

Component Management

Adding/Modifying Components

DDBSP - Dortmund Data Bank Software Package



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1. Introduction

The Dortmund Databank (DDB) contains two major parts, a pure component properties database and several databanks for mixture properties. Both parts have one thing in common – the underlying component list.

The component list contains actually four component lists. One large list for “normal” mostly organic components, a shorter list for electrolytes and salts, and a very short list for adsorptives, and a list for polymers.

A. Content

The main component list contains not only strictly component defining information but also some additional data. The complete list is

- One English name
- One alternative name
- Molecular formula
- CAS registry number (code)
- Two Antoine vapor pressure equation parameter sets
- Critical temperature, pressure, and volume
- Acentric factor
- Heat of fusion
- Melting temperature
- Dipole moment
- Molecular weight
- One liquid(!) density at one temperature (preferably at 25 °C). This density is used for the Wilson g^E model.
- Original UNIFAC and modified UNIFAC (Dortmund) group assignment information
- UNIQUAC r and q values

The electrolyte list data file contains

- Name
- Formula
- Molecular weight
- Dielectric constant with temperature
- Frequency
- One density
- Groups (ions)
- Gibbs energy of formation parameters
- Heat of formation parameters
- Heat capacity parameters
- Melting temperature
- Heat of fusion
- Two heat capacity values for liquid and crystal
- DDB basic number (if the electrolyte or salt is also available in the main component list)
- Volatility flag (yes if electrolyte is volatile, HCl for example)
- Information on associates

The adsorbent list contains

- Name

The polymer list contains

- Name
- List of monomers
- List of polymers (if polymer is a copolymer)

B. Usage

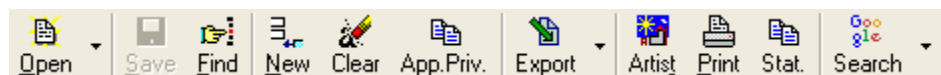
The normal component list is used in every database. The salts list has been introduced for the VLE database containing electrolytes and the salt solubilities database. The adsorptives are used in the adsorbent-adsorptive equilibrium database.

The list have been separated because of using special component- resp. electrolyte-specific parameters for calculation models. This is also the reason for not using a short list of components restricted to names, formula, and maybe CAS registry numbers but to include a multitude of further data. The selection of data is also completely arbitrary since parameters only for a few models are included whereas other models find their parameters in different files.

2. Editing the Main Component List

Components		Salts		Adsorbents		Ions		Groups		Polymers		Flash Points			
Specification															
Component Number:		<input type="text" value="1"/>								24648 components					
English Name:		<input type="text" value="Acetaldehyde"/>													
Alternative Name:		<input type="text" value="Ethanal"/>													
Formula:		<input type="text" value="C2H4O"/>		NIST W.B.		CAS-No.:		<input type="text" value="75-07-0"/>		NIST W.B.					
Antoine Constants T [°C] P [mmHg]															
Low Pressure:		<input type="text" value="7.05640"/>		<input type="text" value="1070.60"/>		<input type="text" value="236.000"/>		Range:		<input type="text" value="-63"/>		<input type="text" value="47"/>		°C Tb=293.55 K	
High Pressure:		<input type="text" value="7.16094"/>		<input type="text" value="1154.01"/>		<input type="text" value="248.700"/>				<input type="text" value="20"/>		<input type="text" value="109"/>		°C Tb=294.07 K	
Values															
Crit. Pressure:		<input type="text" value="5572.875"/>		kPa		Heat of Fusion:		<input type="text" value="3217.5"/>		J/mol					
Crit. Temperature:		<input type="text" value="461.00"/>		K		Melting Point:		<input type="text" value="150.20"/>		K					
Crit. Volume:		<input type="text" value="154.0"/>		cm ³ /mol		Dipole Moment:		<input type="text" value="2.69000"/>		Debye					
Acentric Factor:		<input type="text" value="0.30300"/>				Molecular Weight:		<input type="text" value="44.053"/>							
Density:		<input type="text" value="778.00"/>		kg/m ³ at		<input type="text" value="298.15"/>		K							
UNIFAC Groups and UNIQUAC Parameters															
UNIFAC Groups:		<input type="text" value="2 1001 1020 0 0 0 0 0"/>													
mod. UNIFAC Groups:		<input type="text" value="2 1001 1020 0 0 0 0 0"/>													
UNIQUAC r-value:		<input type="text" value="1.89910"/>				UNIQUAC q-value:		<input type="text" value="1.79600"/>							
<input checked="" type="checkbox"/> Overwrite values by PRIVATE.PCP entries															

A. The Tool Bar

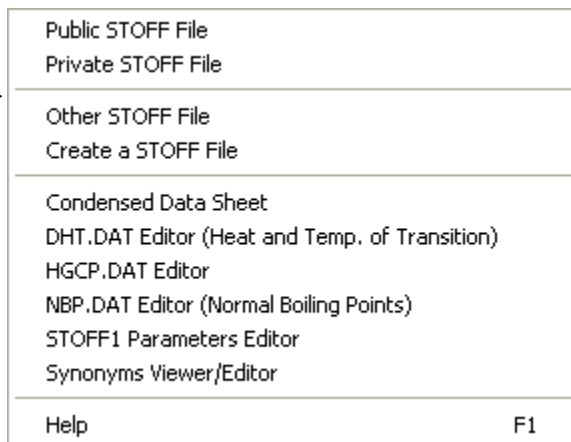




This button opens a context menu which allows to open the public and private component basic file and also to open another file (neither public nor private) or to create a new file.

The other commands open special subdialogs for special data files or to call other programs (“Condensed Data Sheet”) if available. These dialogs are explained later.

The Help command shows the “About” dialog.



The “Save” button is only enabled if changes have been made and allows to store the changes.

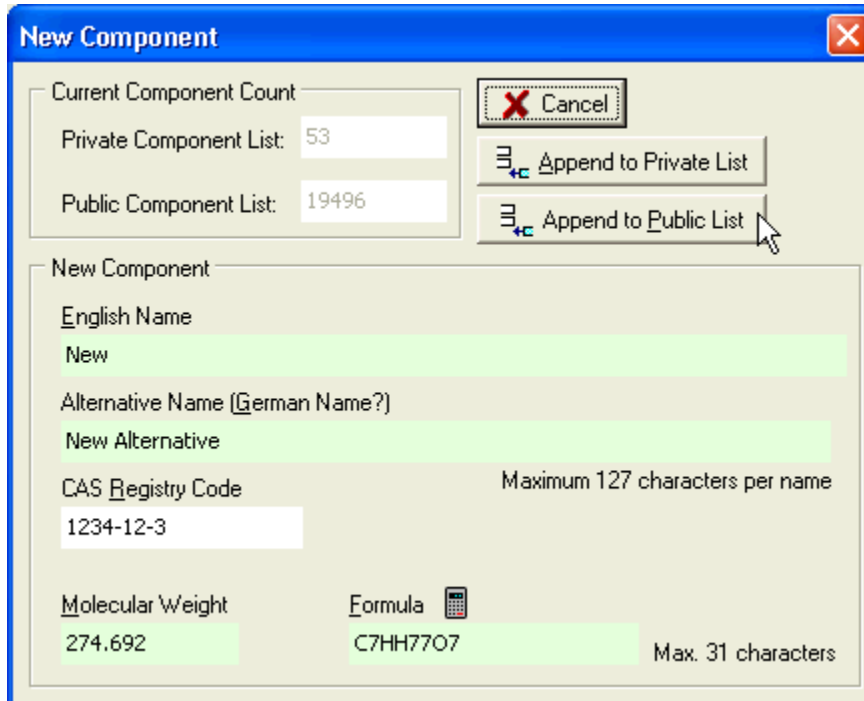


The “Find” button calls the ComponentSelection program which allows to search components by different criteria.



The “New” buttons opens a dialog for entering a new component. The dialog displays the current number of components in the private and the public list and allows to enter two names, the CAS registry code, the molecular weight and a formula. With the exception of the CAS-RN all entries are classified as “necessary”.

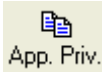
The new component can be append either to the public list or the private list. All additional entries are



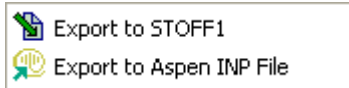
initialized and empty.



The Clear button erases all entries. It is not possible to completely remove an appended component.



This button allows to copy a public (DDBST) component to the private component list. This can be used to add a private component which is the same as a public component but with different additional data like modified T_c , P_c , etc.



The button allows to update an (almost) twin file called STOFF1. This file contains some additional data (parameters) but has to be kept synchronous for some calculations. This synchronization is not done automatically because of some special configuration features which would allow to

screw up these files.

The “Export to Aspen INP File” writes critical temperature, pressure, and volume, melting point, molecular weight, acentric factor, Antoine constants (low pressure), and UNIQUAC constants to an INP file.



The button calls the structure editor Artist – if available. Artist will show the structure of the component – if available.



The Print button allows to print a component sheet but displays it in a dialog beforehand.

```
Data set no. 1 of totally 18487 entries in STOFF
=====
German Name:      Ethanal
English Name:    Acetaldehyde
Empirical Formula: C2H4O
CAS-No.:         75-07-0

Antoine Constants (low):  P [mmHg]  T [°C]
      7.05640    1070.60    236.000
Limits:  -63    47 °C
      Resulting Normal Boiling Point: 293.55 K

Antoine Constants (High): P [mmHg]  T [°C]
      7.16094    1154.01    248.700
Limits:   20   109 °C
      Resulting Normal Boiling Point: 294.07 K

Groups for UNIFAC:
  2 1001 1020    0    0    0    0    0
Groups for mod. UNIFAC (Do):
  2 1001 1020    0    0    0    0    0

r-Value:         1.8991
q-Value:         1.7960

Dipole Moment:   2.6900    Debye
Molecular Weight: 44.053

Density:         778.0000 kg/m3 at T = 298.15 K

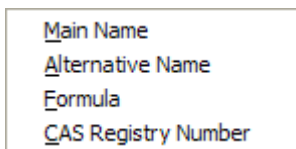
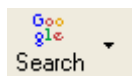
Critical Temperature: 461.00 K
Critical Pressure:    5572.875 kPa
Critical Volume:     154.00 cm3/mol
Acentric Factor:     0.3030
Melting Enthalpy:    3217.50 J/mol
Melting Temperature: 150.20 K
```



This button displays statistics on the component file.

```

Stat.
Number of Components:          22700
394 are PLEASE USE references and
      (2 empty places)
      (-> 22304 normal entries)
CAS-Numbers:                   18285
Molecular Weights:            22246
Melting Points:                3545
Heats of Fusion:               1512
Densities:                     1868
Antoine-Constants (High Pr.):  421
Antoine-Constants (Low Pr.):   3599
UNIFAC-Group Definitions:      12017
UNIFAC (DO)-Group Definitions: 10960
Critical Temperatures:         1374
Critical Pressures:            1108
Critical Volumes:              1083
Acentric Factors:              1069
r-Values for UNIQUAC:          11397
q-Values for UNIQUAC:          11397
Dipole Moments:                  660
  
```



These submenu entries allow searching by the google.com search engine for

- main and alternative name
- the formula and
- the CAS registry number

The search is done by sending an URL to the system's standard web browser. Typical URL for names and CAS-RN search look like

- <http://www.google.com/search?q=Ethanal>
- <http://www.google.com/search?q=71-43-2>

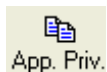
B. Private and Public Compound Files

The Dortmund Data Bank software supports two distinct data bank systems. The first system contains the delivered data banks from DDBST GmbH. The other system contains data banks created by our customers.

