

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

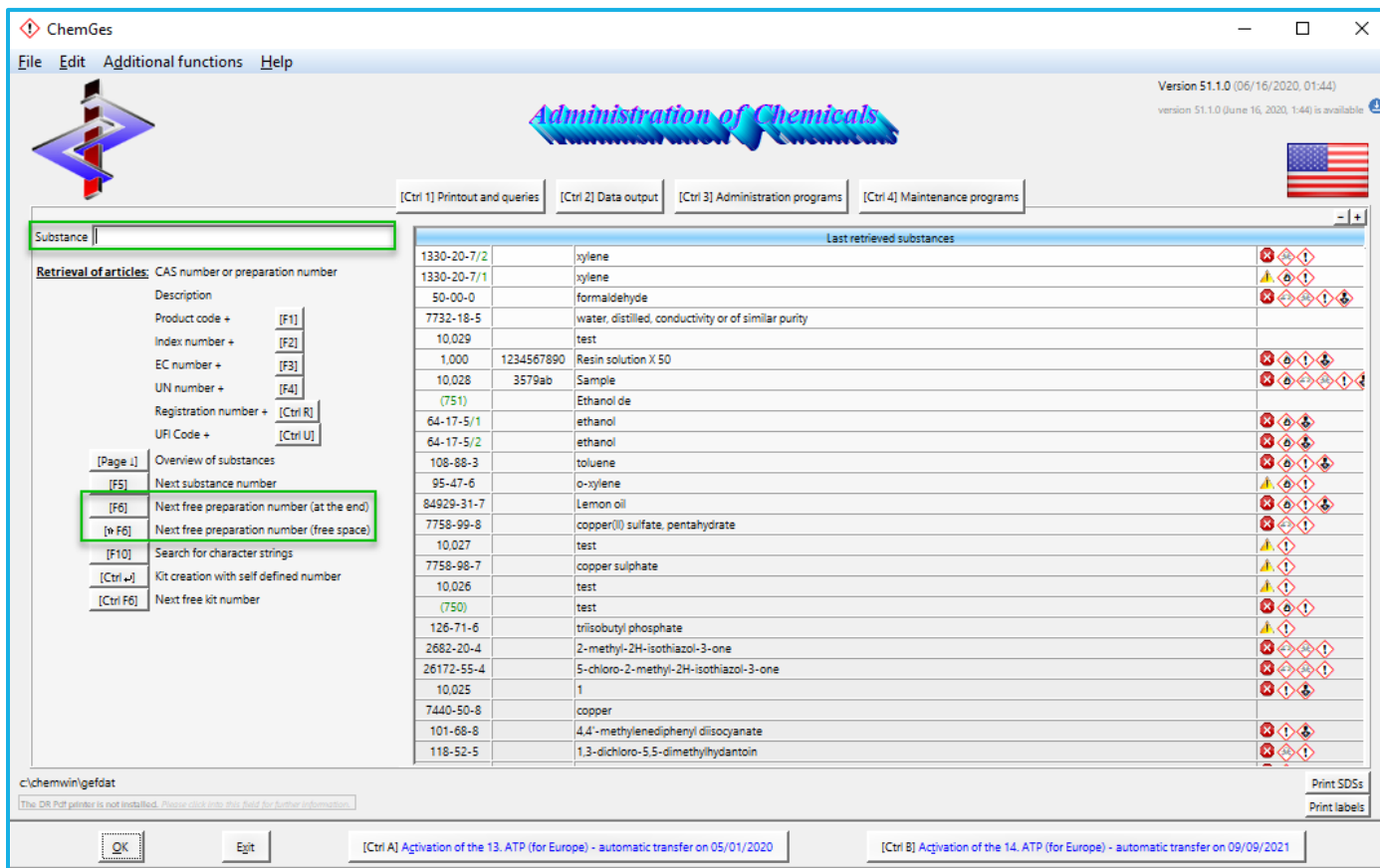
- **ChemGes calculations are based on formulae from the legislation**, as far as they exist and on formulae based on the legislation, generated by our staff of experts.
 - We do not base our calculations or data on ‘Guidance Documents’ (ie ECHA, EPA,...). When there is a discrepancy, the legislation 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.



