

Condensed Data Sheet

DDBSP - Dortmund Data Bank Software Package



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1	Introduction	3
2	Setting up Condensed Data Sheet.....	3
3	Retrieval of temperature independent information.....	4
4	Calculation of temperature dependent properties	5
5	Property options.....	6
6	Calculation results	6
7	Appendix	7
7.1	Unit conversion	7

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

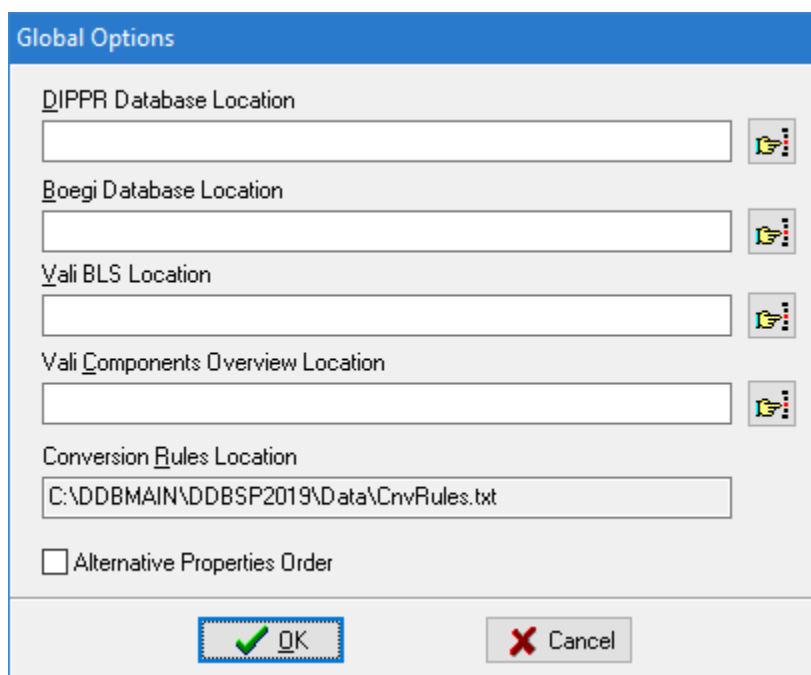
As nearly any DDB program the Condensed Data Sheet program relies on the DDB configuration which can be looked up and modified using the DDB configuration program. The DDB configuration is used to retrieve the public and private pure component information like name, CAS number as well as stored constant 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.

Condensed Data Sheet [Butyl benzoate (CAS: 136-60-7, MW: 178.231)]

File Options View Output Help

Component

Name: DDB Number:

Molecular Weight: [kg/kmol] CAS Number:

Scalar Values Equation Parameters Valid

Critical Temperature	725	K	Solubility Parameter	
Critical Pressure	23.6862	atm	Dipole Moment	
Critical Volume		ccm/mol	Van der Waals Volume	7.326
Critical Compressibility Factor			Van der Waals Area	5.788
Melting Point	-22	C	Refractive Index	
Triple Point Temperature			Flash Point	
Triple Point Pressure			Lower Flammability Limit	
Normal Boiling Point (at 1 atm)	522.95	K	Lower Flamm. Limit Temperature	
Liquid Molar Volume			Upper Flammability Limit	
Liquid Density (at NBP)			Upper Flamm. Limit Temperature	
Liquid Density (at 20°C)			Auto Ignition Temperature	
Solid Density (at 20°C)			Ideal Gas Enthalpy of Formation	-3.67E08
Enthalpy of Vaporization (at NBP)			Ideal Gibbs Energy of Formation	-1.75E08
Std Enthalpy of Formation			Ideal Gas Absolute Entropy	
Std Gibbs Energy of Formation			Lennard Jones Parameter 1	
Std Absolute Entropy			Lennard Jones Parameter 2	
Enthalpy of Fusion		cal/mol	Volume of Diffusion	
Net Enthalpy of Combustion			MAC Value	
Acentric Factor			Dielectric Constant	
Radius of Gyration			Solubility in H2O	

public DDB, Dortmund Data Bank

Public DDB: Private DDB:

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.

Critical Temperature 725 K
 Critical Pressure 725 atm

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.

Critical Temperature 725 K
 Critical Pressure 23.6862 C
 Critical Volume K
 Critical Compressibility Factor R

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.

	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: $A+B/T+C/T^2+D/T^3+E/T^4$	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.

Temp. [C]	Liquid Density [kg/m ³]	Vapor Pressure [bar]	Vapor Pressure [bar]	Enthalpy 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

The possible actions in the *Output* options 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.