The data banks are organized by their location. There's a folder for the public (delivered) data banks and there's a folder for the private (customer's) data banks. Both data banks are integrated seamlessly in the retrieval, plot, prediction, and fit software. The display makes no significant difference between public and private databanks and components. In most cases the numbers changes only the sign. The public components and the data sets from a public data bank have positive numbers and the private components and sets are identified by negative numbers.

Private data banks can be build up with data sets containing information for private and public components. The public data bank contains only public components.

a. Copy Public Components to the Private Component List



This function has been created for a quick update or modification of values stored in the public compound file.

The public component list should be taboo for changes by users for two reasons.

1. The first reason is that this file is changed by DDBST GmbH and will be overwritten if an update is distributed. Every change a customer has made to any fields will be lost.
2. The other reason is that errors introduced by changing delivered values is due to problems when reenacting old calculations. Be aware that other people would have other parameters for the same component. This will lead to confusion.

One solution is to copy the public component into the private component list and add or modify the values there.

Another possibility is implemented by storing different values in a separate file named 'PRIVATE.PCP'. This file is a pure text file containing the same information (and some more) as the compound definition file but it allows to overwrite entries. A detailed description follows later.

C. The Data Fields

a. Component Specification

Specification

Component Number: 20733 components

English Name:

Alternative Name:

Formula: NIST WEB CAS-No.: NIST WEB a+

The "Component Number" is mostly called "DDB number" of the component. The compound list contains two fields, one main name (english) and one alternative name.

Both names have a maximum length of 127 characters. The nomenclature of the components have been following the nomenclature of the authors of the experimental papers. This explains why many names don't follow CAS or IUPAC naming rules.

The formula can have up to 31 characters and digits and the CAS registry number can contain up to eleven digits and hyphens. The CAS registry number is written with hyphens.

The button calls the installed web browser and tries to find information in the NIST web book (<http://webbook.nist.gov>) by the formula or CAS registry number.

The button changes the capitalization of the names.

The program automatically checks the validity of formula and CAS registry number. If a formula contains wrong symbols and the CAS registry number checksum is wrong both entries are displayed in red.

Components with wrong formulas or CAS registry numbers can be stored.

Formula: NIST WEB CAS-No.: NIST WEB

b. Antoine Constants

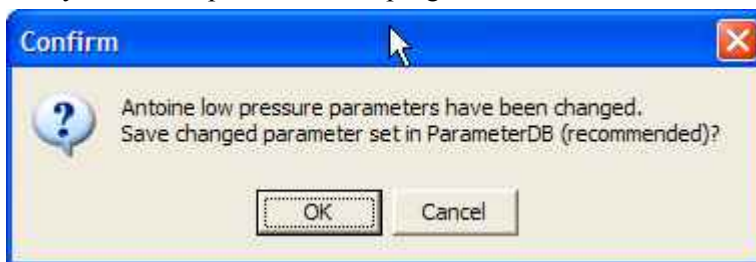
Antoine Constants T [°C] P [mmHg]

Low Pressure: Range: °C Tb=293.55 K

High Pressure: °C Tb=294.07 K

Antoine parameters are given in [°C] as temperature unit and [mmHg] as pressure unit. The component file contains two Antoine parameter sets. One (“Low Pressure”) is normally used for vapor pressure below the normal boiling point and the other (“High Pressure”) is used above the normal boiling point. The “Range” field contain the validity range of both sets. If a parameter set is available the program displays the normal boiling points calculated from the parameters.

Antoine constants are normally stored in the ParameterDDB, the parameter data bank. To ensure consistency between the ParameterDDB and this entry in the component file the program asks to



store changed data also in the ParameterDDB. This is not a compulsory step but it is highly recommended and should only be omitted if the new parameters are stored only for a temporary reason.

c. Values

Values

Crit. Pressure: kPa Heat of Fusion: J/mol

Crit. Temperature: K Melting Point: K

Crit. Volume: cm³/mol Dipole Moment: Debye

Acentric Factor: Molecular Weight:


Density: kg/m³ at K

Most of these values are used for calculations, either fits or predictions. The density entry is only used for the Wilson g^E model and can be hypothetic for components which are solid at approx. 25 °C (= ambient temperature).

Stored and Displayed Units

Value	Shown Unit	Internal Unit
Critical Pressure	kPa	atm
Critical Temperature	K	K
Critical Volume	cm³/mol	cm³/mol
Acentric Factor	-	-
Density	kg/m³	g/cm³
Density Temperature	K	°C
Heat of Fusion	J/mol	cal/mol
Melting Point	K	°C
Dipole Moment	Debye	Debye
Molecular Weight	g/mol	g/mol

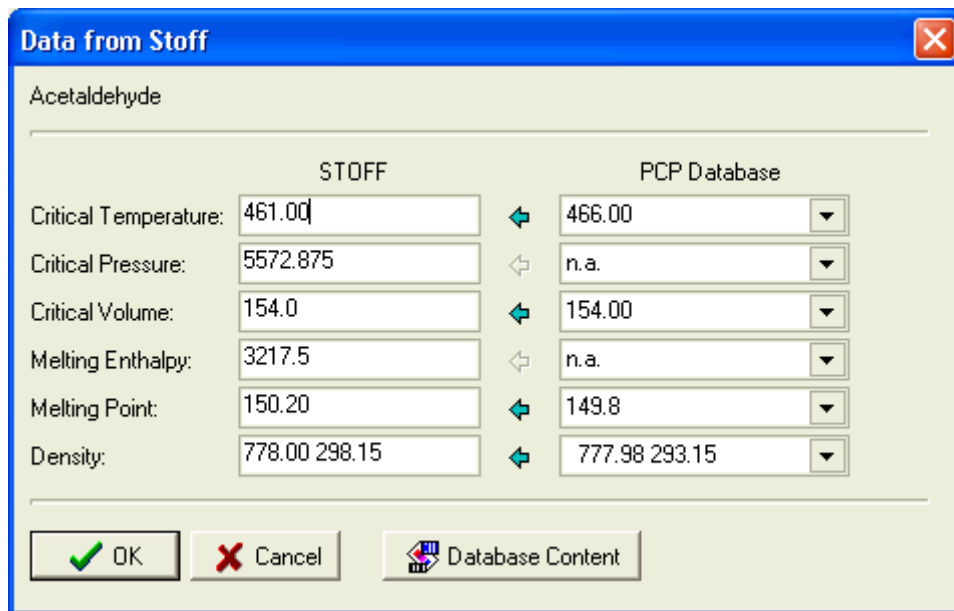
The program displays some of the values in units which are different from the units the values are stored. These units have been selected for being compatible with units used in the pure component properties database.

This was mainly done for being able to compare the component's values with the experimental values. Additionally it is possible to retrieve data from the pure component properties database and update the values in the component file from experimental data. This function can be called by the  button.

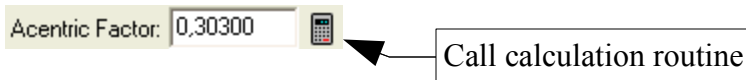


Values from the PCP database can be obtained for six properties shown in the dialog. The drop-down comboboxes below the “PCP Database” title contain all found data points from the PCP database.

The density must be a liquid density near 25 °C.



Obtain the Acentric Factor from Antoine Constants and Critical Data




The dialog displays the old value and two new values from both Antoine parameter sets – if available.

$$\omega = -\log P_{Sr} - 1.000$$

The equation is $\omega = -\log P_{Sr} - 1.000$ with $P_{Sr} = \frac{P_S}{P_c}$ at $T_r = 0.7$

Calculate the Molecular Weight from Formula and Structure

Molecular Weight: 

The dialog displays the original value and two calculated values. The second molecular weight has been obtained from molecular structure (by an Automatic Incrementation function). The structure is only available if the Artist program package is present.

The third field shows the molecular weight calculated from the empirical formula stored in the component file (C₂H₄O in the example).

d. UNIFAC Groups and UNIQUAC Parameters

The groups for both UNIFAC models are encoded. The first number is the amount of different groups (subgroups) in the molecule. The following numbers list the single group as 'count times thousand plus subgroup number'. "1020"

UNIFAC Groups and UNIQUAC Parameters

UNIFAC Groups:	2 1001 1020 0 0 0 0 0	
mod. UNIFAC Groups:	2 1001 1020 0 0 0 0 0	
UNIQUAC r-value:	1.89910	
UNIQUAC q-value:	1.79600	

means one time subgroup 20. The maximum number of different subgroups is seven (eight numbers including the group count).

Obtain UNIFAC Groups from Molecular Structure

The button displays the dialog.

Automatic Group Assignment

Acetaldehyde

UNIFAC

Groups from STOFF:	2 1001 1020 0 0 0 0 0
Groups from A.I.:	2 1001 1020

mod. UNIFAC (Dortmund)

Groups from STOFF:	2 1001 1020 0 0 0 0 0
Groups from A.I.:	2 1001 1020

Accept both A.I. Assignments

Accept UNIFAC Assignment

Accept mod. UNIFAC Assignment

Cancel

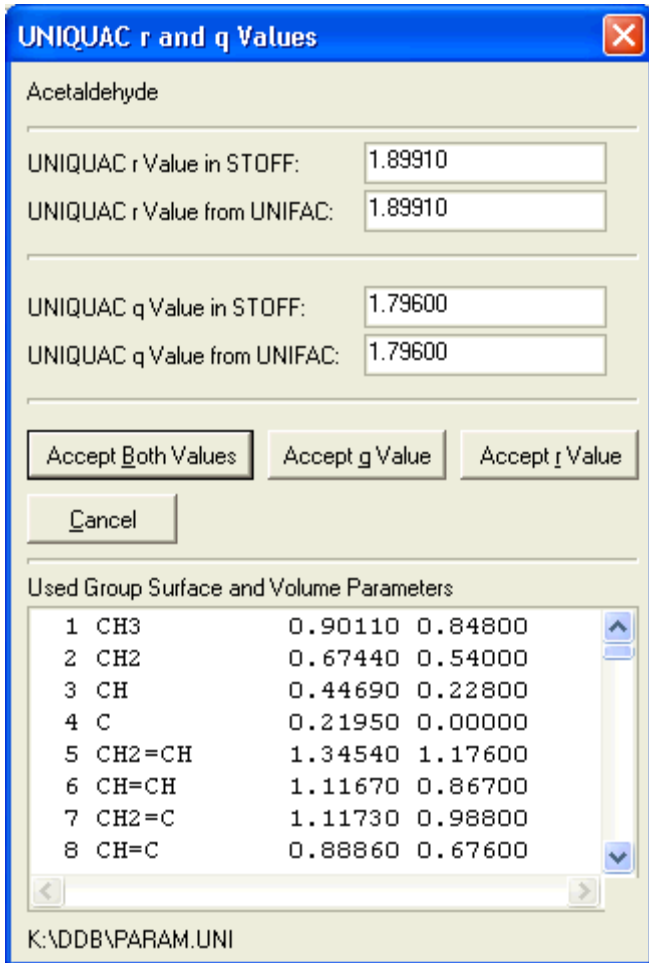
This function uses the automatic fragmentation (also called *automatic incrementation* – A.I.) algorithms. Therefore the Artist program package – including the structure database – has to be available.