The screenshot shows the ChemGes software interface. The main window is titled "Administration of Chemicals" and displays a list of substances. The left sidebar contains a "Retrieval of articles" section with various search options. The "Next free preparation number (free space)" option is highlighted in green. The main window displays a table of substances with columns for CAS number, description, and various icons.

CAS number	Description	Icons
1330-20-7/2	xylene	⚠️
1330-20-7/1	xylene	⚠️
50-00-0	formaldehyde	⚠️
7732-18-5	water, distilled, conductivity or of similar purity	⚠️
10,029	test	⚠️
1,000	1234567890 Resin solution X 50	⚠️
10,028	3579ab Sample	⚠️
(751)	Ethanol de	⚠️
64-17-5/1	ethanol	⚠️
64-17-5/2	ethanol	⚠️
108-88-3	toluene	⚠️
95-47-6	o-xylene	⚠️
84929-31-7	Lemon oil	⚠️
7758-99-8	copper(II) sulfate, pentahydrate	⚠️
10,027	test	⚠️
7758-98-7	copper sulphate	⚠️
10,026	test	⚠️
(750)	test	⚠️
126-71-6	trisobutyl phosphate	⚠️
2682-20-4	2-methyl-2H-isothiazol-3-one	⚠️
26172-55-4	5-chloro-2-methyl-2H-isothiazol-3-one	⚠️
10,025	1	⚠️
7440-50-8	copper	⚠️
101-68-8	4,4'-methylenediphenyl diisocyanate	⚠️
118-52-5	1,3-dichloro-5,5-dimethylhydantoin	⚠️

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.

Formulation 1,000 Resin solution X 50

Classification for USA: H203-H224-H315-H319-H317-H361-H336-H373-H304

Substance number	Description	Symbols	Percent
25068-38-6	reaction product: bisphenol-A-(epichlorohydrin) epoxy resin (number average molecular weight <= 700)		50.00
108-88-3	toluene		20.00
78-92-2	butanol		5.00
67-83-0	propan-2-ol		5.00
141-78-6	ethyl acetate		20.00

Substance 141-78-6
Index number 607-023-00-5
EC number 205-500-4
State Liquid
Flash point -4
Boiling point 77-78
Melting point -83.57
Density 0.9 g/cm³
Miscibility/solubility (water) No
Molecular weight 88
Vapor pressure 97 hPa (20) °C
Viscosity 360 mPa (50) °C
Explosion limits 0.44 mbar (20) °C
Explosion limits 2.1-11.5 Vol %
Explosion limits 75-420 g/m³
Ignition temperature 460 °C

Formulation 1,000 Resin solution X 50

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108-88-3	toluene		20.00
78-92-2	butanol		5.00
67-83-0	propan-2-ol		5.00
141-78-6	ethyl acetate		20.00

Standard butan-2-ol
EU list butan-2-ol
butyl alcohol (except tert-butyl alcohol)
1-Methyl-1-propanol
Ethylmethyl carbinol
sec-Butyl alcohol

Formulation 1,000 Resin solution X 50

Classification for USA: H203-H224-H315-H319-H317-H361-H336-H373-H304

Substance number	Description	Symbols	Percent
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108-88-3	toluene		20.00
78-92-2	butanol		5.00
67-83-0	propan-2-ol		5.00
141-78-6	ethyl acetate		20.00

Danger
2.6/2 Flam. Liq. 2 H225 Highly flammable liquid and vapour.
3.2/2 Skin Irrit. 2 H315 Causes skin irritation.
3.7/2 Repr. 2 H361 Suspected of damaging fertility or the unborn child.
3.8/3/0 STOT SE 3 H336 May cause drowsiness or dizziness.
3.9/2 STOT RE 2 H373 May cause damage to organs through prolonged or repeated exposure.
3.10/1 Asp. Tox. 1 H304 May be fatal if swallowed and enters airways.

