

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 by definition 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.
 - Therefore, when using intermediates in preparations, the following must be taken into consideration 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). The formulae in the legislation are based on Raw Material data.


- **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

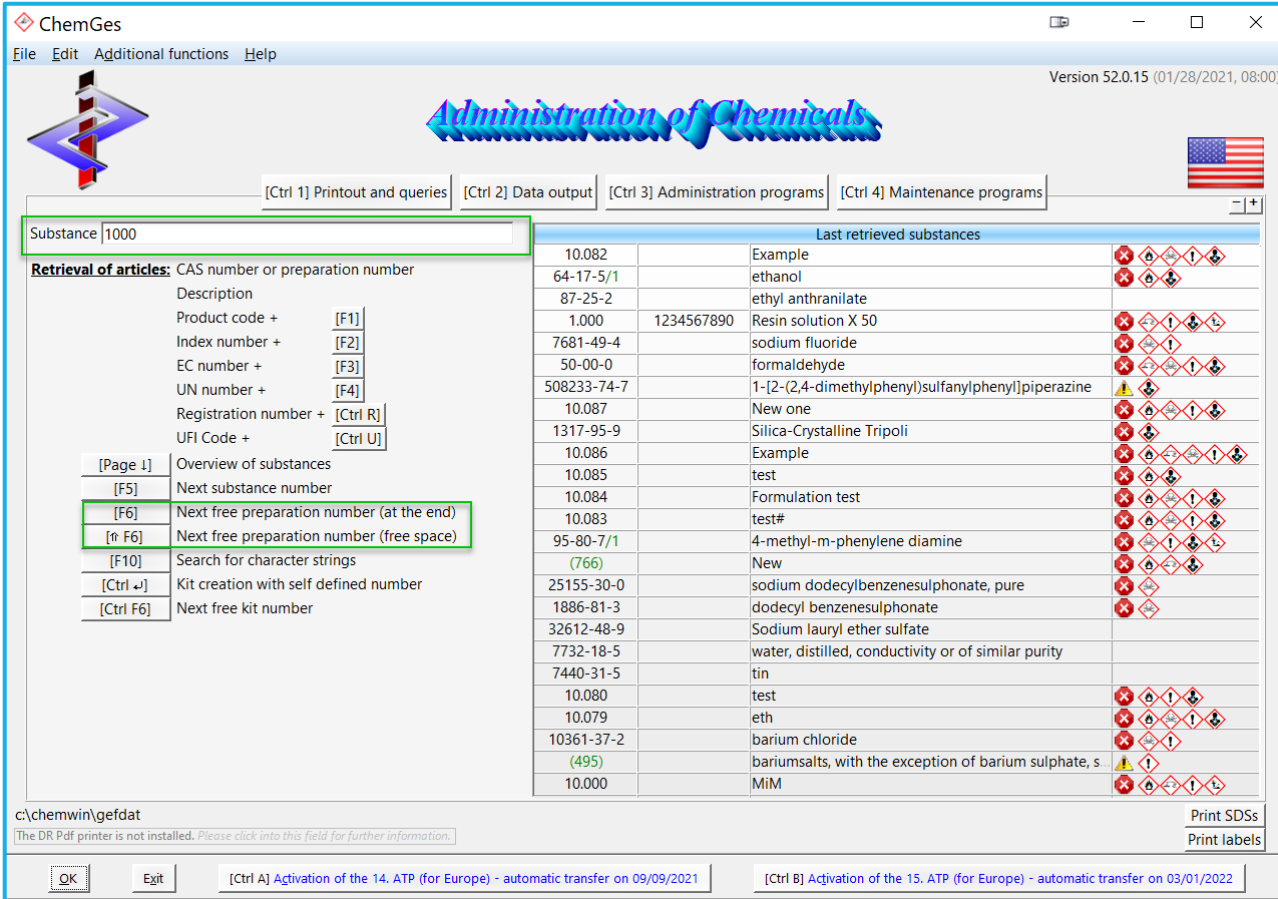
Introduction

- **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.
- **Calculation of transport classification**
 - 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 or accessible through the *Help* option in ChemGes (*General Help*) or in the **Transport** power point.