The fragmentation schemes only contain published group definitions – not any additional groups from the UNIFAC consortium.

Calculate UNIQUAC r and q Values from UNIFAC Group Surfaces and Volumes


UNIQUAC r-value:	1.89910	UNIQUAC q-value:	1.79600	
------------------	---------	------------------	---------	--

Call calculation routine



The dialog displays the originally stored values and the recalculated values obtained by summing up the surfaces and volumes of the original UNIFAC subgroups. The used group values are listed below.

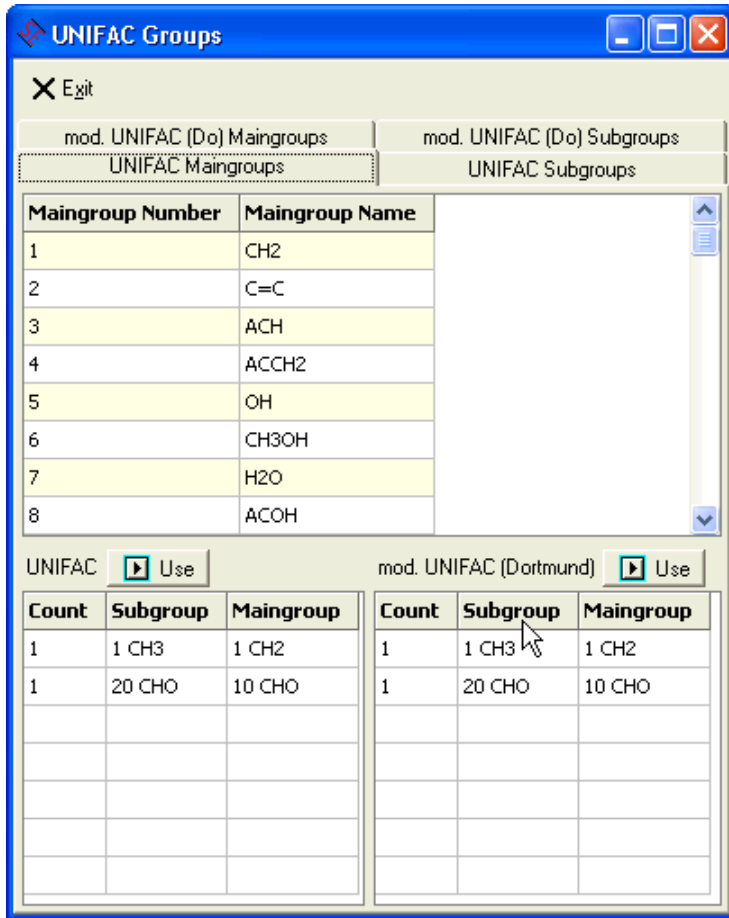
Details Display

Selecting the button  open a dialog with a detailed display of the groups. The upper part display the complete list of main and subgroup of both the original UNIFAC and the modified UNIFAC (Dortmund) models. The lower grid show the current group assignment.

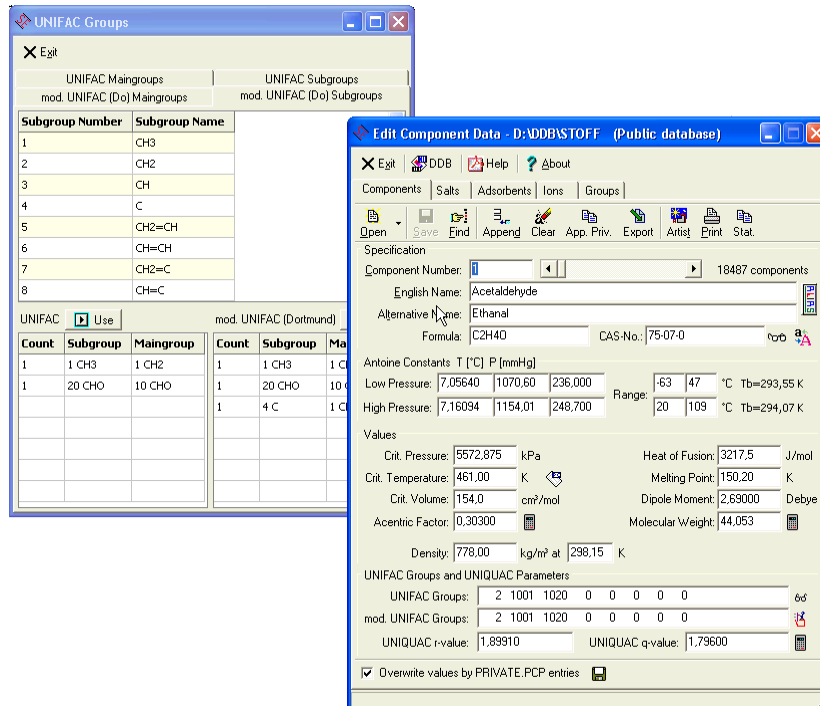
This dialog allows to edit the list of group by dragging **sub**groups from the complete list above to the component's list below.

The 'Count' column in the component's UNIFAC or mod. UNIFAC list is editable.

The  Use button allows to copy the modified list of groups to main editing window.

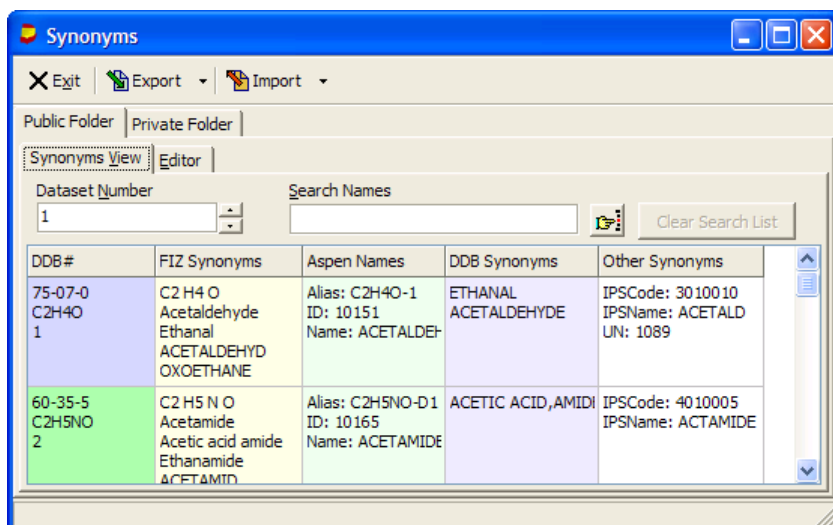


This dialog is non-modal, therefore it is possible to have both the main and this dialog displayed together:



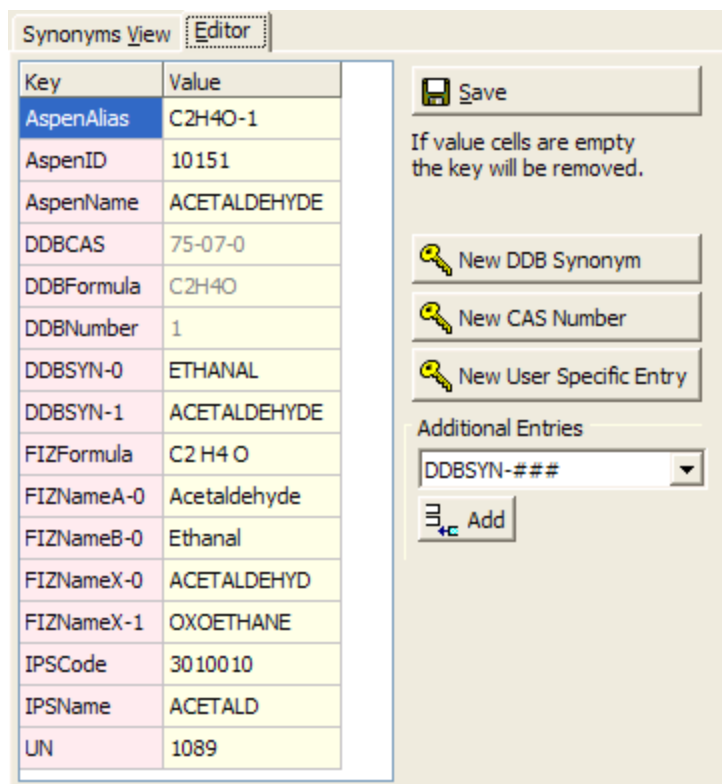
D. Synonyms Management

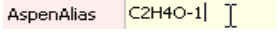
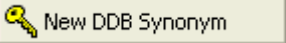
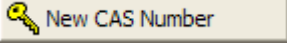

The main DDB component file only contains two names for every component. The synonyms database allows to store any amount of additional names and numbers and whatever.



Three types of synonyms are displayed separately from 'other' synonyms. These are old DDB synonyms, synonyms entered by the FIZ CHEMIE, and Aspen names resp. aliases.

A synonyms dataset is a list of key/value pairs. The keys specify the type of synonym or data and the value specifies the name.



The synonyms editor displays these key/ value pairs in a grid. The light red column contains the key and the light yellow column contains the values. Only the values can be edited directly in the grid(). New keys have to be added by the buttons ,  or . The box 'Additional Entries' contains a list of predefined keys which are read from an “ini” file (STOFFEditor.ini), The file contains four blocks.

```
[StandardPredefinedKeysUnique]
1=AspenAlias
[StandardPredefinedKeysNumbered]
1=DDBSYN-
[AdditionalPredefinedKeysUnique]
1=UN
[AdditionalPredefinedKeysNumbered]
1=DDBSYN-
```

The [StandardPredefinedKeys...] are always inserted in the editing grid if none of these entries are available. The value cell is empty.

The [AdditionalPredefinedKeys...] are only displayed in the drop-down-selection control.

The [...Numbered] entries can occur multiple times – numbers are appended - whereas the [...Unique] entries can occur only one time.

Keys cannot be deleted directly but the program removes keys with an empty value cell when saving.

E. Additional Files

Some of the pure component data are not stored in the main component file. For some of these files additional dialogs have been added. These dialogs can be opened by the drop-down-menu entries.

