

Components



DDBST

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1 Introduction

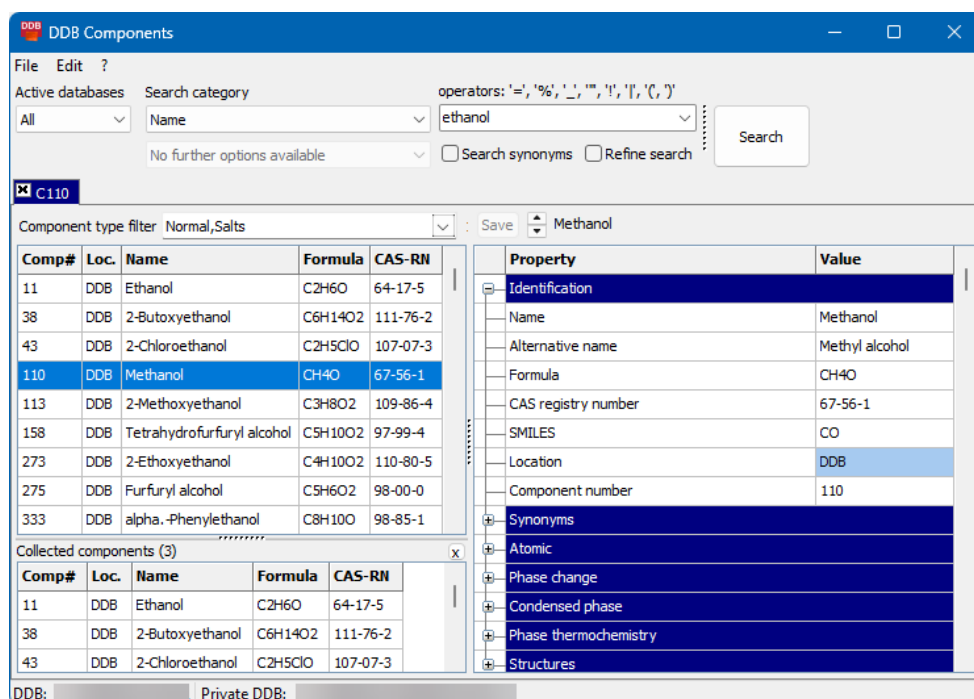
DDB Components is the standard application to store and search for components in the DDB. It interacts with other DDB applications to provide the search functionality.

Examples are:

- Dortmund Data Bank
- DDB Regression Mix
- DDB Regression Pure

New private components can be defined either using *DDB Components* or in interaction with *DDB Predict Pure*.

An overview of the application is shown in the screenshot below.



DDB Components is organized in different parts to provide the above-mentioned functionalities.

The combined *search result* and *editor* area is organized in pages. Each page has at least an *editor* part. The *search result* may be hidden until a search was performed. With the context menu entry “New page” another page with a blank editor area can be opened. With a click on the “X” symbol a page is closed. When the last page is closed, then the application is closed as well. This does also happen when a tab is automatically closed by sending components to another application (see section *Search Result* on page 6).

1.1 Global Options

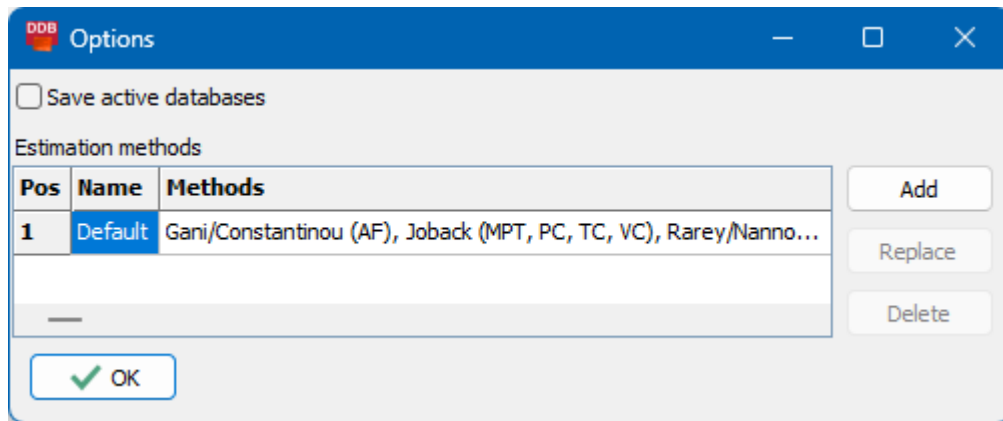
1.1.1 File Menu

The *Open component list* function in the *File* menu allows the user to load component lists from DDB conform formats (*.ddbpr, *.stl, *.stx and *.txt).

The *Exit* menu item closes *DDB Components*.

1.1.2 Edit Menu

In the *Edit* menu, options are accessible.

