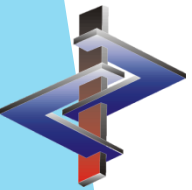


# Creating a Preparation

# Introduction

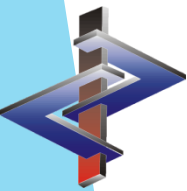
- **Raw Materials are those with a CAS number and Preparations are a combination of Raw Materials.**
  - Many companies have Raw Materials that are in actuality intermediate products consisting of Raw Materials (CAS Numbers).
  - It is necessary to set up these intermediates in ChemGes as preparations, so that, for calculation, as is legislatively required, they can be broken down into their Raw Materials.
  - This also means that data/classification changes need to be done at the lowest level of the breakdown, so that they carry through. (i.e. Changing the classification of an intermediate will not carry through to the final product – it is necessary to change the Raw Material Data so that it leads to the desired change).
- **ChemGes does not contain any Preparations by default.**

**Please direct additional questions to our hotline**  
**Via telephone at +1 (902) 832-3425 or +43 2628 619 00**  
**Via email to [info@dr-software.com](mailto:info@dr-software.com)**



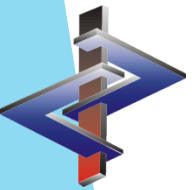
# Introduction

- **ChemGes calculations are based on formulae from the legislation**, as far as they exist and on formulae based on the legislation, generated by our staff of experts.
  - We do not base our calculations or data on 'Guidance Documents' (ie ECHA, EPA,...). When there is a discrepancy, the legislation takes precedence.
- **Transport legislation calculation**
  - In most cases, it is possible to calculate a specific transport classification, but some classes, as well as often the UN Numbers, require human input. In such cases, ChemGes will make an educated and logical suggestion.
  - Our Programmers, Chemists and Transport experts have created a system for 'calculating' the transport classification based on the data of the preparation (classification, physical data,...) and the data, or lack thereof, of the individual raw materials, where clear formulae are not present in the legislation.
  - We recommend that you review the transport classification output by ChemGes. Feel free to make changes to the transport classification and/or to the settings for transport, if these are based on sound data from another source.
  - Further details about transport classifications in ChemGes, can be found in the manual located on the downloads page of our Website [www.dr-software.com](http://www.dr-software.com) or accessible through the *Help* option in ChemGes (*General Help*) or in the **Transport** power point.



## Table of Contents

- 1. Entering the Formula**
- 2. Entering Additional Data**
- 3. Understanding the Calculation Results**
- 4. Further Data Entry**
- 5. Using a Preparation as an Intermediate**



# 1. Entering the Formula

- Ingredients can be entered by their CAS Number, their name, a partial search string or an internal Product Code.
- For each ingredient, enter the percentage at which it is contained in the preparation.
- Even though non-hazardous ingredients do not have to appear on your SDS, it is recommended to input all ingredients when generating the formulation, as this way calculations performed by ChemGes can be more exact.
- You can enter ranges and  $<$ ,  $>$ ,  $\leq$ ,  $\geq$  and  $\sim$ . ChemGes then performs all calculations (classification, physical data,...) using these range values.
- By hovering your mouse over the various fields pertaining to each substance, you can view additional information.

The screenshots illustrate the ChemGes software interface for entering a formulation. The main window shows a list of substances with their CAS numbers and descriptions. The 'Formulation' screen displays a table of substances and their percentages. A tooltip for 'formaldehyde ... %' shows its hazard classification and special limits.

Substance	Description	Percent
25068-38-6	reaction product: bisphenol-A-(epichlorhydrin) epoxy resin (number average molecular weight <= 700)	> 30 - < 40
108-88-3	toluene	≤ 15
78-92-2	butanol	5 - ≥ 10
67-63-0	propan-2-ol	~ 4
141-78-6	ethyl acetate	≥ 15 - 25
7732-18-5	water, distilled, conductivity or of similar purity	> 6 - < 10
1330-20-7/1	xylene	3 - 6
122-57-6	Benzalacetone	≤ 10
12468	formaldehyde ... %	≥ 5 - ≤ 10

EU - Special limits

3.1.0	Acute Tox. 3	H301 Toxic if swallowed.
3.1.D	Acute Tox. 3	H311 Toxic in contact with skin.
3.1.1	Acute Tox. 3	H331 Toxic if inhaled.
3.2	Skin Corr. 1B	H314 Causes severe skin burns and eye damage.
3.4.5	Skin Sens. 1	H317 May cause an allergic skin reaction.
3.5	Muta. 2	H341 Suspected of causing genetic defects.
3.6	Carc. 1B	H350 May cause cancer.