1. DHT.DAT Editor
Heats of transitions and transition temperatures in the solid phase, used for SLE calculations. Up to three temperature/heat pairs can be added.
2. HGCP.DAT Editor
Heat and Gibbs Energy of Formation, and parameters for a heat capacity equation.
3. NBP.DAT Editor
Normal boiling points
4. STOFF1 Parameters
Editor for a variety of equations for vapor pressures, liquid densities, second virial coefficient and heat of vaporization. The equation numbers are “DIPPR numbers – 99”, e. g. equation DIPPR no. 100 is no. 1 in the STOFF1 file.

3. Replace Component Definition File Entries for Calculations

As stated in chapter “Private and Public Compound Files” the data entries in the public compound definition files are not allowed.

One possibility to modify the data nevertheless has been mentioned already. Public components can be copied into the private component list. This doesn't solve the problem entirely because the data bank contains public components and a user would have to alter the component list in public data banks in order to use the private component duplicate.

There's another solution: All calculation programs (and the `StoffEditor`) are looking for a file named `PRIVATE.PCP` in the `DDB` folder for private data banks. This file contains selected data for specified components.

This file has to be edited currently by hand. Its format is pure text and the single values are identified by tags.

The possible tags are

Tag	Description
DDB#	DDB component number
COM	Comment
INIT	Initialize all value for a component (see description of the 'Clear' button)
GNAM	German name (up to 48 characters)
EMPF	Empirical formula (up to 12 characters)
ENAM	English name (up to 48 characters)
CASN	CAS registry number
ANTN	Low pressure Antoine constants (P [mm Hg], T [°C]), Line entries: A, B, C, lower temperature limit, upper temperature limit
ANTH	High pressure Antoine constants (P [mm Hg], T [°C]), Line entries: A, B, C, lower temperature limit, upper temperature limit
CRID	critical properties and dipole moment Line entries: Tc [K], Pc [atm], Vc [cm ³ /mol], acentric factor, and dipole moment Values can be separated by semicoli.
MPT	Melting temperature in [°C]
HFSN	heat of fusion [cal/mol]
UNRQ	UNIQUAC r and q values
INKU	Structural information of original UNIFAC. Groups are encoded
INKM	Structural information of mod. UNIFAC (Dortmund variant).
MWGH	molecular weight [g/mol]
LDEN	Liquid density [g/cm ³] and temperature [°C]
INK# ¹	Structural information of ASOG, mod. UNIFAC (Lyngby) and both PSRK models. Structural information is preceded by model numbers: 1: mod. UNIFAC (Lyngby) 2: ASOG 3: PSRK and PSRK2 13: PSRK extended (32 Groups)
TRAN ¹	Transition temperature and heat Line Entries: T _{Tr} [K], H _{Tr} [J/mol]
MCRK ¹	Mathias-Copeman constants for Soave-Redlich-Kwong equation of state used in PSRK. Line entries: c ₁ , c ₂ , c ₃ , T _{min} , T _{max} [K]

¹ This information is not available in the compound definition file.

The following frame shows the content of a PRIVATE.PCP file. In this special case every entry is written. This is not necessary. If some tags are not given, the calculation programs always use the entries from the compound definition file.

```

DDB# 11
INIT
GNAM ETHANOL
ENAM ETHANOL
EMPF C2H6O
CASN 64-17-5
ANTN      8.20417    1642.89    230.341    -57    80
ANTH      7.68117    1332.04    199.177    77    243
CRID      516.2000    63.0000    167.0000    0.6350    1.6900
MPT      -114.500
HFSN      1199.200
UNRQ      2.10550    1.97200
INKU          3      1001      1002      1014
INKM          3      1001      1002      1014
MWGH          46.069
LDEN          0.785000      25.00
;
INK# 1          3      1001      1002      1012
INK# 2          2      2001      1006
INK# 3          3      1001      1002      1014
TRAN      0.00      0.0    0.00      0.0    0.00      0.0
MCRK      1.3327    0.9695    -3.1879      206      490
    
```

The screenshot shows the 'Component Editor' window for Acetaldehyde. The 'Specification' section includes fields for Component Number (19496), English Name (Acetaldehyde), Alternative Name (Ethanal), Formula (C2H4O), and CAS-No. (75-07-0). The 'Antoine Constants' section shows parameters for Low Pressure (7.05640, 7.06, 1070.600) and High Pressure (7.16094, 7.16, 1154.010). The 'Values' section includes Crit. Pressure (46710.830 kPa), Heat of Fusion (3217.5 J/mol), Crit. Temperature (461.00 K), Melting Point (150.20 K), Crit. Volume (55.0 cm³/mol), Dipole Moment (0.30300 Debye), Acentric Factor (154.00000), and Molecular Weight (44.053). The 'UNIFAC Groups and UNIQUAC Parameters' section shows UNIFAC Groups (2, 2, 1001, 1020, 0, 0, 0, 0) and UNIQUAC r-value (1.89910). The 'Density' is 778.00 kg/m³ at 273.93 K. The 'Overwrite values by PRIVATE.PCP entries' checkbox is checked.

If entries have been replaced by entries from the "Private.PCP" file the component editor shows blue background on the affected data fields.

Additionally, both names are prefixed by an exclamation mark if at least one entry has been modified.





Saves changes



Export all data sets to old-style salt files (needed in other programs).

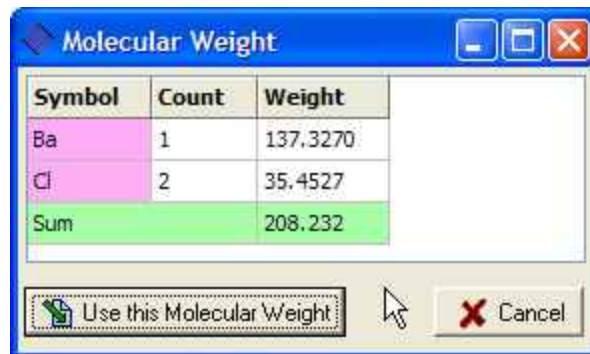
B. Basic Entries

The electrolyte list contains

- a single name entry
- a formula
- a DDB basic number. Many electrolytes are also part of the main component list (for the EGLE - gas solubilities - and PCP - pure component properties - databanks). The button  opens a component selection dialog and the button  displays the connected entry of the main component list.
- a molecular weight. The molecular weight can be calculated from the formula.


The program displays the molecular weight calculated from the formula and a click on the blue label open a details dialog.

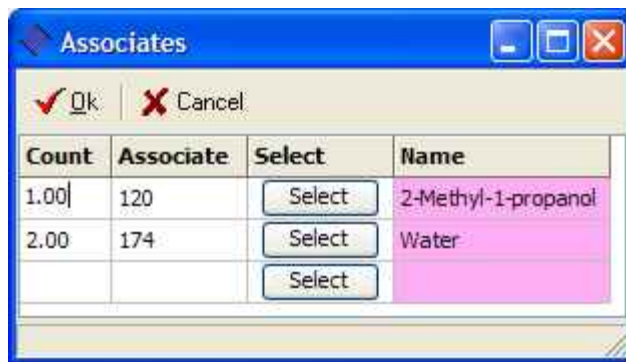
Molecular Weight
208,240
From Formula: [208,23](#)
Gibbs Energies of Form.



Symbol	Count	Weight
Ba	1	137.3270
Cl	2	35.4527
Sum		208.232

- a dielectric constant (with temperature)
- a single density value (with temperature)
- a frequency (Hz)
- heat capacities
- energies and enthalpies of formation
- a melting temperature
- a heat of fusion
- a list of ions in encoded form. The first number gives the number of different ions and the following specify the ions count (thousands) plus ions number ("2012" means 2 times ion no. 12 - CO₃).

- a list of associates. This is a list of number pairs. The first is the count and the second is the main component number (“2.5 174” means two and half water molecules). The button  opens a small editing dialog for the associates.
- a flag if the electrolyte is volatile (true for HCl, false for NaCl).

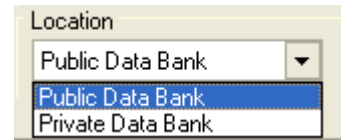


C. Private and Public Salts and Electrolytes Lists

Like the normal component's list the salt editor supports two distinct electrolytes lists. One public list delivered from DDBST GmbH, and a private list created by customers.

The two buttons allow to switch between both lists. If a private file does not yet exist it will be created on the fly.

Private ESLE and ELE databanks can be build from private and public components and electrolytes whereas the public databases only contain public components and electrolytes.



D. ELE Parameters

#	Component 1	Component 2	Interaction Parameter 1-2	Interaction Parameter 2-1
1	-11	-19	0.00	0.00
2	-11	-21	0.00	0.00
3	-11	-23	0.00	0.00
4	-11	-2	0.00	0.00
5	-11	-5	0.00	0.00
6	-11	174	-593.70	-956.90
7	-11	110	-74.20	631.50

The ELE parameters dialog is a preliminary version. It only allows to view the parameters for several models for the estimation of vapor-liquid equilibria of electrolyte containing systems. The possibility to edit the parameters and a more concise display will be added.

5. Ions

The component editor provides an editor for an ions list. These ions are the “groups” of a salt and are widely used for different models.

Number	Ion	Charge (Z)	Mol.Weight [g]	Radius of Ion [Ångström]	Delta-Hf 298.15 K [KJ/mol]	Delta-Gf 298.15 K [KJ/mol]	Delta-cP 298.15 K [J/(mol K)]
1	Ba	2	137.33	1.98	0.000	0.000	0.000
2	Cl	-1	35.45	0.99	-167.159	-131.228	-136.400
3	F	-1	19.00	0.72	-332.630	-278.790	-106.700
4	I	-1	126.90	2.20	-55.190	-51.570	-142.300
5	NO3	-1	62.00	0.00	-207.400	-111.300	-86.600
6	SO3	-2	80.06	0.00	0.000	0.000	0.000
7	Be	2	9.01	0.90	0.000	0.000	0.000
8	Br	-1	79.91	1.14	-119.570	-104.160	-72.300
9	SO4	-2	96.06	0.00	-909.270	-744.530	-293.000

The list contains the formula (without charges), the charge, the molecular weight, the radius of the ions, and some thermodynamic properties. The grid is editable.

NO3

The context menu of the grid

- Display all salts containing "Ba"
- Copy Hf, Gf, cP values in salt file for "Ba"
- Calculate molecular weight of Ba

allows

1. searching for all salts containing the ion of the selected line. The salts found will be displayed in the standard component selection program.
2. updating the salts basic file with the H_f , G_f , and c_p values.
3. Calculating the molecular weight of an ion

Gibbs Energies of Form.			kJ/mol
Salt	Cation	Anion	
-810.400	-560.770	-131.228	
Enthalpies of Formation			kJ/mol
Salt	Cation	Anion	
-868.600	-537.640	-167.159	
Heat Capacities			J/mol*K
Salt	Cation	Anion	
75.000	0.000	-136.400	

6. Groups

The “Groups” page allows to edit group list for the implemented mixture group contribution methods.

Public file K:\DDB\INKR.PSX with 15732 entries - Private file K:\DDBPRV\INKR.PSX with 15732 entries

This dialog displays the name, formula, CAS-RN and the DDB number of the currently edited component.

The group assignment is displayed in a read-only field because editing the list of groups is performed in the grid below that display field.