Creating a Preparation:

In order to generate a **Preparation**, enter a preparation number in the main screen of ChemGes and press  *Enter* or let ChemGes assign an automatic database entry number:

- via  **Next free preparation number (at the end)**: ChemGes assigns the next preparation number after the highest number already used.
- via   **Next free preparation number (free space)**: ChemGes uses the next available number, after the number 1.



ChemGes
File Edit Additional functions Help
Version 52.0.15 (01/28/2021, 08:00)

Administration of Chemicals

[Ctrl 1] Printout and queries [Ctrl 2] Data output [Ctrl 3] Administration programs [Ctrl 4] Maintenance programs

Substance 1000

Retrieval of articles: CAS number or preparation number
Description
Product code + [F1]
Index number + [F2]
EC number + [F3]
UN number + [F4]
Registration number + [Ctrl R]
UFI Code + [Ctrl U]

[Page 1] Overview of substances
[F5] Next substance number
[F6] Next free preparation number (at the end)
[F6] Next free preparation number (free space)
[F10] Search for character strings
[Ctrl ↵] Kit creation with self defined number
[Ctrl F6] Next free kit number

Last retrieved substances	
10.082	Example
64-17-5/1	ethanol
87-25-2	ethyl anthranilate
1.000	1234567890 Resin solution X 50
7681-49-4	sodium fluoride
50-00-0	formaldehyde
508233-74-7	1-[2-(2,4-dimethylphenyl)sulfanylphenyl]piperazine
10.087	New one
1317-95-9	Silica-Crystalline Tripoli
10.086	Example
10.085	test
10.084	Formulation test
10.083	test#
95-80-7/1	4-methyl-m-phenylene diamine
(766)	New
25155-30-0	sodium dodecylbenzenesulphonate, pure
1886-81-3	dodecyl benzenesulphonate
32612-48-9	Sodium lauryl ether sulfate
7732-18-5	water, distilled, conductivity or of similar purity
7440-31-5	tin
10.080	test
10.079	eth
10361-37-2	barium chloride
(495)	bariumsalts, with the exception of barium sulphate, s
10.000	MiM

c:\chemwin\gefdat
The DR Pdf printer is not installed. Please click into this field for further information.

Print SDSs
Print labels

OK Exit [Ctrl A] Activation of the 14. ATP (for Europe) - automatic transfer on 09/09/2021 [Ctrl B] Activation of the 15. ATP (for Europe) - automatic transfer on 03/01/2022

Entering the Formulation:

- 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:
 - You can enter **exact percentages** (i.e. 10.5%) and / or **ranges** with or without $<$, $>$, \leq , \geq and \sim .
 - ChemGes then performs all calculations (classification, physical data,...) using these range values.
 - As long as your formulation is below 100%, ChemGes will show you, when clicking into the percentage field, what the difference to 100% is, allowing you to adopt that number via **[F1]**.

Note: While it is not necessary to enter the formulation to exactly 100%, and higher and lower sums are permitted, the more exact the formulation is, the more exact your calculations can be.

- 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.
- By hovering your mouse over the various fields pertaining to each substance, you can view additional information.

The image displays three overlapping screenshots of the ChemGes software interface, illustrating the 'Formulation' window. The leftmost screenshot shows the 'Physical data' tab for a substance, with a green box highlighting the 'CAS number' field. The middle screenshot shows the 'Formulation' table with a green box highlighting the 'Standard, EU list' dropdown menu. The rightmost screenshot shows the 'Country specific classifications' tab with a green box highlighting a 'Danger' tooltip for a substance.