## 2. Entering Additional Data

The image shows two overlapping windows from the ChemGes software. The background window is titled "Physical values and general information" and has tabs for "Basic screen", "Formulation", "Physical data", "Flammability", "Country specific classifications", "Land transport", and "Sea and air transport". The "Physical data" tab is active, showing a list of properties with values entered in yellow boxes. The foreground window is titled "Fire and explosion risks" and has tabs for "Country specific classifications", "Land transport", "Sea and air transport", "Basic screen", "Formulation", "Physical data", and "Flammability". The "Flammability" tab is active, showing a list of risk assessment criteria with checkboxes and some values entered in blue boxes.

**Physical values and general information**

1 State	liquid
2 Flash point	-4 °C
3 Boiling point	77 - 78 °C
04 Melting point	4 °C
5 Water miscible/water soluble	<input type="checkbox"/>
6 Density	> 0.66692 - < 1.29473 g/cm <sup>3</sup>
7 Bulk density	> 666.9 - < 1294.7 kg/m <sup>3</sup>
8 pH-value	4 - 6
9 Solids	≤ 10.0 %
10 Flammable substances	~ 42 - ≤ 60 %
11 Ignition temperature	~ 300 °C
12 Chemical heat of combustion	
13 Viscosity bei 20°C	
14 at 40°C	
15 Vapor pressure bei 20.0 °C	97 hPa
16 bei 50.0 °C	360 hPa
17 Explosion limits	1.2 - 73 Vol%
18	46 - 910 g/m <sup>3</sup>
19 Contains ≥ 10 % nitro cellulose	<input type="checkbox"/>

**Fire and explosion risks**

Please check the system made proposal

- 1 The product is flammable or explosive
- 2 The product is explosive  3 Extremely explosive
- 4 The product is fire promotive or contains peroxides
- 5 The product contains organic peroxides
- 6 The product forms flammable gas with water or air
- 7 The product is dusty and has an explosive range with air
- 8 The product has its ignition range at 1 bar and room temperature
- 9 The gas is liquefied
- 10 The product is self igniting in the air at room temperature
- 11 Flash point 30 °C 12 The boiling point is under 35 °C
- 13 The product promotes burning
- 14 During usage an ignition risk exists

Black indicated fields are without significance for the calculation

- After inputting the formulation, ChemGes automatically takes you to two screens, where you are shown some initial calculations.
- Here, please input any additional data for your preparation, that you might have, and check the data provided by ChemGes.
- ChemGes has marked the data provided automatically, based on the ingredients, in yellow and blue.
- Appropriate formulae are used when applicable.
- Certain data, such as Flash Point, cannot be calculated. Therefore, the worst-case-scenario is output.

### 3. Understanding the Calculation Results

**GHS Classification:** Here you can see the details to the classification results based on the different forms of the GHS. (see [',GHS in Brief' Power Point for details](#))

If you wish to change these classifications, that is certainly possible, but be aware that any such changes must have solid reasons to back them up.

**DPD Classification:** These are the results based on the old system, using R and S Phrases.

**Transport:** The transport classification for the ADR, DOT, IMDG, and IATA are output here. (see [',Transport' Power Point for details](#))

On this screen, you can also find **WHMIS 1988** and **NFPA/HMIS**.