The grid allows to enter the group count directly in the left column. Adding subgroups is done by dragging a line from the list of groups to editing grid. Lines are removed by double-clicking.

Count	Subgroupnumber	Subgroupname
1	1	CH3
23	2	CH2
5	9	ACH
1	12	ACCH2

This group can also be used for the original UNIFAC and modified UNIFAC (Dortmund) group assignments.

7. Polymers

A. List of Polymers

#	Names	Monomer	Copolymer Parts
5	poly(n-butyl methacrylate)		
6	poly(vinyl acetate)		
7	ethylene/vinyl acetate copolymer poly[ethylene-co-(vinyl acetate)]		1 Ethylene 2 Vinyl acetate
8	poly(methyl methacrylate)		
9	polypropylene polypropene Poly(1-methylethylene), PP	(C ₃ H ₆) _n	

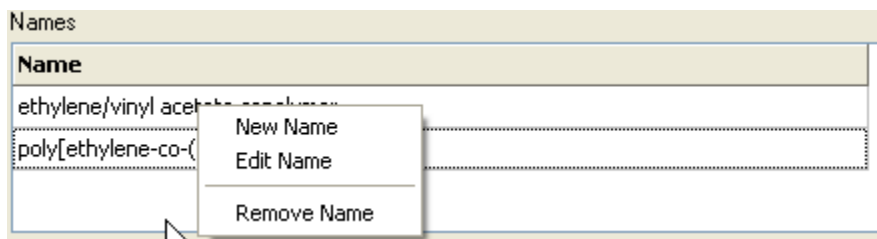
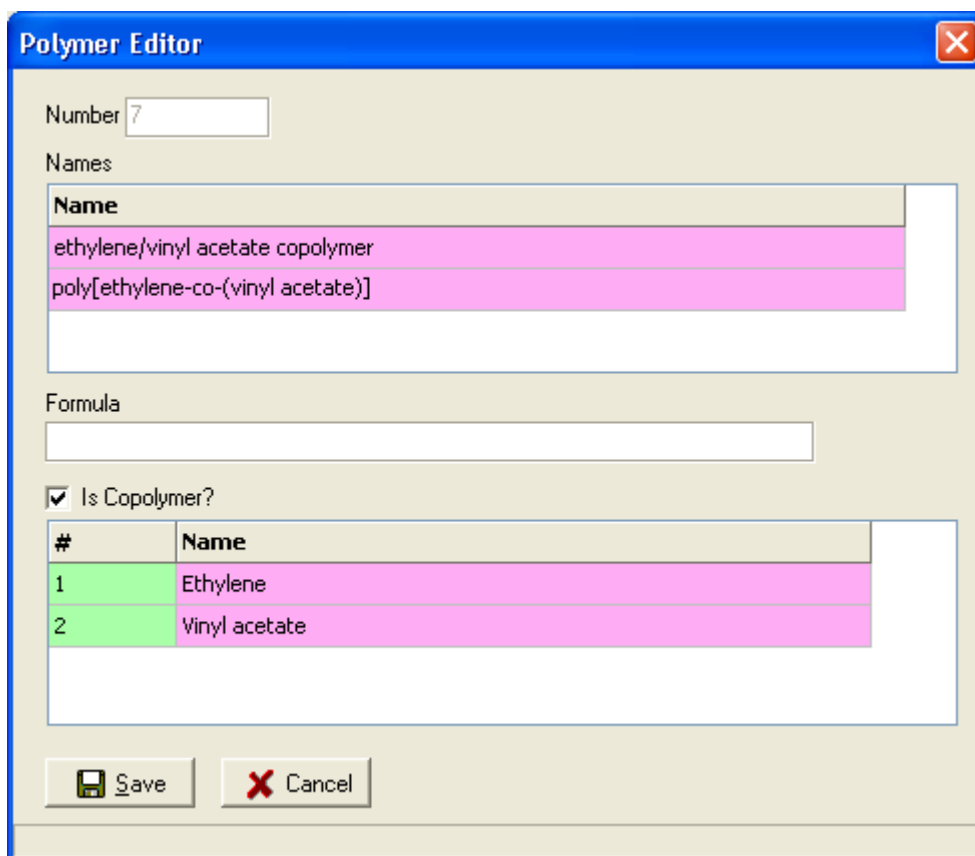
The list of polymers contains names for the polymer, a description of its monomers, and, in case of copolymers, the polymer's monomers. Details like mean molecular weights, mean chain length, supplier, and other details are stored within the single polymer data sets only.

B. Editing Polymers

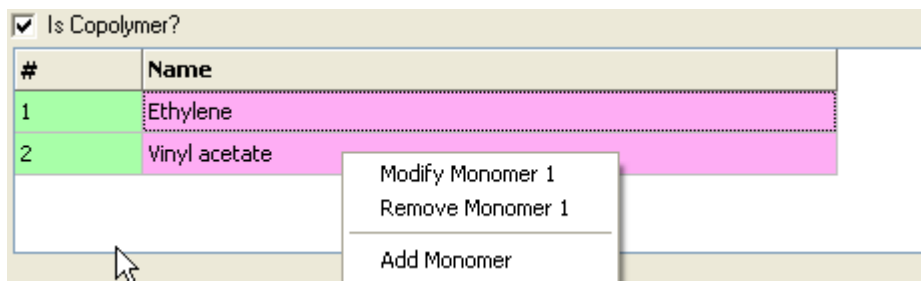
The editor for a single polymer can be opened by a double-click on the grid line or by a context menu.

6	poly(vinyl acetate)		
7	ethylene/vinyl acetate copolymer poly[ethylene-co-(vinyl acetate)]		1 Ethylene 2 Vinyl acetate
8	poly(methyl methacrylate)		

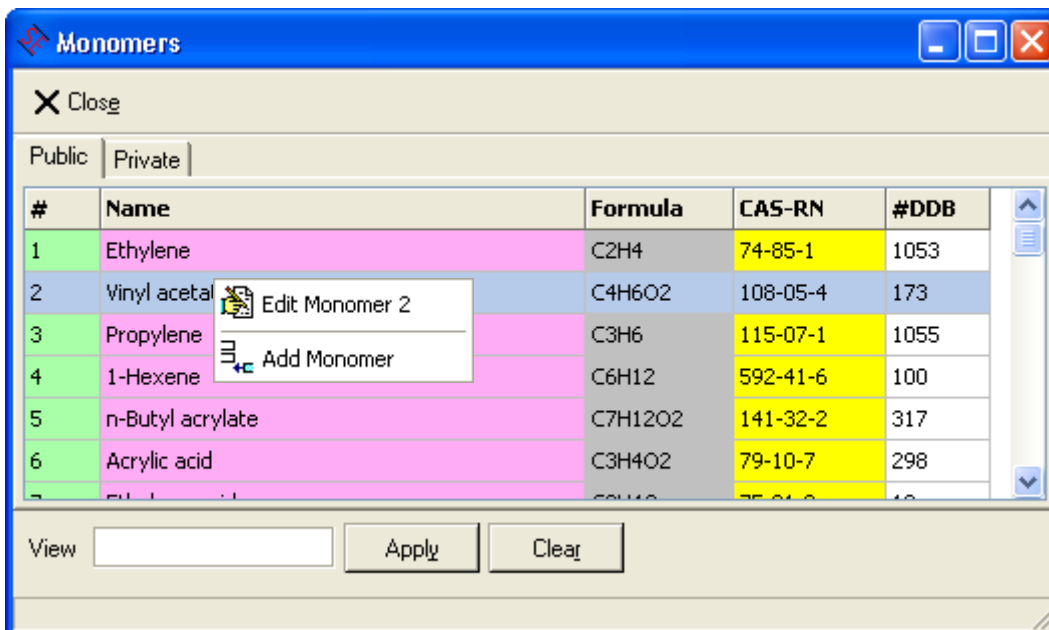
The editor allows to enter several names (one main name and an unlimited number of synonyms). The formula is intended for the description of the monomer's formula. If the polymer described is actually a copolymer the list of building monomers can be added.




The editing functions are all in context menus. The names can be in the grid, whereas the monomers in the copolymer block must be edited by a sub dialog.

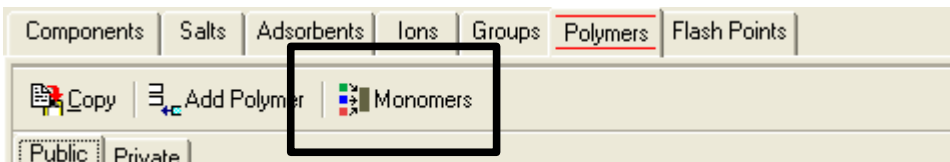


C. Editing Monomers

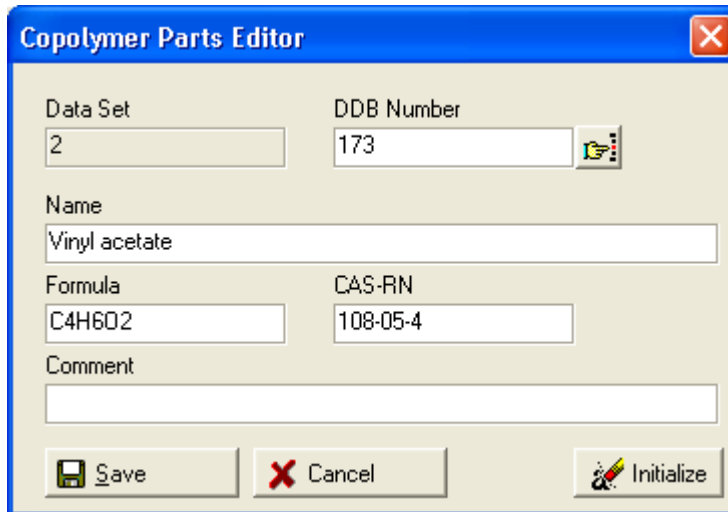


Monomers are managed in a separate list. This list is used in the copolymer editor (part of the polymer editor dialog) but can also be displayed by the button

 Monomers in the tool bar if the polymer list display. The editor for single monomers can be called through the context menu of the monomer's grid.



The editor allows to edit a single name, a formula, a CAS registry numbers and a comment.

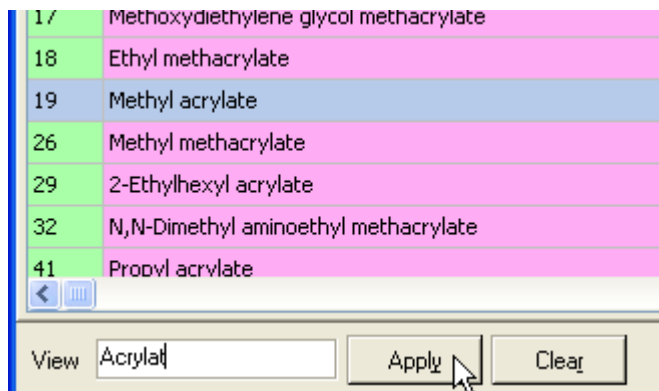


If the monomer is part of the normal DDB component list its DDB number can and should be specified. If a DDB number has been selected it is possible to use the entries from the component basic file to fill the entries of this dialog.