Substance number	Description	Symbols	Percent
25068-38-6	reaction product: bisphenol-A-(epichlorhydrin) epoxy resin (number average molecular weight <= 700)	▲ ⚠ ⚡	40.0000
108-88-3	toluene	⚠ ⚡	21.0526
78-92-2	butanol	▲ ⚠ ⚡	5.2632

Substance number	Description	Symbols	Percent
25068-38-6	reaction product: bisphenol-A-(epichlorhydrin) epoxy resin (number average molecular weight <= 700)	▲ ⚠ ⚡	40.0000
108-88-3	toluene	⚠ ⚡	21.0526
78-92-2	butanol	▲ ⚠ ⚡	5.2632
67-63-0	propan-2-ol	▲ ⚠ ⚡	5.2632
141-78-6	ethyl acetate	▲ ⚠ ⚡	0.0100
10,000	MIM	▲ ⚠ ⚡	5.0000

Substance number	Description	Symbols	Percent
25068-38-6	reaction product: bisphenol-A-(epichlorhydrin) epoxy resin (number average molecular weight <= 700)	▲ ⚠ ⚡	40.0000
108-88-3	toluene	⚠ ⚡	21.0526
78-92-2	butanol	▲ ⚠ ⚡	5.2632
67-63-0	propan-2-ol	▲ ⚠ ⚡	5.2632
141-78-6	ethyl acetate	▲ ⚠ ⚡	0.0100
10,000	MIM	▲ ⚠ ⚡	5.0000

Entering Additional Data:

After inputting the formulation, ChemGes automatically takes you to the **Physical Data** screen.

- This screen contains calculated and estimated values, based on the raw materials (marked in yellow). The yellow marked fields should be checked and verified by the user.

Note:

Certain data, such as the Flash Point, cannot be calculated but can only be properly identified via laboratory tests. In such cases, ChemGes estimates the worst-case-scenario.

- Please input any additional data for your preparation, that you might have.

The screenshot displays the 'Physical data' window of ChemGes software. The interface includes a menu bar (File, Edit, Help) and a tabbed navigation system with 'Physical data' selected. The main area is divided into several sections:

- Physical Properties:** Fields for State (liquid), Flash point (4.45 °C), Boiling point (78 °C), Melting point, Density (0.837 g/cm³), Bulk density, pH-value, Solids (20 %), Flammable substances (80 %), Ignition temperature (~300 °C), and Chemical heat of combustion (kJ/g).
- Thermal Properties:** Viscosity at 20°C and 40°C, and Vapor pressure at 20.0 °C (59 hPa) and 50.0 °C (280 hPa).
- Explosion Limits:** Explosion limits (1.2-73 Vol%) and Lower Explosive Limit (46-910 g/m³).
- Safety and Classification:** Checkboxes for 'Purpose' (Public, Industry or trade), 'Ready-to-use product for the final customer', 'The product will be applied by spraying or splattering', 'Product is in aerosol package or container with sealed spray attachment', 'Pressure > 29 psig', 'The aerosol is' (extremely flammable, flammable, non-flammable), 'The product promotes burning', 'During use, an ignition risk exists', 'The product is spontaneously flammable in air at room temperature', 'The product is explosive' (Extremely explosive), 'The product is fire promotive or contains peroxides' (Organic peroxides), 'The product forms flammable gas with water or air', 'The product is dusty and has an explosive range with air', 'The product has its ignition range at 1 bar and room temperature', and 'The gas is liquefied'.
- Form and Odor:** Input fields for Form, Color, and Odor.

At the bottom, there are keyboard shortcuts: [Ctrl F4] Recalculate physical values, [Ctrl P] Additional physical-/chemical values, [Ctrl I] Physical data of contents, [F10] Settings for physical values, and a 'Basic screen' button. A red text prompt at the bottom center reads: 'Please check the color-coded suggestions'.

Calculated results:

The screenshot displays the 'Maintenance of preparations' software interface. The main window shows the 'GHS classification' section with various hazard and warning symbols and text. To the right, there are fields for physical and chemical data such as State (liquid), Flash point (25 °C), and Boiling point (77 °C). Below this, the 'Transport' section shows ADR, DOT, IMDG, and IATA codes. At the bottom, a 'Listing status' table is visible, showing the status of various regulatory listings for the preparation.

