

Codensed Data Sheet

DDBSP - Dortmund Data Bank Software Package



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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.

Setting up Condensed Data Sheet

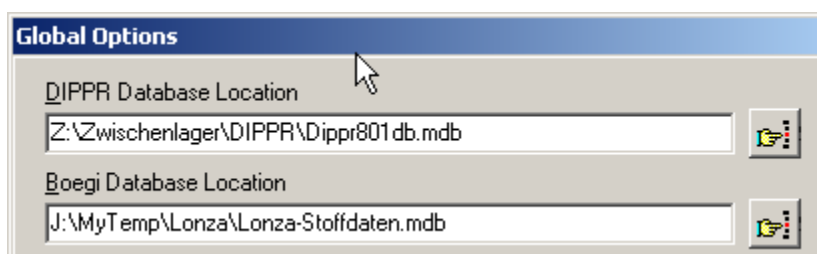
As nearly any DDB program the Condensed Data Sheet program relies on the DDB configuration which can be looked up and modified using the DDB configuration program. The DDB configuration is used to retrieve the public and private pure component information like name, CAS number as well as stored constant 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 not found, only data stored in DDB is available.

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 2008 [Butyl benzoate (CAS: 136-60-7, MW: 178.231)]

File Options View Output Help

Component

Name:

Molecular Weight: [kg/kmol] CAS Number:

DDB Number:

Scalar Values Equation Parameters Vali

Critical Temperature	<input type="text" value="724"/>	<input type="text" value="K"/>	Radius of Gyration	<input type="text" value="5.505E-07"/>	<input type="text" value="mm"/>
Critical Pressure	<input type="text" value="2590"/>	<input type="text" value="kPa"/>	Solubility Parameter	<input type="text" value="18250"/>	<input type="text" value="(J/m^3)^(1/2)"/>
Critical Volume	<input type="text" value="555"/>	<input type="text" value="ccm/mol"/>	Dipole Moment	<input type="text" value="1.8303"/>	<input type="text" value="Debye"/>
Critical Compressibility Factor	<input type="text" value="0.239"/>	<input type="text" value=""/>	Van der Waals Volume	<input type="text" value="6.94792"/>	<input type="text" value="."/>
Melting Point	<input type="text" value="-21.5"/>	<input type="text" value="C"/>	Van der Waals Area	<input type="text" value="5.48"/>	<input type="text" value="."/>
Triple Point Temperature	<input type="text" value="251.65"/>	<input type="text" value="K"/>	Refractive Index	<input type="text" value="1.494"/>	<input type="text" value=""/>
Triple Point Pressure	<input type="text" value="0.0452286"/>	<input type="text" value="Pa"/>	Flash Point	<input type="text" value="379.15"/>	<input type="text" value="K"/>
Normal Boiling Point (at 1 atm)	<input type="text" value="523.15"/>	<input type="text" value="K"/>	Lower Flammability Limit	<input type="text" value="0.8"/>	<input type="text" value="vol % in air"/>
Liquid Molar Volume	<input type="text" value="0.177898"/>	<input type="text" value="m^3/kmol"/>	Lower Flamm. Limit Temperature	<input type="text" value="379"/>	<input type="text" value="K"/>
Liquid Density (at NBP)	<input type="text" value="0.769138"/>	<input type="text" value="kg/l"/>	Upper Flammability Limit	<input type="text" value="5.4"/>	<input type="text" value="vol % in air"/>
Liquid Density (at 20°C)	<input type="text" value="0.9716"/>	<input type="text" value="kg/l"/>	Upper Flamm. Limit Temperature	<input type="text" value="424"/>	<input type="text" value="K"/>
Solid Density (at 20°C)	<input type="text" value=""/>	<input type="text" value=""/>	Auto Ignition Temperature	<input type="text" value="713.15"/>	<input type="text" value="K"/>
Enthalpy of Vaporization (at NBP)	<input type="text" value="101.029"/>	<input type="text" value="kcal/kg"/>	Ideal Gas Enthalpy of Formation	<input type="text" value="-3.67E08"/>	<input type="text" value="J/kmol"/>
Std Enthalpy of Formation	<input type="text" value="-4.29055E08"/>	<input type="text" value="J/kmol"/>	Ideal Gibbs Energy of Formation	<input type="text" value="-1.75E08"/>	<input type="text" value="J/kmol"/>
Std Gibbs Energy of Formation	<input type="text" value="-2.001E08"/>	<input type="text" value="J/kmol"/>	Ideal Gas Absolute Entropy	<input type="text" value="539000"/>	<input type="text" value="J/(kmol*K)"/>
Std Absolute Entropy	<input type="text" value="414100"/>	<input type="text" value="J/(kmol*K)"/>	Lennard Jones Parameter 1	<input type="text" value="8.58865"/>	<input type="text" value="A"/>
Enthalpy of Fusion	<input type="text" value="4708.3"/>	<input type="text" value="cal/mol"/>	Lennard Jones Parameter 2	<input type="text" value="547.388"/>	<input type="text" value="K"/>
Net Enthalpy of Combustion	<input type="text" value="-5.59E09"/>	<input type="text" value="J/kmol"/>	Volume of Diffusion	<input type="text" value="194.5"/>	<input type="text" value=""/>
Acentric Factor	<input type="text" value="0.576708"/>	<input type="text" value=""/>			