View

The part of the dialog allows to shorten the list of monomers by filtering the names by the text entered. For example, if the filter is set to “Acrylat” only monomers with the name's part “Acrylat” are displayed. Capitalization is ignored.

removes the filter and display the entire list again.



8. Flash Points

Components | Salts | Adsorbents | Ions | Groups | Polymers | **Flash Points**

Save | Copy

Name
Acetaldehyde

Formula: C₂H₄O DDB Number: 1

Property	Value
Flash Point [°C]	
Soluble in Water at 15°C [yes/no]	yes
Lower Explosion Limit [g/cm ³]	73
Lower Explosion Limit [Vol-%]	4
Upper Explosion Limit [g/cm ³]	1040
Upper Explosion Limit [Vol-%]	57
O ₂ Limiting Concentration [Vol-%]	
Max. Explosion Pressure [bar]	8.20
Ignition Temperature [°C]	155
Max. Experimental Safe Gap [mm]	0.92
Temperature Class	T4
Explosion Group	IIA

Most of the entries are from

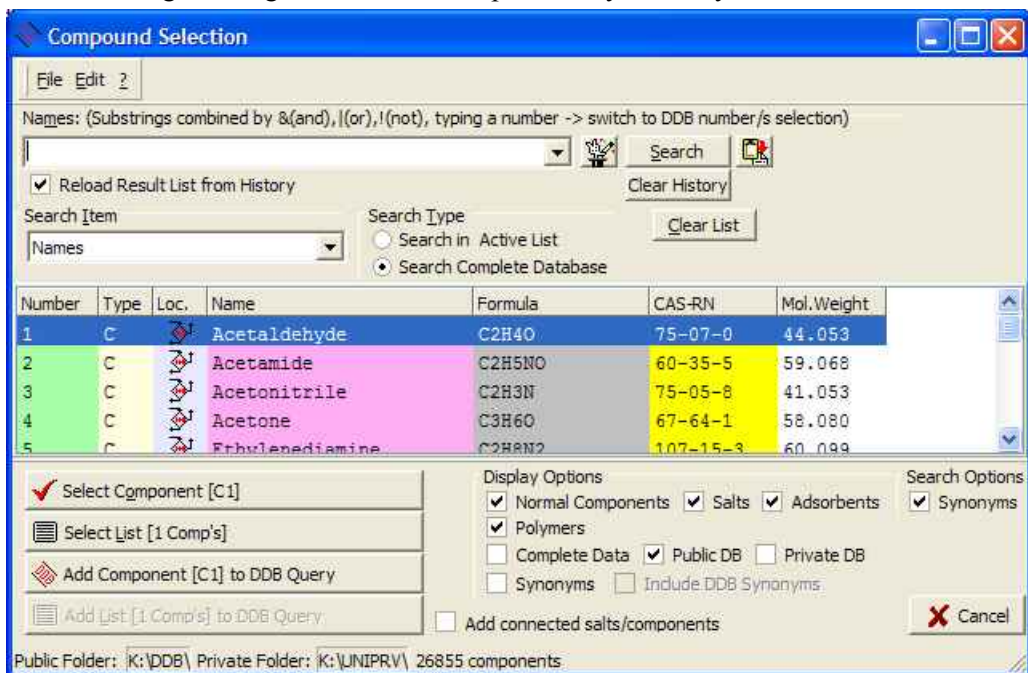
Brandes E., Möller W., “Sicherheitstechnische Kenngrößen”, Band 1: Brennbare Flüssigkeiten und Gase”,
Wirtschaftsverlag NW, Verlag für neue Wissenschaft GmbH, Bremerhaven

(“Safety-related characteristics”, Volume 1: “Inflammable Liquids and Gases”)

Data are available for almost 1900 components – but the data sets are rarely complete.

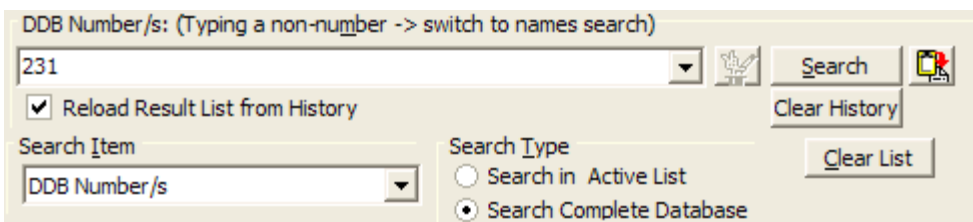
9. Searching Components

The DDB software uses a single dialog to search for components by a variety of criteria.



A. Dialog Parts

a. Search Queries



This part allows to specify a search by different criteria.

b. Component List

Number	Type	Loc.	Name	Formula	CAS-RN	Mol.Weight
1	C		Acetaldehyde	C2H4O	75-07-0	44.053
2	C		Acetamide	C2H5NO	60-35-5	59.068
3	C		Acetonitrile	C2H3N	75-05-8	41.053
4	C		Acetone	C3H6O	67-64-1	58.080
5	C		Ethylenediamine	C2H8N2	107-15-3	60.099
6	C		1,2-Dibromoethane	C2H4Br2	106-93-4	187.870
7	C		Ethyl bromide	C2H5Br	74-96-4	108.970
8	C		1,2-Ethanediol	C2H6O2	107-21-1	62.068
9	C		Ethyl iodide	C2H5I	75-03-6	155.970
10	C		5-Ethyl-2-norbornol	C11H20O	103-08-2	172.310

This part displays the list of components – either the complete list or a search result

c. Options

Display Options			Search Options				
<input checked="" type="checkbox"/>	Normal Components	<input checked="" type="checkbox"/>	Salts	<input checked="" type="checkbox"/>	Adsorbents	<input type="checkbox"/>	Synonyms
<input checked="" type="checkbox"/>	Polymers	<input type="checkbox"/>	Complete Data	<input checked="" type="checkbox"/>	Public DB	<input type="checkbox"/>	Private DB
<input type="checkbox"/>	Synonyms	<input type="checkbox"/>	Include DDB Synonyms				

The display options change the component display:

- Component types. The DDB know four types of components:
 - Normal components
 - Salts
 - Adsorbents
 - Polymers
- Complete Data. This option extends the display of normal components by several properties like T_c , P_c , V_c , etc.
- DDB Location. Two locations are supported. The public list is the data bank distributed by DDBST and the private list is from the user.
- Synonyms. This option allows to display synonyms directly in the component list. The DDB synonyms are normally not very useful and can be showed or hidden separately.

Number	Type	Loc.	Name	Form
1	C		ACETALDEHYD Acetaldehyde AspenAlias: C2H4O-1 AspenID: 10151 AspenName: ACETALDEHYDE C2 H4 O Ethanal OXOETHANE UN: 1089	C2H

The search option “Synonyms” allows switching the synonyms search on or off. The synonyms search is rather slow and if the names are simple a search in the main names might be sufficient.

d. Commands

<input checked="" type="checkbox"/> Select Component [C2]	<input type="checkbox"/> Add connected salts/components
<input type="checkbox"/> Select List [2 Comp's]	
<input checked="" type="checkbox"/> Add Component [C2] to DDB Query	
<input type="checkbox"/> Add List [2 Comp's] to DDB Query	

These buttons allow to

- select a single component (the currently selected component, the component's code is appended to the button's caption)
- select a list of components (the list's size is appended to the button's caption)
- add a single component to the Dortmund Data Bank query
- add a list of components to the Dortmund Data Bank query.

The first two buttons will close the dialog but the latter two will keep the search result window open.

The option “Add connected salts/components” is necessary for components that are both in the normal component list and in the salt list. The reason is that salts are treated as normal components in most data banks. Salts are treated as separate components only in the salt solubilities (ESLE) data bank and in the vapor-liquid equilibria data bank containing salts (ELE). The reason is that only for these kind of data salt-specific parameters are needed.

B. Search Criteria

The different search types can be set by the drop-down menu in the “Search Item” area of the dialog.

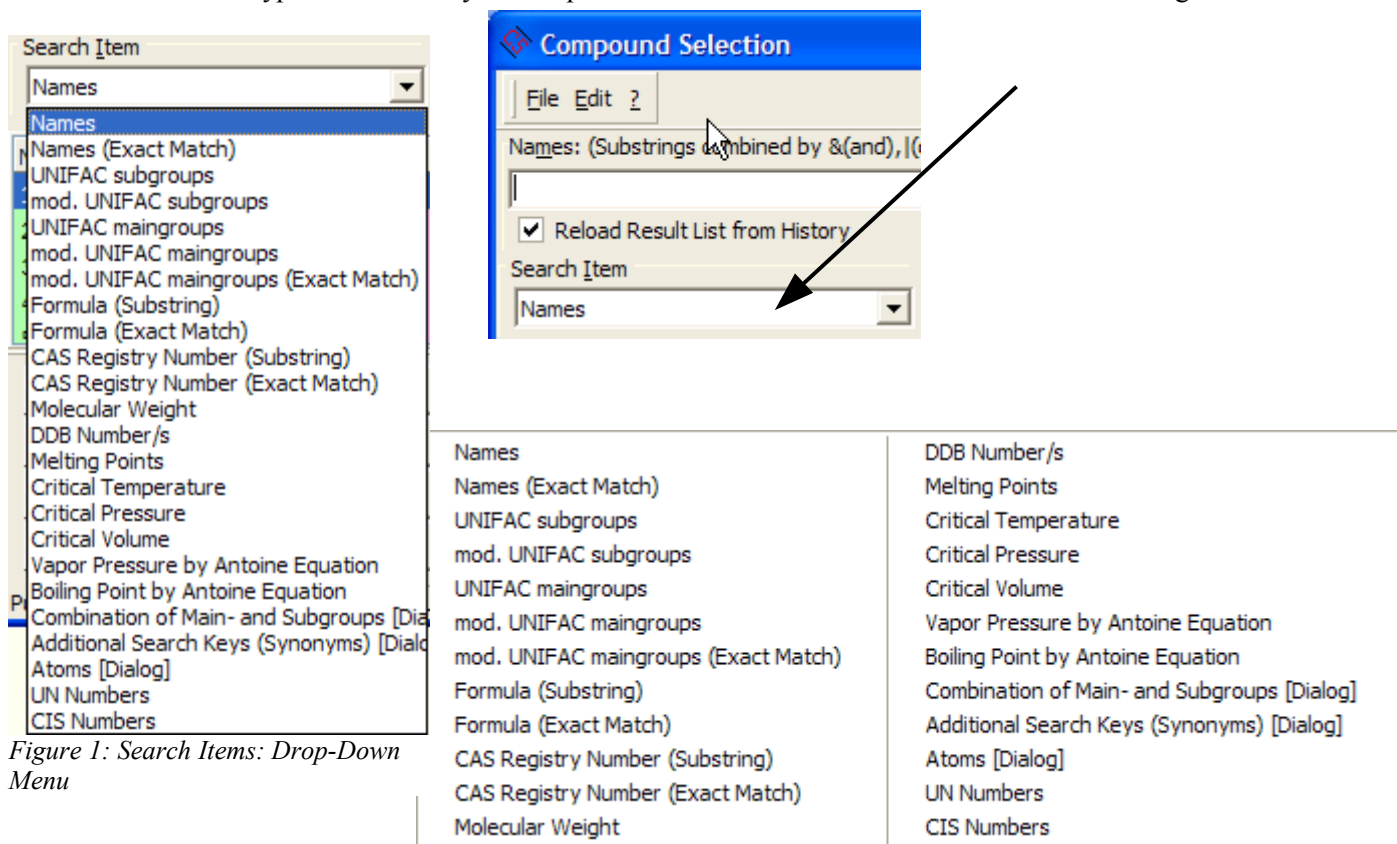


Figure 1: Search Items: Drop-Down Menu

Figure 2: Search Items: Context Menu

a. Search for Names

The search for names can either be a sub-string search or an exact match search. In case of a sub-string search several operators can be used to combine the parts:

<i>Operator</i>	<i>Used to</i>
!	NOT Excludes strings. If a string is prefixed with the exclamation sign it must not be part of the name
&	AND Tells the search routine that both parts before and behind the ampersand must be given.
	OR (Pipe symbol) Tells the search routine that either one or the other part or both parts must be present.