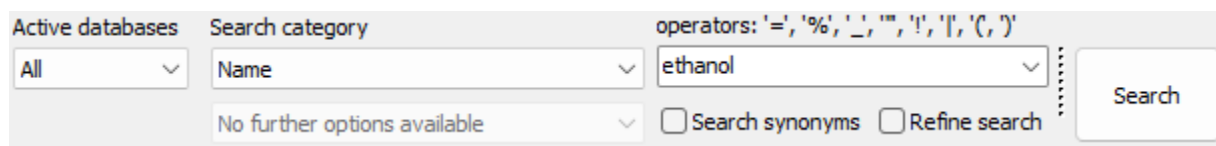


If the *Save active databases* option is activated, the application remembers the active database (*All*, *Public DDB* and *Private DDB*) for the next start. *All* is used by default.

In the lower part of the menu, estimation methods can be defined which will be used to automatically calculate pure component properties. The precondition is a license of *DDB Predict Pure*. The *Add* and *Replace* button allows the user to load methods from *.ini files, which can be created by *DDB Predict Pure*. *Delete* removes the selected entry. The default method cannot be removed.

2 Component Search

To use the component search functions, *DDB Components* can be started directly for example from the *DDB JumpStart* or the Windows start menu. It can also be opened via the *Add Component* button from other DDB applications. The global search options can be found at the top of the window.



The screenshot shows a search interface with the following elements:

- Active databases:** A dropdown menu currently set to "All".
- Search category:** A dropdown menu currently set to "Name".
- Search text:** A text input field containing "ethanol".
- operators:** A label above the search text field listing operators: '=', '%', '_', '"', '!', '|', '(', ')'. A small dropdown arrow is visible to the right of the search text field.
- Search button:** A button labeled "Search" located to the right of the search text field.
- Options:** Below the search category dropdown, there is a dropdown menu showing "No further options available" and two checkboxes: "Search synonyms" (unchecked) and "Refine search" (unchecked).

The *Active databases* drop down menu allows the user to select the database to be searched for components. If the option *All* is selected, the search will use both, the public and the private DDB database. If *Public DDB* is active, private overwrites of public components will not be recognized.

The *Search category* defines the property to be searched. It can be modified by an automatic analysis of the search text (e.g., an integer number in the typing field leads to the *Component number(s)* category). The following categories are available:

- *Name*: Search in *Name* and *Alternative Name* entries. If the *Search synonyms* option is active, also the synonyms will be checked.
- *Formula*: Search in the formula entry.
- *CAS registry number*: Search for components with the given CAS number. Invalid CAS number entries will be colored red if the “exact match” operator “=” is used (see below).
- *Component number(s)*: Search for the DDB Number. Operators (see below) can define the component type or range.
- *Scalar Property*: Search for components with a specific pure component property value within the defined range.
- *Synonym key*: Search in the selected synonyms category.
- *Component class*: The result contains all components of the selected category.

The search item is defined in the typing field and operators can be used for a more accurate search:

Symbol	Definition	Example
=	Exact search	=ethanol
%	Placeholder for a substring (order is important)	ethyl%, %iodide, dimethyl%butan
_	Placeholder for a character (order is important)	b_tyl
""	Defines an exact substring	"ethyl iodide"
Space	AND function	phenyl propanol
!	NOT function	!amide
	OR function	methanol butanol
()	Grouping of search statements	2- (methanol butanol)
/	Search for a number range	15/45, 101s/105s
s	Search for a salt number	15s
a	Search for an adsorbent number	10a
p	Search for a polymer number	512p
i	Search for an ion number	19i
m	Search for a monomer number	82m

Refine Search limits the next search to the obtained search result. The search can be started by the *Search* button or the *Enter* key.

The divider to the left of the search button can be used to change the width of the search text field. The size is remembered in the settings.

2.1 Search Result

The *Search Result* tab shows the results in form of a component list for the last search.

The component editor shows detailed information for the selected component on the right. If the data sheet is currently modified, then the data sheet will be blocked from being updated by a selecting a different item in the search result.

A double-click on a component in the list will send it as selected component to the calling application and close the tab. If the tab does not have a calling application, then the information is sent to the *Dortmund Data Bank* application and the tab is not closed.

Above the component list is the *Component type filter*. The filter can be used to exclude or include specific component types. Excluded components are just hidden and can be included after a search. If there are excluded components, then next to the filter the number of visible components and the total number of the search result are displayed. The text in a component number column that is excluded by the filter will become gray.

The search result can be sorted by a click on a column header. Use *Shift + Click* to use multiple sort columns.

The columns can be moved by drag and drop.

The context menu of the result sheet offers several options, the number of "Send to" entries is flexible and depends on how many pending add or edit requests from other applications are active.

- *Send to DDB: DDB Components* sends the selected component(s) to the *Dortmund Data Bank* application. If *DDB Components* was opened with another DDB application, this option is also available for that application.