The **Quotients** Button, at the bottom of the screen, lets you examine the calculations that have lead to the classification of your preparation. (see [',Quotients' Power Point for details](#))

The screenshot shows the 'Maintenance of preparations' software interface. The window title is 'Maintenance of preparations'. The menu bar includes 'File', 'Edit', 'Preparation screens', 'Print programs', 'Additional functions', and 'Help'. The status bar shows '(44.4.7) 6,236, 2,756(+)' (85%), 496(-), 14(=), 1 User, M 2.76MB, HD 0.37MB, C

The main content area is divided into several sections:

- Basic screen:** Includes fields for 'Preparation' (1,000), 'Resin solution X 50', 'Product code' (1234567890), 'Article group', and 'Flag' (Internal Storage Code: 123/456/789).
- GHS classification:** Lists hazard statements such as '3.10/1; Asp. Tox. 1 - H304 May be fatal if swallowed and enters airways.', '3.7/2; Repr. 2 - H361 Suspected of damaging fertility or the unborn child.', and '3.9/2; STOT RE 2 - H373 May cause damage to organs through prolonged or repeated exposure.'
- Warning:** Lists hazard statements such as '2.6/3; Flam. Liq. 3 - H226 Flammable liquid and vapour.', '3.2/2; Skin Irrit. 2 - H315 Causes skin irritation.', and '3.3/2; Eye Irrit. 2 - H319 Causes serious eye irritation.'
- DPD classification:** Shows 'Xn', 'N', and 'R10-36/38-43-48/20-51/53-63-65-67; S2-13-23-24/25-26-29/56-37-43h-46-51-52-57-60-64; Z2'.
- Transport:** Shows 'ADR: 3', 'ADR Code: F1, PG: III, UN: 1866', 'DOT: 3', 'PG: III, UN: 1866', 'IMDG: 3', 'PG: III, UN: 1866, EmS: F-E, S-E', and 'IATA: 3', 'PG: III, UN: 1866'.
- WHMIS 1988:** Shows hazard symbols for 'B2, D2A'.
- NFPA:** Shows a diamond-shaped hazard label with '3' in the top blue section, '1' in the bottom left red section, and '0' in the bottom right yellow section.

The bottom of the screen features a toolbar with various function keys: [Ctrl G] GHS-Ableitung, [Alt F8] PDF files (-), [F10] Classification, [Ctrl N] NFPA+HMIS, [F9] Texts, [Alt F3] Variants (4), [Page ↓] Quotients, [F5] JPI, [F6] Label, [F8] SDS, [F7] Temcard, [↓] Next page, [Ctrl T] Tox values, [Ctrl X] Lock, [Alt F11] Memo, [Ctrl K] Copy, [F1] Names, [Ctrl F8] SDS versions, [←, Esc] End, [Ctrl F6] Delete, [Home] Price.

## 4. Further Data Entry

**Tox Values:** Here you can enter Toxicological Value Data for the preparation itself.

**Names:** In this field, you can enter/edit the names of the Preparation in various languages and with various markings for application.

**Country specific classification:** This screen allows for the input and viewing of country specific data, such as VOCs or Water Hazard Class.

At any time, it is possible to return to any of the screens of your formulation and add or change information/data. After changes, please ensure that these changes are actually applied, by means of recalculations and reclassification of affected areas. (see ,Updating and Updates' Power Point for details)

Maintenance of preparations

File Edit Preparation screens Print programs Additional functions Help (44.4.7) 6,236, 2,756(+), (85%), 496(-), 14(=), 1 User, M 2,76MB, HD 0,37MB, C

Basic screen Formulation Physical data Flammability **Country specific classifications** Land transport Sea and air transport

Preparation 1,000 Resin solution X 50

Product code 1234567890 Article group Flag Internal Storage Code: 123/456/789

**GHS classification**

**Danger**

3.10/1; Asp. Tox. 1 - H304 May be fatal if swallowed and enters airways.

3.7/2; Repr. 2 - H361 Suspected of damaging fertility or the unborn child.

3.7/2; Repr. 2 - H361d Suspected of damaging the unborn child.

3.9/2; STOT RE 2 - H373 May cause damage to organs through prolonged or repeated exposure.

**Warning**

2.6/3; Flam. Liq. 3 - H226 Flammable liquid and vapour.