Example searches:

brom&chlor	Searches for names where both “brom” and “chlor” is present. 2-Bromo-2-chloro-pentane Bromochloromethane [R30B1]
brom chlor	Searches for names where “brom” or “chlor” is present. 2-Bromo-pentane 3-Chloro-hexane
brom&!chlor	Searches for names containing “brom” but “chlor” must not be present.

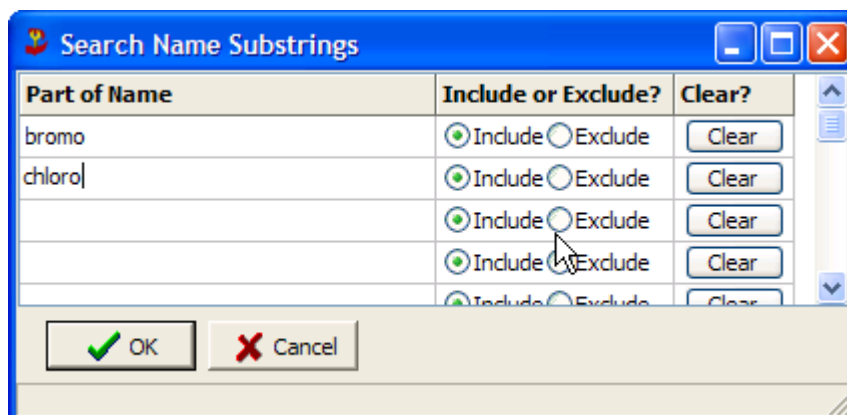
All searches are case-**ins**ensitive.

If a substring search finds an exact match the search result list will contain these exact matches as first matches.

For names sub string search a special dialog is available.



The dialog

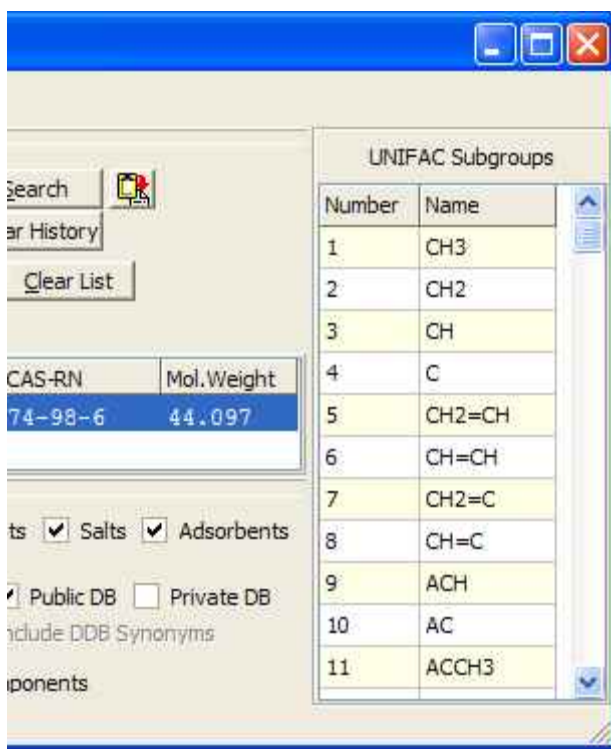


allows the specification of search strings without these somewhat awkward operators.

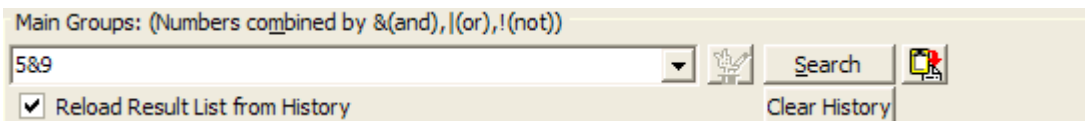
b. UNIFAC sub group and main group searches

The group searches allow some kind of structural search because the UNIFAC groups are mostly defined by standard functional groups like ketone, alcohols, etc.

The component selection is extended by the selected group list.



These numbers have to be entered in the main query edit field:



The number can be combined with the same operators that have been explained for the sub string search.

c. Empirical Formulas

The search for formulas be performed as substring or as exact match search.

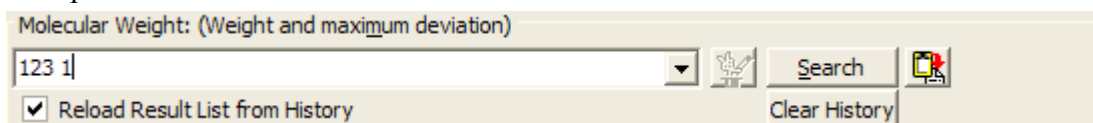
d. CAS Registry Number

The search for registry numbers be performed as substring or as exact match search. The search requires that the numbers are entered including the hyphens (513-86-0 instead of 513860).



e. Molecular Weight

The molecular weight search requires two numbers separated by blanks: The wanted molecular weight and a value for an acceptable deviation which can be 0.



f. DDB Numbers

This search allows to search components directly by the DDB definition numbers (4 for acetone, 31 for benzene, 95 for 2-Propanol, etc.). It is possible to enter multiple numbers. These numbers have to be separated by blanks.

g. Critical Temperature, Pressure, Volume

This search requires two values separated by blanks: A wanted critical value and an acceptable deviation.

h. Vapor Pressure by Antoine

This search allows to find components with a wanted saturated vapor pressure at a given temperature. The component selection program opens a special dialog where the data can be entered.

After pressing the Okay button the values are moved to the query edit control and the search can be started.

In this example we will find Ethyl benzene which has a vapor pressure of $P=151.6$ kPa at 425 K.

i. Boiling Point by Antoine

This is the reverse search. A dialog opens where a wanted boiling temperature and a pressure can be specified.

If the pressure is set to 101.325 kPa the search will yield components with normal boiling points near the entered temperature.

Boiling Point: (T [K], maximum deviation in T [K], P [kPa])

400 5 101.325

Reload Result List from History

Search Clear History

The example will return 2-Methyl pyridine which has a normal boiling of $T_B=402$ K.

j. Combination of main and subgroups

This search opens directly a dialog:

CODSNT

Group Contribution Method

UNIFAC ASOG

mod. UNIFAC (Do) PSRK

mod. UNIFAC (Ly)

List of allowed maingroups (leave empty to allow all)

List of necessary subgroups (leave empty to allow all)

Search

This search allows to search for components with some special combinations of main and sub groups. This search is mainly used internally for the UNIFAC development and is of little use for normal queries.

k. Additional Search Keys (Synonyms)

This search allows to search special entries in the synonyms file.

Search For Additional Keys

Search for

AspenAlias

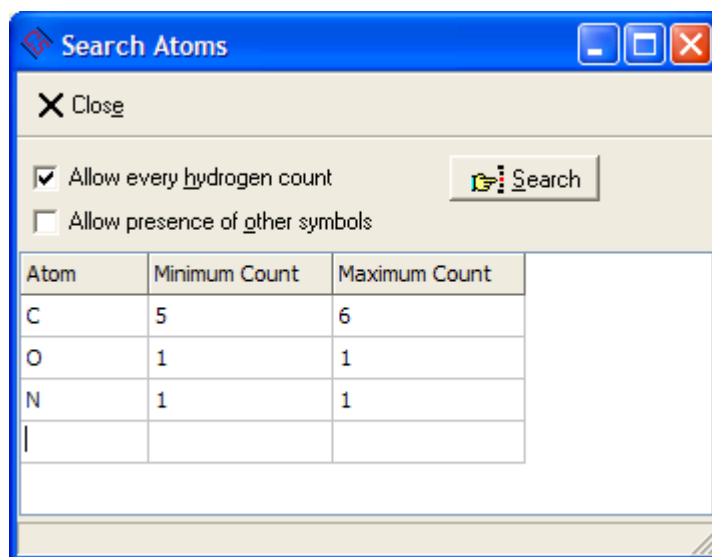
Search Text:

C2H4O-1

Typically search entries are the Aspen Alias, the Aspen ID, and the Aspen Name.

l. Atoms

This search mode open directly an additional dialog where atoms and their counts can be entered. This search analyzes the empirical formula and searches for components with specified atom types.



The search options are:

- “Allow every hydrogen count”: Hydrogens are not specified in the table and can be present in the component in every number.
- “Allow presence of other symbols”: This option decides whether the search criterion is “exact match” or not.

The example will find ϵ -Caprolactam (C₆H₁₁NO).

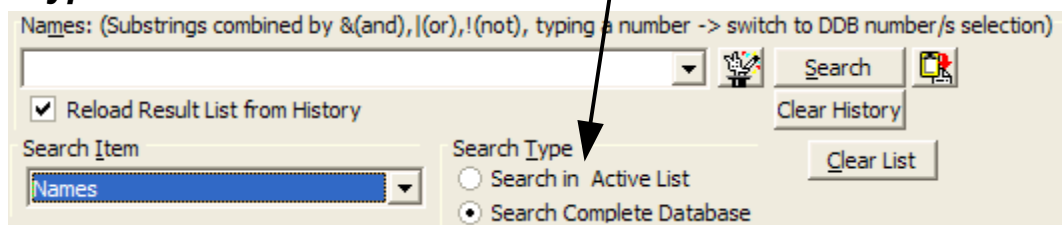
m. UN Numbers

The UN numbers are numbers with four digits specifying some special components and some component class.

n. CIS Numbers

CIS number are specific numbers of the Lonza AG and are only available on request and on special affirmation.