- *Send as list to DDB*: The marked components are sent as list to the *Dortmund Data Bank* application. The target application has to be able to handle a component list.
- *Add to collected components*: Adds the selected component to a separate list, shown in an area below the search result items. It is possible add items to the list by drag and drop.
- *Remove selection*: The selected components are removed from the search result.
- *Remove all but selection*: All components but the selected are removed from the search result.
- *Save*: Saves the component list of the search result as DDB component list (*.ddbpr, *.stl, *.stx and *.txt). *Save selection* saves only the selected components.
- *Visible columns*: Define the properties of a component to be shown in the search result.
- *Search DDB*: Initiates a pure component property or mixture data search for systems containing any of the selected components.

2.2 Collected Components

The *Collected Components* area can be used to collect components from different search results. It will be shown, when the first component is added to the *Collected components*.

Some calling applications restrict the total number of components it accepts. The limit is also applied to the *Collected components*.

A double-click on a component in the list acts as a double-click on a search result entry.

The sorting and removing capabilities are the same as for the search result.

The context menu offers with *Send to ...*, *Send as list to ...*, *Save...* and *Save selection...* the same functionalities as the context menu in the *Search Result* sheet.

3 Components Editor

The *Components Editor* shows detailed component information as data sheet. Dependent on the component type, the properties are grouped in main categories:

- *Identification*: Contains the main identifier for the component like the name, the CAS registry number, and more. It also shows the storage location (“DDB” = public, “PRV” = private) of the component.
- *Synonyms*: Contains additional identifiers like synonyms.
- *Component class*: Shows if a component is assigned to a component class.
- *Atomic*: General information about the molecule that are (often) necessary for calculations.
- *Phase change*: Information about the phase change important for the calculation of phase equilibria.
- *Condensed phase*: Density information of the liquid phase at a given temperature.
- *Phase thermochemistry*: Additional thermophysical properties.
- *Structure*: Displays a drawing of stored structural information.

The datasheet itself can be modified via the context menu:

- *Display all*: Shows the entries of a category that are currently not available for the selected component. Some entries like the CAS Number or synonyms create an additional entry and allow the storage of multiple values.
- *Add structure*: Loads a structure from a DDB structure or MOL file (only available for private components).
- *Add structure with editor*: Opens *DDB Predict Pure*. A new structure can be returned to *DDB Components* using the *Save structure to the database* function (only available for private components).
- *Edit structure with editor*: Opens *DDB Predict Pure*. A modified structure can be returned to *DDB Components* using the *Save structure to the database* function (only available for private components).
- *New substance*: Creates a nearly empty data sheet, prepared for data input. Details can be found in the next chapter.
- *Clear*: Creates a blank data sheet, no input is possible. This can be used to cancel data input or to have the data sheet updated again when an item in the search result is selected.
- *Clone substance to Private DDB*: Make a copy of the currently displayed public component and add it as new component to the Private DDB (including structures, group assignments and parameters).
- *Display max.*: Shows the last component of a specific component class.
- *Expand all*: Expand all categories.
- *Collapse all*: Collapse all categories.
- *Show all data fields*: If the option is set, then all fields for all categories are always shown, no matter if data is present or not. It is still possible to collapse categories. This option is useful especially for data comparison.
- *Calculate missing values*: Uses one of the defined methods in the options menu to calculate missing values. The precondition is a license for *DDB Predict Pure*. Depending on the structure and the license, not all selected properties can be calculated. The hint for a calculated property will display the used method and properties (if any).

- *Search DDB*: Initiates a pure component property or mixture data search for systems containing the displayed component.
- *Show*: Calls external applications, like the *Group Editor* or the *Parameter DDB Organizer*.

3.1 Create a new Component

A new empty data sheet can be created by the *New Substance* option in the *DDB Component Editor* context menu. If the option *Show all data fields* is not set, then only the basis entries will be available as empty cells and additional information can be added by selecting *Display all*.

Either the user can fill the gaps manually or use *DDB Predict Pure* to calculate some of the missing properties automatically. For the calculation, a license of *DDB Predict Pure* and a structure is needed. The structure can be loaded from a file using the *Add structure* option from the context menu. Alternatively, *DDB Predict Pure* can be used as it was described previously. If OpenBabel is installed, then a missing structure is automatically created when a SMILES value is entered (or modified).

After defining the component name, the new component can be added using the *Save* button at the top of the data sheet. This assigns a unique identification number and the component is now part of the private database.

3.2 Modify an Existing Component

Private components can directly be modified by editing in the corresponding cell. The color of a modified cell turns light green. *Save* stores the modifications of the private component information.

Public component entries can be *overwritten* by private entries only. However, for technical reasons is this not possible for all properties. To use the overwrite option all databases have to be active. If a cell has been modified, its color changes to turquoise. The modification can then be stored using the *Save* button. Modified entries will be marked by a bluish color.

Overwriting can be reverted by deleting all information in the respective cell. After leaving the cell, its color will change to light grey and the originally value will be shown. *Save* will finish the reset.

Overwritten data will (also) be stored in the PRIVATE.PCP file. Do *not* modify this file manually!