Country	Listing	Description	Limit	Type	Status
USA	EPA	Environmental Protection Agency	>0 %	Value	2 / 6 of the substances are included
	HAPs	Hazardous Air Pollutants	>0 %	Value	Yes/No 2 / 6 of the substances are included
	Prop 65 RT	Inactive listing - Prop 65 - reproductive toxicity	>0 %	Value	Yes/No One substance is included
	TSCAnew	Inactive listing - TSCA new	>0 %	Value	All substances are included
	IARC	International Agency for Research on Cancer	>0 %	Value	3 / 6 of the substances are included
	NIOSH-Ca	National Institute for Occupational Safety and Health - carcinogen	>0 %	Value	No substance is included
	NTP	National Toxicology Program	>0 %	Value	No substance is included
	RTK-NJ	New Jersey Right-to-Know List	>0 %	Value	Yes/No One substance is not included
	SHSL-NJ	New Jersey Special Hazardous Substances List	>0 %	Value	One substance is not included
	OSHA-Ca	Occupational Safety and Health Administration - carcinogen	>0 %	Value	Yes/No No substance is included
	PAC-1	PACs - Protective Action Criteria for Chemicals 1	>0 %	Value	All substances are included
	PAC-2	PACs - Protective Action Criteria for Chemicals 2	>0 %	Value	All substances are included
	PAC-3	PACs - Protective Action Criteria for Chemicals 3	>0 %	Value	All substances are included
	RTK-PA	Pennsylvania Right-to-Know List	>0 %	Value	Yes/No One substance is not included
	SHSL-PA	Pennsylvania Special Hazardous Substances List	>0 %	Value	One substance is not included
	Prop 65 C	Prop 65 - Chemicals known to cause cancer	>0 %	Value	Yes/No No substance is included
	Prop65 DT	Prop 65 - Developmental toxicity	>0 %	Value	Yes/No One substance is included
	Prop65 RTF	Prop 65 - Reproductive toxicity for females	>0 %	Value	Yes/No No substance is included
	Prop65 RTM	Prop 65 - Reproductive toxicity for males	>0 %	Value	Yes/No No substance is included
	RCRA	RCRA (Resource Conservation and Recovery Act)	>0 %	Value	3 / 6 of the substances are included
	SARA 313	SARA Section 313 (specific toxic chemical listings)	>0 %	Value	Yes/No 4 / 6 of the substances are included
	SARA 355	SARA Section 355 (extremely hazardous substances)	>0 %	Value	Yes/No No substance is included

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)

Note: 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. As well, since the classification is calculated based on the ingredients and other data, it would be best to change the source of the calculated classification, rather than just the final result, so that the information can be carried through in the future in other formulations as well.


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

The **Page ↓ Quotients** button, at the bottom of the screen, lets you examine the calculations that have led to the classification of your preparation. (see ,Quotients' Power Point for details)

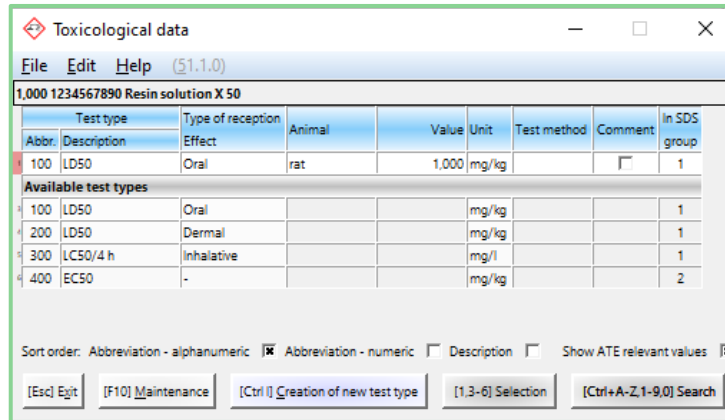
The **Ctrl L Substance Listings** screen shows the listing status of the various ingredients of your formulation.