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.

Physical data

File Edit Help (51.1.0)

Basic screen Formulation Physical data Country specific classifications Transport

1 State liquid

2 Flash point ≤ 93 °C

3 Boiling point unknown °C

4 Melting point °C

5 Water miscible/water soluble

6 Density 0.81 g/cm³

7 Bulk density kg/m³

8 pH-value

9 Solids 50 %

10 Flammable substances 50 %

11 Ignition temperature -300 °C

12 Chemical heat of combustion kJ/g

13 Viscosity at 20°C mPas

at 40°C mm²/s

14 Vapor pressure at 20.0 °C 1.7 hPa

at °C hPa

15 Explosion limits 7-73 Vol% 87-910 g/m³

16 Contains ≥ 10 % nitro cellulose

Purpose: 21 Public
22 Industry or trade

23 Ready-to-use product for the final customer

24 The product will be applied by spraying or splattering

25 Product is in aerosol package or container with sealed spray attachment

26 Pressure > 29 psig

The aerosol is: 27 extremely flammable
28 flammable
29 non-flammable

30 The product promotes burning

31 During use, an ignition risk exists

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

33 The product is explosive 34 Extremely explosive

35 The product is fire promotive or contains peroxides 36 Organic peroxides

37 The product forms flammable gas with water or air

38 The product is dusty and has an explosive range with air

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

40 The gas is liquefied

20 Form

21 Color

22 Odor

Please check the color-coded suggestions

[<] [Esc] Basic screen [Ctrl F4] Recalculate physical values [Ctrl P] Additional physical-/chemical values [Ctrl L] Physical data of contents

Calculated results:

The screenshot shows the 'Maintenance of preparations' software interface. The main window displays the 'GHS classification' for a preparation named 'Resin solution X 50'. The classification includes several hazard statements (H302, H312, H314, H332, H334, H335) and warning symbols. A 'Transport' tab is also visible, showing classification codes like 'ADR: 3, 3', 'DOT: 3', 'IMDG: 3', and 'IATA: 3'. Below the main window, a 'Listing status for 1234567890 Resin solution X 50' table is shown, listing various regulatory criteria and their status.