3.2/2; Skin Irrit. 2 - H315 Causes skin irritation.

3.3/2; Eye Irrit. 2A - H319 Causes serious eye irritation.

3.3/2; Eye Irrit. 2 - H319 Causes serious eye irritation.

3.4/1; Skin Sens. 1 - H317 May cause an allergic skin reaction.

3.8/3; STOT SE 3 - H336 May cause drowsiness or dizziness.

**Transport**

ADR: 3

ADR Code: F1, PG: III, UN: 1866

DOT: 3

PG: III, UN: 1866

IMDG: 3

PG: III, UN: 1866, EmS: F-E, S-E

IATA: 3

PG: III, UN: 1866

**WHMIS**

B2, D2A

**NFPA**

1 3 0

**DPD classification** Xn N; R10-36/38-43-48/20-51/53-63-65-67; S2-13-23-24/25-26-29/56-37-43h-46-51-52-57-60-64; Z2

Creation - Last alteration 05/09/2017 Last classification 05/09/2017

[Ctrl G] GHS-Ableitung [Alt F8] PDF files (-) [F10] Classification [Ctrl N] NFPA+HMIS [F9] Texts [Alt F3] Variants (4) [Page 1] Quotients [F5] IPI [F6] Label [F8] SDS [F7] Trzcard [L] Next page [Ctrl T] Tox values [Ctrl X] Locks [Alt F11] Memo [Ctrl K] Copy [F1] Names [Ctrl F8] SDS versions [Esc] End [Ctrl F6] Delete [Home] Price

Country specific classifications

File Edit Preparation screens Help (45.2.26) 116,820 disk operations, C

Basic screen Formulation Physical data Flammability **Country specific classifications** Land transport Sea and air transport

BetrSichV (D) Flammable liquid VbF (D) - VbF (A) - Storage class (LGK) acc. to TRGS510 (Germany) 3

WHC (Water hazard class) 2 D 2 NL Z(1) Danish MAL-Code 5-6

Seveso III: Qualified quantities: 200 t, 500 t, Categories: E2, P5c, CAS 50-00-0/1

Disposal key numbers 6 EU 08 01 11\* 7 Austria 55.503

8 Switzerland (if different)

9 Relevant waste hazards HP 3, HP 5, HP 6, HP 7, HP 8, HP 10, HP 11, HP ...

10 Coating  VOC value: 11 EU-VOC > 330.3 - < 1,050.8 g/l 12 ≥ 47.55 - ≤ 70.65 % 13 Wood preservative

14 US-VOC > 290.4 - < 966.5 g/l 15 Swiss VOCV-content ≥ 47.55 - ≤ 70.65 %

Detergent Regulation: 16 Fragrance  17 Essential oil  18 Dye

Cosmetic Regulation: 19 Cosmetic product according to Regulation 1223/2009/EC  20 Leave-on Product