Additional Data:

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

Descriptions: In this field, you can enter/edit the description(s) of the preparation and by clicking on the  you can define the translations thereof.

Alt 5 Country specific values: This screen allows for the input and viewing of country specific data, such as VOCs or Water Hazard Class.



Toxicological data (51.1.0)

1,000 1234567890 Resin solution X 50

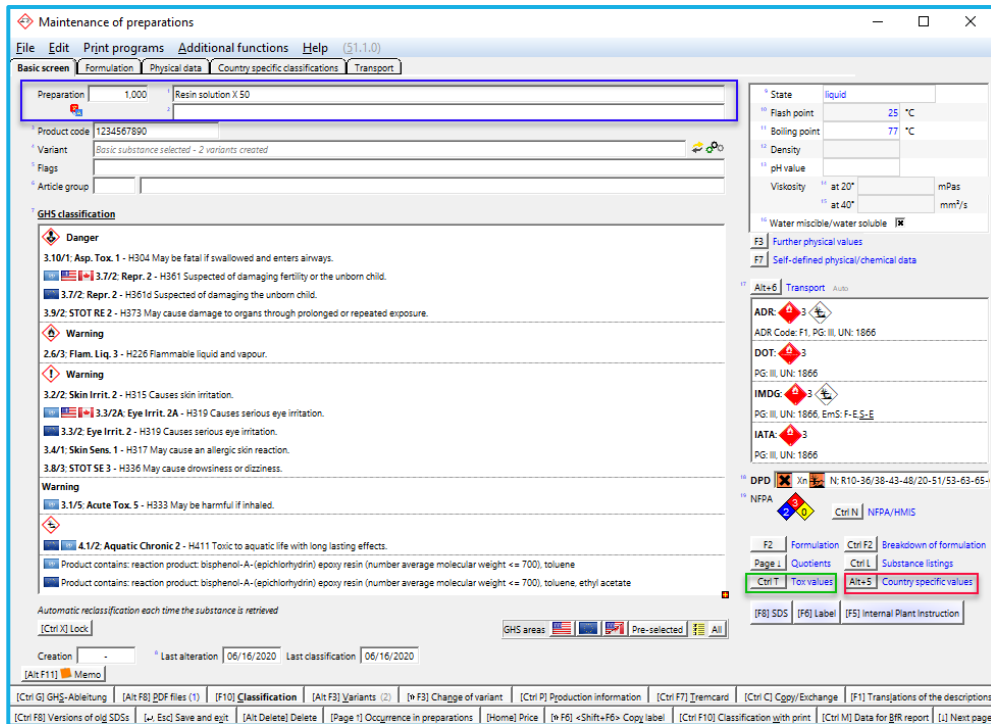
Abbr.	Description	Type of reception	Animal	Value	Unit	Test method	Comment	In SDS group
100	LD50	Oral	rat	1,000	mg/kg			1

Available test types

Abbr.	Description	Type of reception	Animal	Value	Unit	Test method	Comment	In SDS group
100	LD50	Oral			mg/kg			1
200	LD50	Dermal			mg/kg			1
300	LC50/4 h	Inhalative			mg/l			1
400	EC50	-			mg/kg			2

Sort order: Abbreviation - alphanumeric Abbreviation - numeric Description Show ATE relevant values

[Esc] Exit [F10] Maintenance [Ctrl I] Creation of new test type [1,3-6] Selection [Ctrl+A-Z,1-9,0] Search



Maintenance of preparations (51.1.0)

Preparation: 1,000 Resin solution X 50

Product code: 1234567890

Variant: Basic substance selected - 2 variants created

State: liquid

Flash point: 25 °C

Boiling point: 77 °C

Density: []

pH value: []

Viscosity: [] at 20° mPas [] at 40° mm²/s

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.
- 3.3/2A: 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.

Warning

- 3.1/5: Acute Tox. 5 - H333 May be harmful if inhaled.

4.1/2: Aquatic Chronic 2 - H411 Toxic to aquatic life with long lasting effects.

