-Unit |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Liquid Density | -21.50 | 450.85 | 105: A/B^(1+(1-T/C)^D) | DIPPR (old) | < 5% | 0.47624 | 0.26431 | 724 | 0.2971 | | kmol/m^3 | kg/m^3 |
| Vapor Pressure | -21.50 | 450.85 | 101: exp(A+B/T+C*ln(T)+D*T^E) | DIPPR (old) | < 10% | 63.668 | -9088.8 | -5.5595 | 1.807E-18 | 6 | Pa | bar |
| Vapor Pressure | 100.00 | 201.00 | -4: A-B/(C+T) | public DDB | unknown accuracy | 6.41411 | 1348.78 | 130.33 | | | mmHg | bar |
| Enthalphy of Vaporization | -21.50 | 450.85 | 106: A*(1-Tr)^(B+C*Tr+D*Tr^2+E*Tr^3) | DIPPR (old) | < 10% | 7.304E07 | 0.3071 | | | | J/kmol | kJ/kmol |
| Ideal Gas Heat Capacity | 26.85 | 1226.85 | 107: A+B*(C/T/sinh(C/T))^2+D*(E/T/cosh(E/T))^2 | DIPPR (old) | < 25% | 146880 | 496380 | 1903.6 | 405100 | 844 | J/kmol*K | kJ/(kg*K) |
| Second Virial Coefficient | 88.85 | 3338.85 | 104: A+B/T+C/T^3+D/T^8+E/T^9 | DIPPR (old) | < 25% | 0.41525 | -521.11 | -1.8853E08 | -3.2899E21 | 8.193E23 | m^3/kmol | m^3/kg |

## 4 Calculation of temperature dependent properties

The calculation page shows all properties for which parameters are available.

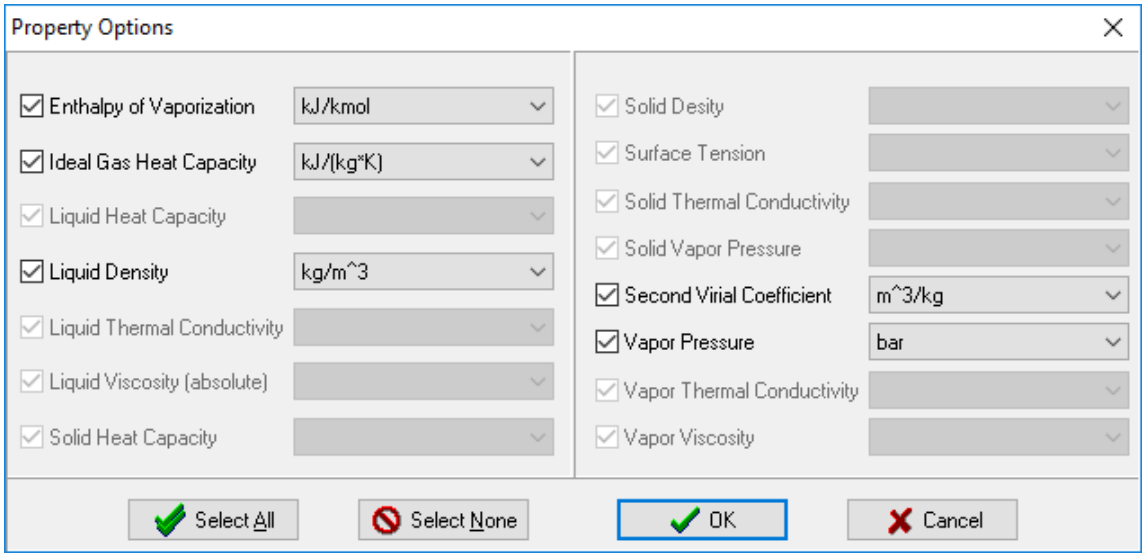
By default, all available properties will be considered when a calculation is started. The active properties and the target unit (displayed in the last column of the grid) can be changed by selecting the *Options* button. Parameters for properties that are excluded from calculation will be grayed out.

In the calculation area of the window you can select the *Start Temperature*, the *End Temperature* and the *Step Width* for the calculation. The temperature range can be given in several units. Use the *Temperature Unit* selection box to switch to another unit for the next calculation.

Press the *Calculate* button to start the calculation.

# 5 Property options

In the *Property Options* dialog the preferred units for a calculated property can be selected.




A property option is grayed out if there are no parameters available for it for the currently selected component.

Uncheck a property to exclude the property from the calculation.

As for the selectable units the settings will be used in all further calculations and stored when the program is exited.

# 6 Calculation results

The *Calculation Results* page is visible after a calculation has been performed. All calculated properties for the specified range are displayed.

Scalar Values | Equation Parameters | Calculation Results | Vali

| Temp. [C] | Liquid Density [kg/m^3] | Vapor Pressure [bar] | Vapor Pressure [bar] | Enthalphy of Vaporization [kJ/kmol] | Ideal Gas Heat Capacity [kJ/(kg*K)] | Second Virial Coefficient [m^3/kg] |
|---|---|---|---|---|---|---|
| 20 | 1004.6163 | 2.9548786E-05 | 3.6888011E-06 | 62296.221 | 1.06159 | -0.10056251 |
| 21 | 1003.8259 | 3.2218333E-05 | 4.2283773E-06 | 62251.885 | 1.0646383 | -0.099684195 |
| 22 | 1003.0348 | 3.5106247E-05 | 4.8381999E-06 | 62207.478 | 1.0676991 | -0.09879589 |
| 23 | 1002.243 | 3.822844E-05 | 5.526252E-06 | 62162.999 | 1.0707722 | -0.097898983 |
| 24 | 1001.4506 | 4.1601839E-05 | 6.3012863E-06 | 62118.448 | 1.0738574 | -0.09699477 |
| 25 | 1000.6575 | 4.524443E-05 | 7.1728845E-06 | 62073.824 | 1.0769546 | -0.096084467 |
| 26 | 999.86375 | 4.917532E-05 | 8.1515208E-06 | 62029.129 | 1.0800634 | -0.095169211 |
| 27 | 999.06928 | 5.3414793E-05 | 9.2486289E-06 | 61984.36 | 1.0831838 | -0.094250066 |
| 28 | 998.27414 | 5.7984371E-05 | 1.0476672E-05 | 61939.519 | 1.0863153 | -0.093328028 |
| 29 | 997.4783 | 6.2906874E-05 | 1.1849218E-05 | 61894.604 | 1.089458 | -0.092404028 |
| 30 | 996.68177 | 6.8206493E-05 | 1.3381015E-05 | 61849.615 | 1.0926114 | -0.091478933 |

Print... Print Black/White

The possible actions are:

- Print all available data: The data sheet (temperature independent parameters), the calculation results as text table and as plots will be send to the specified printer.
- Copy the calculation results as text table to an Excel file
- View all plots as preview

# 7 Appendix

## 7.1 Unit conversion

There is a file called *CnvRules.txt* distributed with the Condensed Data Sheet program. The unit conversion is controlled by the contents of that file. It consists of three sections:

- *Measurands*
- In this sections for any property that shall be displayed or calculated by Condensed Data Sheet an associated measurand must be given.
- *Complex Conversion Rules*
- This section contains rules that need additional information to convert one unit into another. Only conversions between SI-Units (see section 3) have to be specified. In order to be able to convert back, a separated rule for the back-conversion must be given.
- *Aliases*: To overcome typographical differences between units specified in the file and units stored in a used database this entry can be used to introduce alias names.
- *Simple Conversion Rules*
- The last section contains rules to convert one unit into another using only a factor and/or an addend.

Please feel free to extend the file to fit your needs.