C. Search Type

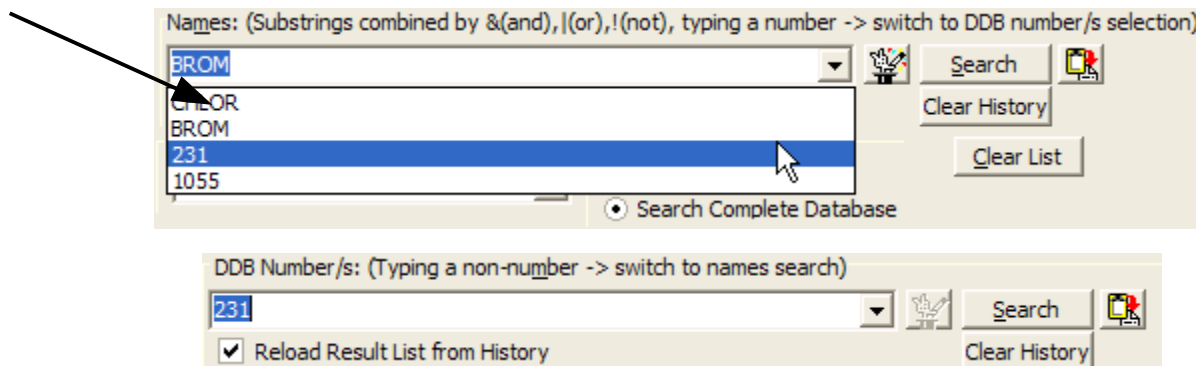


A search can be restricted to the result list of a previous search. This allows to perform different searches sequentially.

D. Search History

The component selection stores the last ten searches. These latest queries are listed in the drop-down menu of the query edit control.

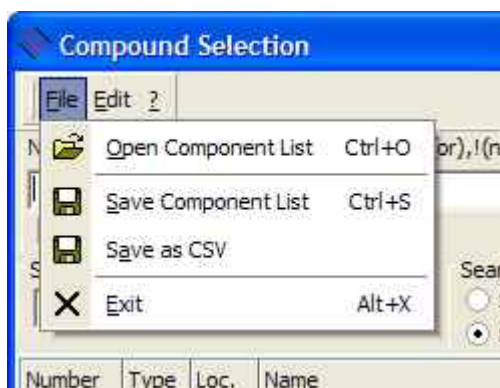
Besides the queries the search result lists are also stored. These list are recovered if the “Reload Result List from History” box is checked.



The complete history can be deleted by the “Clear History” button.

E. The Menus

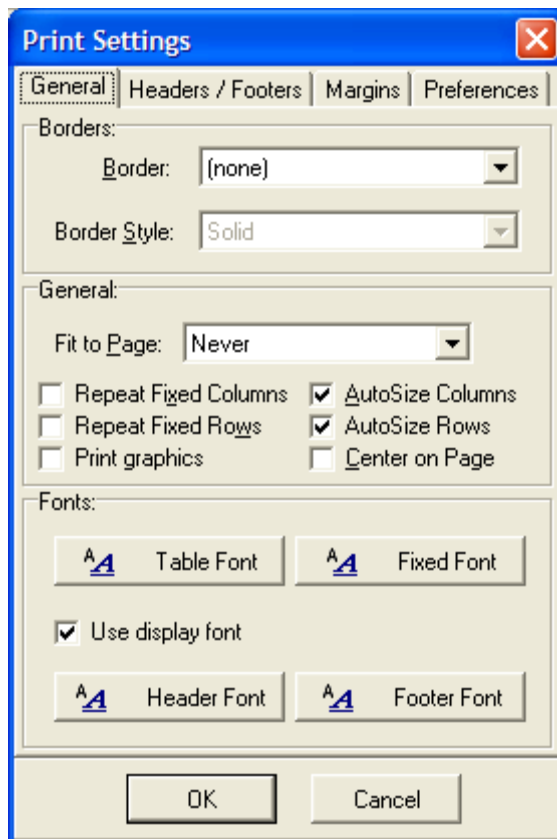
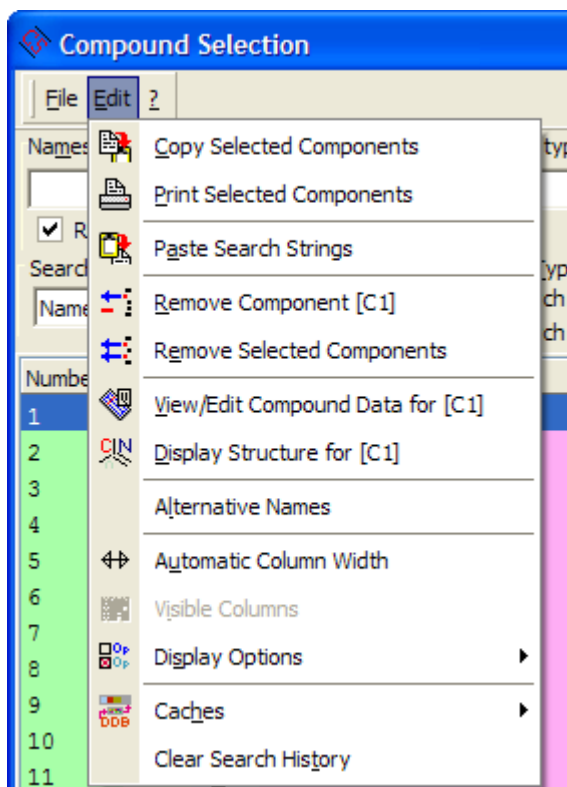
a. File Menu



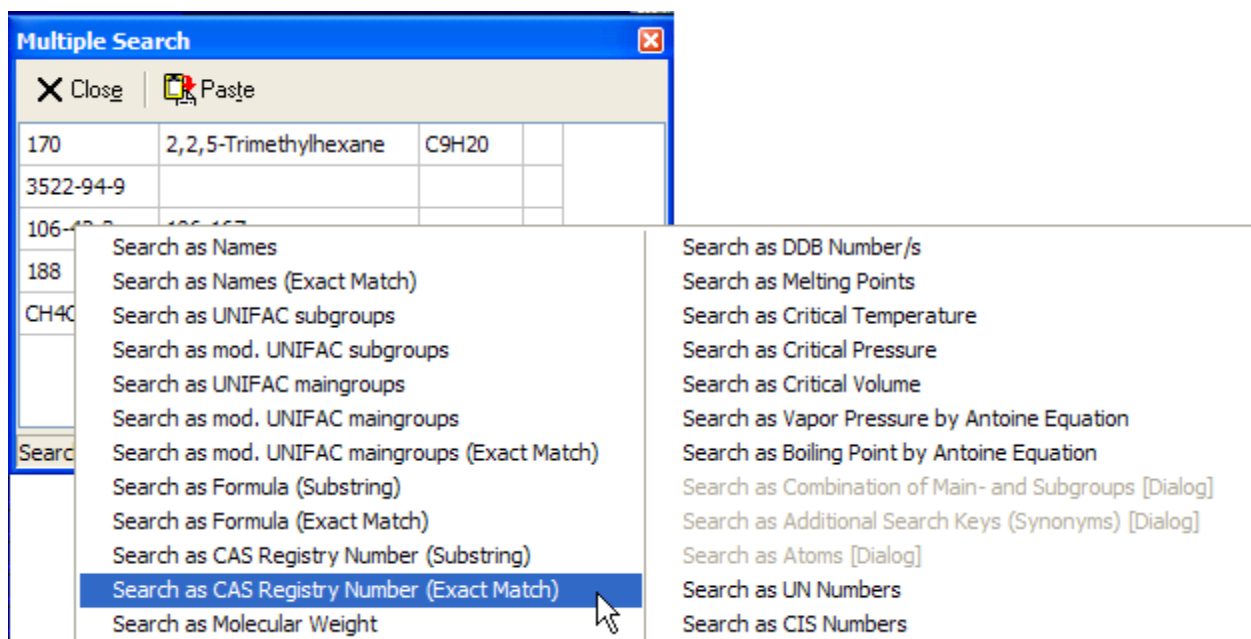
The file menu allows to open and save component list in a DDB specific format containing DDB component numbers. A CSV (comma-separated values) will contain the content of the component grid and can be easily loaded in spread sheet programs like Microsoft Excel or OpenOffice Calc.

b. Edit Menu

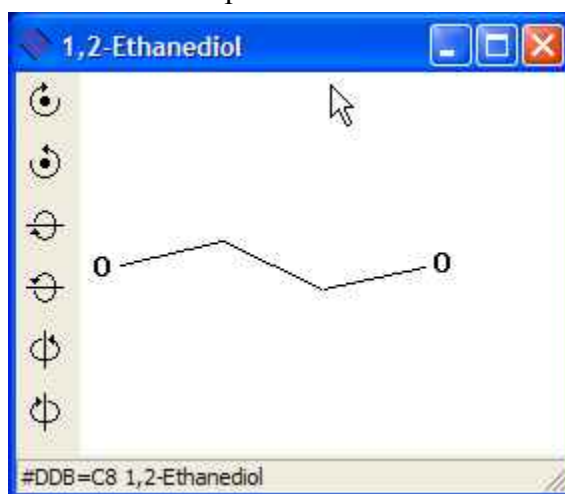
1. “Copy Selected Components”
Copies the selected lines of the component grid to the Windows clipboard.



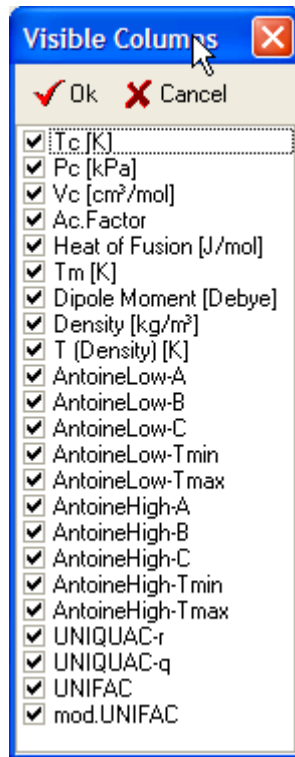
2. “Print Selected Components”
Print the selected line of the component grid. The programs open a “Print Settings” dialog where several options are available.
3. “Paste Search Strings”
This dialog can be used to perform multiple searches for strings pasted from the Windows clipboard. A left-click or a right-click in one of the table cells opens a context menu with the different search options.
4. “Remove (Selected) Components”
Removes single or selected lines from the component list



5. “View/Edit Compound Data” for [????]
Starts the component editor.
6. “Display Structure for [????]”
Displays a simple plot of the selected component.

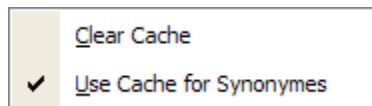


7. “Alternative Names”
The basic component list (without synonyms) contain two names – one main and one alternative (formerly mainly German names)
8. “Automatic Column Widths”
This function adjusts the column widths of the component grid to the size of the contents.
9. “Visible Columns”
If “Complete Data” (see Display Options) is selected this function allows selecting the visible columns.
10. “Display Options”
See chapter “Display Options”.



11. “Caches”

The synonyms cache accelerates the search in the synonyms dramatically but needs a fair amount of memory. Clearing the cache allows to free some memory but mainly it is important if changes done in the main component editor must be visible in the component selection.



12. “Clear Search History”

Removes all saved queries.