Public DDB: F:\DDB\ Private DDB: F:\DDBPRV\

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	724	K
Critical Pressure	724 729.85	kPa

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	724	K
Critical Pressure	2590	C
Critical Volume	555	F
Critical Compressibility Factor	0.239	K

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.

Calculation of Temperature Dependent Properties

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

	Tmin [C]	Tmax [C]	Equation	Source	Error	A	B	C	D	E	SI-Unit	Target-Unit
Enthalpy of Vaporization	0.01	373.98	106: $A*(1-Tr)^{(B+C*Tr+D*Tr^2+E*Tr^3)}$	DIPPR801	< 1%	5.2053E07	0.3199	-0.212	0.25795		J/kmol	kJ/kmol
Ideal Gas Heat Capacity	-173.15	2000.00	107: $A+B*(C/T)/sinh(C/T)^2+D*(E/T/cosh(E/T))^2$	DIPPR801	< 1%	33363	26790	2610.5	8896	1169	J/kmol*K	kJ/(kg*K)
Liquid Heat Capacity	0.01	260.00	100: $A+B*T+C*T^2+D*pT^3+E*T^4$	DIPPR801	< 1%	276370	-2090.1	8.125	-0.014116	9.3701E-06	J/kmol*K	kJ/(kg*K)
Liquid Density	0.01	373.98	116: $A+B*(1-Tr)^{0.35+C*(1-Tr)^{(2/3)}+D*(1-Tr)+E*(1-Tr)^4/3}$	DIPPR801	< 1%	17.863	58.606	-95.396	213.89	-141.26	kmol/m^3	kg/m^3
Liquid Density	0.01	60.00	100: $A+B*T+C*T^2+D*pT^3+E*T^4$	DIPPR801	< 0.2%	-13.851	0.64038	-0.0019124	1.8211E-06		kmol/m^3	kg/m^3
Liquid Thermal Conductivity	0.01	360.00	100: $A+B*T+C*T^2+D*pT^3+E*T^4$	DIPPR801	< 1%	-0.432	0.0057255	-8.078E-06	1.861E-09		W/m*K	W/(m*K)
Liquid Viscosity (absolute)	0.01	373.00	101: $exp(A+B/T+C*ln(T)+D*T^E)$	DIPPR801	< 3%	-52.843	3703.6	5.866	-5.879E-29	10	Pa*s	cP
Solid Heat Capacity	-270.00	0.00	100: $A+B*T+C*T^2+D*pT^3+E*T^4$	DIPPR801	< 3%	-262.49	140.52				J/kmol*K	kJ/(kg*K)
Solid Density	-40.00	0.00	100: $A+B*T+C*T^2+D*pT^3+E*T^4$	DIPPR801	< 1%	53.03	-0.0078409				kmol/m^3	kg/m^3
Surface Tension	0.01	373.98	106: $A*(1-Tr)^{(B+C*Tr+D*Tr^2+E*Tr^3)}$	DIPPR801	< 1%	0.18548	2.717	-3.554	2.047		N/m	N/m

Start Temperature: 169 End Temperature: 185 Step Width: 1 Temperature Unit: C [Calculate] [Options...]