Biocidal Products Regulation: 21

ECHA notification: 22 Reference Number

UFI code: 23 Company DR Software GmbH 24 Code P800-W02K-500V-TCXM

25 Chemical Safety Assessment available

26 This product is a raw material with impurities  (overrides default value)

27 Main raw material

28 Output of the main raw material in the SDS

29 CAS of the preparation

30 GISCode (BG BAU (D))

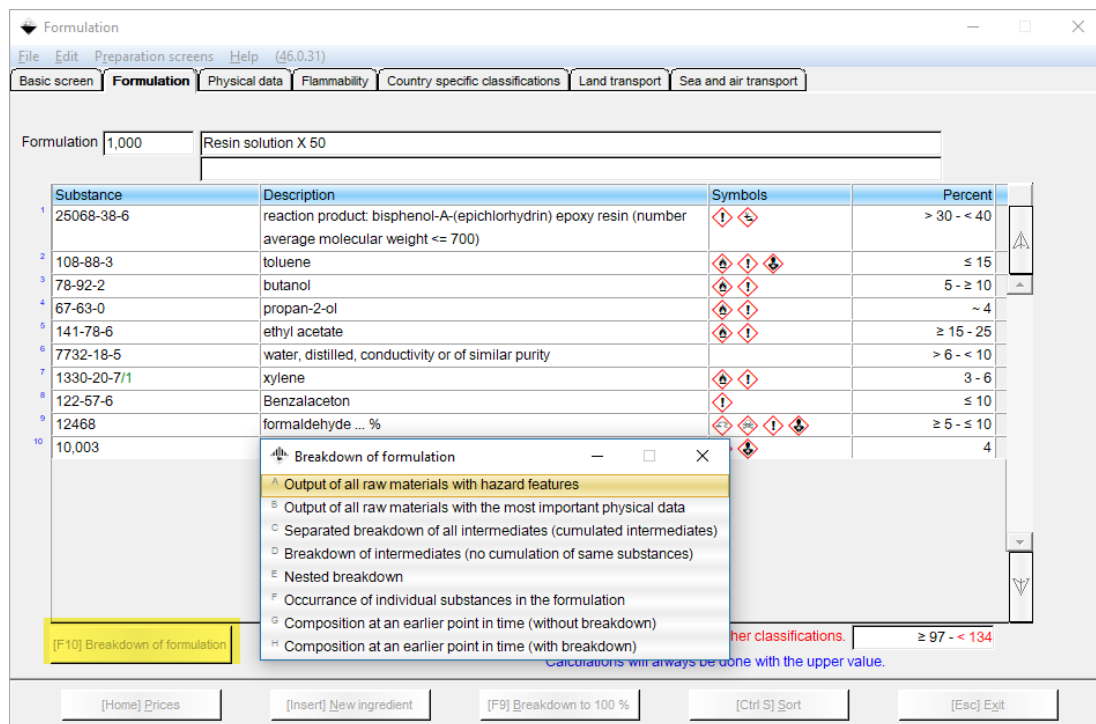
31 Limit table for the SDS acc. to presettings

[Esc] End [Ctrl F4] Calculate the WHC (D) [F4] Printout of documentation for WHC



## 5. Using a Preparation as an Intermediate

In order to use a preparation as an intermediate, simply create the preparation first and then enter it in the formulation screen of a new preparation, with the percentage at which it is contained.



The screenshot shows the 'Formulation' window with the 'Formulation' tab selected. The main area displays a table of substances and their percentages. A dialog box titled 'Breakdown of formulation' is open, showing options for displaying raw materials and intermediates.

Substance	Description	Symbols	Percent
25068-38-6	reaction product: bisphenol-A-(epichlorhydrin) epoxy resin (number average molecular weight <= 700)	⚠	> 30 - < 40
108-88-3	toluene	⚠	≤ 15
78-92-2	butanol	⚠	5 - ≥ 10
67-63-0	propan-2-ol	⚠	~ 4
141-78-6	ethyl acetate	⚠	≥ 15 - 25
7732-18-5	water, distilled, conductivity or of similar purity		> 6 - < 10
1330-20-7/1	xylene	⚠	3 - 6
122-57-6	Benzalacetone	⚠	≤ 10
12468	formaldehyde ... %	⚠	≥ 5 - ≤ 10
10,003		⚠	4

The 'Breakdown of formulation' dialog box options include:

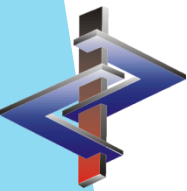
- Output of all raw materials with hazard features
- Output of all raw materials with the most important physical data
- Separated breakdown of all intermediates (cumulated intermediates)
- Breakdown of intermediates (no cumulation of same substances)
- Nested breakdown
- Occurrence of individual substances in the formulation
- Composition at an earlier point in time (without breakdown)
- Composition at an earlier point in time (with breakdown)

When such an intermediate preparation is used, the data from the raw materials (CAS Numbers) is what will be used for the calculations of the resulting preparation.

Changes made in the intermediate preparation will not carry through into the next preparation.

This is what the legislation requires.

The **Breakdown of formulation** option allows for an easy overview of the ingredients contained in the whole preparation, including the intermediate preparations.



**More detailed Information can be found in the Manual to ChemGes**

**@ [www.dr-software.com](http://www.dr-software.com) - Downloads**