Product contains: reaction product: bisphenol-A-(epichlorohydrin) epoxy resin (number average molecular weight <= 700), toluene

Product contains: reaction product: bisphenol-A-(epichlorohydrin) epoxy resin (number average molecular weight <= 700), toluene, ethyl acetate

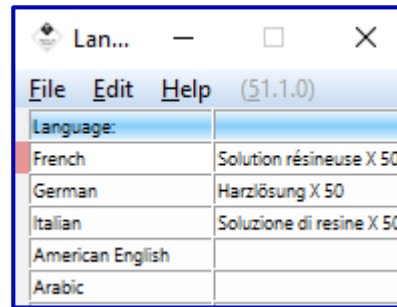
Automatic reclassification each time the substance is retrieved

[Ctrl X] Lock

Creation: [] Last alteration: 06/16/2020 Last classification: 06/16/2020

[Alt F11] Memo

[Ctrl G] GHS-Ableitung [Alt F8] PDF files (1) [F10] Classification [Alt F3] Variants (2) [W F3] Change of variant [Ctrl P] Production information [Ctrl F7] Inreicard [Ctrl C] Copy/Exchange [F1] Translations of the descriptions [Ctrl F8] Versions of old SDSs [W Esc] Save and edit [Alt Delete] Delete [Page 1] Occurrence in preparations [Home] Price [W F6] +Shift+F6+ Copy label [Ctrl F10] Classification with print [Ctrl M] Data for BR report [1] Next page

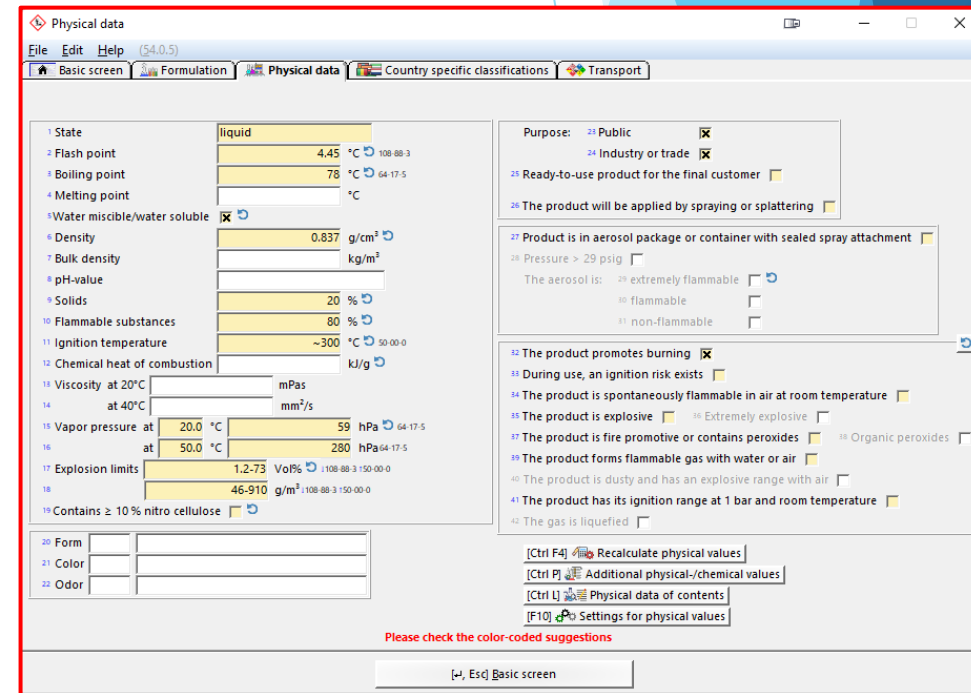


Lan... (51.1.0)

File Edit Help

Language:

- French: Solution résineuse X 50
- German: Harzlösung X 50
- Italian: Soluzione di resine X 50
- American English
- Arabic



Physical data (54.0.5)

Basic screen Formulation Physical data Country specific classifications Transport