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.

Properties Options

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

Property Options

<input checked="" type="checkbox"/> Enthalpy of Vaporization	<input type="text" value="kJ/kmol"/>	<input checked="" type="checkbox"/> Solid Density	<input type="text" value="kg/m^3"/>
<input checked="" type="checkbox"/> Ideal Gas Heat Capacity	<input type="text" value="kJ/(kg*K)"/>	<input checked="" type="checkbox"/> Surface Tension	<input type="text" value="N/m"/>
<input checked="" type="checkbox"/> Liquid Heat Capacity	<input type="text" value="kJ/(kg*K)"/>	<input checked="" type="checkbox"/> Solid Thermal Conductivity	<input type="text" value=""/>
<input checked="" type="checkbox"/> Liquid Density	<input type="text" value="kg/m^3"/>	<input checked="" type="checkbox"/> Solid Vapor Pressure	<input type="text" value=""/>
<input checked="" type="checkbox"/> Liquid Thermal Conductivity	<input type="text" value="W/(m*K)"/>	<input checked="" type="checkbox"/> Second Virial Coefficient	<input type="text" value=""/>
<input checked="" type="checkbox"/> Liquid Viscosity (absolute)	<input type="text" value="cP"/>	<input checked="" type="checkbox"/> Vapor Pressure	<input type="text" value="bar"/>
<input checked="" type="checkbox"/> Solid Heat Capacity	<input type="text" value="kJ/(kg*K)"/>	<input checked="" type="checkbox"/> Vapor Thermal Conductivity	<input type="text" value=""/>
		<input checked="" type="checkbox"/> Vapor Viscosity	<input type="text" value=""/>

Select All
 Select None

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.

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]	Enthalpy of Vaporization [kJ/kmol]	Ideal Gas Heat Capacity [kJ/(kg*K)]	Liquid Heat Capacity [kJ/(kg*K)]	Liquid Density [kg/m^3]	Liquid Density [kg/m^3]	Liquid Thermal Conductivity [W/(m*K)]	Liquid Viscosity (absolute) [cP]	Solid Heat Capacity [kJ/(kg*K)]	Solid Density [kg/m^3]	Surface Tension [N/m]
169	37061.559	1.9225351	4.3622358	900.33484	951.91102	0.68117077	0.15848811	3.4342158	892.89495	0.044363541
170	36998.744	1.9230752	4.3653499	899.34361	952.23181	0.68083875	0.15753476	3.4420158	892.75369	0.044153717
171	36935.641	1.9236165	4.3685084	898.34695	952.57092	0.68049552	0.15659458	3.4498159	892.61243	0.043943577
172	36872.248	1.9241589	4.3717121	897.34482	952.92856	0.68014109	0.15566728	3.4576159	892.47118	0.043733118
173	36808.564	1.9247025	4.3749617	896.33722	953.30492	0.67977547	0.15475263	3.465416	892.32992	0.04352234
174	36744.586	1.9252473	4.3782582	895.32412	953.7002	0.67939868	0.15385037	3.473216	892.18866	0.04331124
175	36680.312	1.9257932	4.3816025	894.30549	954.11459	0.67901073	0.15296027	3.481016	892.04741	0.043099817
176	36615.74	1.9263402	4.3849954	893.28131	954.5483	0.67861162	0.15208208	3.4888161	891.90615	0.04288807
177	36550.868	1.9268883	4.3884378	892.25156	955.00151	0.67820138	0.15121557	3.4966161	891.7649	0.042675998
178	36485.694	1.9274375	4.3919306	891.21621	955.47443	0.67778	0.15036051	3.5044161	891.62364	0.042463599

 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

Appendix

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.

Aliase: 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.