State: liquid

Flash point: 4.45 °C 108.88.3

Boiling point: 78 °C 64.17.5

Melting point: °C

Water miscible/water soluble:

Density: 0.837 g/cm³

Bulk density: kg/m³

pH-value: []

Solids: 20 %

Flammable substances: 80 %

Ignition temperature: ~300 °C 50.00.0

Chemical heat of combustion: kJ/g

Viscosity at 20°C: mPas

at 40°C: mm²/s

Vapor pressure at 20.0 °C: 59 hPa 64.17.5

at 50.0 °C: 280 hPa 64.17.5

Explosion limits: 1.2-73 Vol% 108.88.3 150.00.0

46-910 g/m³ 108.88.3 150.00.0

Contains ≥ 10 % nitro cellulose:

Form: []

Color: []

Odor: []

Purpose: Public Industry or trade

Ready-to-use product for the final customer

The product will be applied by spraying or splattering

Product is in aerosol package or container with sealed spray attachment

Pressure > 29 psig

The aerosol is: extremely flammable flammable non-flammable

The product promotes burning

During use, an ignition risk exists

The product is spontaneously flammable in air at room temperature

The product is explosive Extremely explosive

The product is fire promotive or contains peroxides Organic peroxides

The product forms flammable gas with water or air

The product is dusty and has an explosive range with air

The product has its ignition range at 1 bar and room temperature

The gas is liquefied

[Ctrl F4] Recalculate physical values

[Ctrl P] Additional physical-/chemical values

[Ctrl L] Physical data of contents

[F10] Settings for physical values

Please check the color-coded suggestions

[-, Esc] Basic screen

Using a preparation as an Intermediate:

General Information:

An intermediate is a preparation that is used as an ingredient in a preparation.

Therefore, intermediates must first be generated in ChemGes as preparations, so that, as legislatively required, the final formulation can be broken down to the raw material level and the proper data applied to the legislative formulae.

Note:

When using intermediates, the following needs to be taken into consideration:

- As legislative required, the classification needs to be calculated at the raw material level. Therefore, a classification change is to also be applied at the raw material level.

The screenshot shows the 'Formulation' window with the 'Formulation' tab selected. The 'Formulation' field contains '10.025' and 'Example'. Below it, the 'Classification for USA' is listed as 'H227-H302-H331-H315-H319-H317-H341-H350-H361-H373'. A table displays the breakdown of the formulation:

Substance number	Description	Symbols	Percent
50-00-0	formaldehyde ... %	☠☠☠☠☠	10.00
7732-18-5	water, distilled, conductivity or of similar purity	☠☠☠☠☠	70.00
1234567890	Resin solution X 50	☠☠☠☠☠	20.00

Below this table, a detailed breakdown of the resin solution is shown:

Substance number	Product code	Description	% in intermediate	% in product
25068-38-6		reaction product: bisphenol-A-(epichlorhydrin) epoxy resin (number average molecular weight <= 700)	50%	10%
108-88-3		toluene	20%	4%
78-92-2		butanol	5%	1%
67-63-0		propan-2-ol	5%	1%
141-78-6		ethyl acetate	20%	4%

The '[F10] Breakdown of formulation' button is highlighted in the bottom left corner.

The option **[F10] Breakdown of formulation** allows for an easy overview of the ingredients contained in the whole preparation, including those part of the intermediate preparation(s).

Note:

The **Breakdown of formulation** can also be accessed in the *Maintenance of preparations* via **Ctrl F2**.

The 'Breakdown of formul...' dialog box is shown with the following options:

- 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)

The 'Maintenance of preparations' dialog box shows the following keyboard shortcuts:

- F2** Formulation
- Ctrl F2** Breakdown of formulation
- Page 1** Quotients
- Ctrl L** Substance listings
- Ctrl T** Tox values
- Alt+5** Country specific values
- [F8] SDS**
- [F6] Label**
- [F5] Internal Plant Instruction**

More detailed Information can be found in the Manual to ChemGes

@ www.dr-software.com - *Downloads*