Country	Listing	Description	Limit	Type	Status
USA	EPA	Environmental Protection Agency	>0%	Value	One substance is included
USA	NARA	Hazardous Air Pollutants	>0%	Yes/No	One substance is included
USA	Prop 65	Inactive listing - Prop 65 - reproductive toxicity	>0%	Yes/No	One substance is included
USA	TSCAnew	Inactive listing - TSCA new	>0%	Value	All substances are included
USA	IARC	International Agency for Research on Cancer	>0%	Value	2/3 of the substances are included
USA	NIOSH-Ca	National Institute for Occupational Safety and Health - carcinogen	>0%	Yes/No	No substance is included
USA	NTP	National Toxicology Program	>0%	Value	No substance is included
USA	RTK-NU	New Jersey Right-to-know List	>0%	Yes/No	One substance is not included
USA	SHSL-NU	New Jersey Special Hazardous Substances List	>0%	Value	One substance is not included
USA	OSHA-Ca	Occupational Safety and Health Administration - carcinogen	>0%	Yes/No	No substance is included
USA	PAC-1	PAC - Protective Action Criteria for Chemicals 1	>0%	Value	All substances are included
USA	PAC-2	PAC - Protective Action Criteria for Chemicals 2	>0%	Value	All substances are included
USA	PAC-3	PAC - Protective Action Criteria for Chemicals 3	>0%	Value	All substances are included
USA	RTK-PA	Pennsylvania Right-to-know List	>0%	Yes/No	One substance is not included
USA	SHSL-PA	Pennsylvania Special Hazardous Substances List	>0%	Value	One substance is not included
USA	Prop 65 C	Prop 65 - Chemicals known to cause cancer	>0%	Yes/No	No substance is included
USA	Prop 65 D	Prop 65 - Developmental toxicity	>0%	Yes/No	One substance is included
USA	Prop 65 F	Prop 65 - Reproductive toxicity for females	>0%	Yes/No	No substance is included
USA	Prop 65 M	Prop 65 - Reproductive toxicity for males	>0%	Yes/No	No substance is included
USA	RCL	RCL (Resource Conservation and Recovery Act)	>0%	Value	2/3 of the substances are included
USA	SARA 302	SARA Section 302 (specific toxic chemical listings)	>0%	Yes/No	3/4 of the substances are included
USA	SARA 303	SARA Section 303 (extremely hazardous substances)	>0%	Yes/No	No substance is included
USA	TLV	Threshold Limit Value	>0%	Value	2/3 of the substances are included
USA	TSCA	TSCA (Toxic Substances Control Act)	>0%	Value	All substances are included
USA	AD-DL	Aerospace and Defense Declassifiable Substance List	>0%	Value	No substance is included
USA	SAGSL	Global Automotive Declassifiable Substance List	>0%	Value	One substance is included
Australia	ACS	Australian Inventory of Chemical Substances	>0%	Yes/No	All substances are included
Australia	PEC	Priority Existing Chemicals	>0%	Yes/No	No substance is included
Australia	SUMP	Standard for the Uniform Scheduling of Medicines and Poisons	>0%	Value	One substance is included
Australia	A	A	>0%	Yes/No	No substance is included
Canada	DCL	Canadian Domestic Chemicals List (DCL)	>0%	Yes/No	All substances are included
Canada	CDN 1%	Canadian Ingredient disclosure list (limit 0.1%)	>0.1%	Yes/No	No substance is included
Canada	CDN 1%	Canadian Ingredient disclosure list (limit 1%)	>1%	Yes/No	One substance is not included
China	ChaoChem	Catalogue of Hazardous Chemicals	>0%	Value	One substance is not included
China	IECC	Chinese Chemical Inventory of Existing Chemical Substances	>0%	Yes/No	All substances are included
China	ENECs	ENECs	>0%	Yes/No	One substance is not included
China	BLNCS	BLNCS	>0%	Yes/No	No substance is included
China	PBT	PBT	>0%	Yes/No	No substance is included
China	PC	PC	>0%	Value	No substance is included
China	POP	POP	>0%	Value	No substance is included
China	ANNEX IV	REACH - Annex IV	>0%	Value	No substance is included
China	REACH-RE	REACH - Pre-registered substances	>0%	Yes/No	All substances are included
China	REACH-REUK	REACH - Registered substances UK only	>0%	Yes/No	No substance is included
China	RoHS 2	RoHS Directive - Annex II	>0.1%	Yes/No	No substance is included
China	SVHC	Substances of very high concern	>0.1%	Yes/No	No substance is included
China	HPB	HPB	>0%	Yes/No	No substance is included
Germany	MAK	Maximum Allowable Concentration	>0%	Value	No substance is included
Germany	ASCL	Air Pollution Control Law	>0%	Yes/No	One substance is included
Germany	BECS	Biodegradation and Bioaccumulation of Existing Substances	>0%	Yes/No	All substances are included
Germany	CSPN	Chemical Substances Relating to a Public Notice	>0%	Yes/No	No substance is included
Germany	BNCS	Existing Chemical Substances	>0%	Value	All substances are included
Germany	IFA	Fire Services Act	>0%	Yes/No	One substance is not included
Germany	ISHA-DSCG	ISHA - Dangerous Substances (Combustible gases)	>0%	Yes/No	No substance is included
Germany	ISHA-DSCS	ISHA - Dangerous Substances (Combustible substances)	>0%	Yes/No	No substance is included
Germany	ISHA-DSES	ISHA - Dangerous Substances (Explosive substances)	>0%	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)

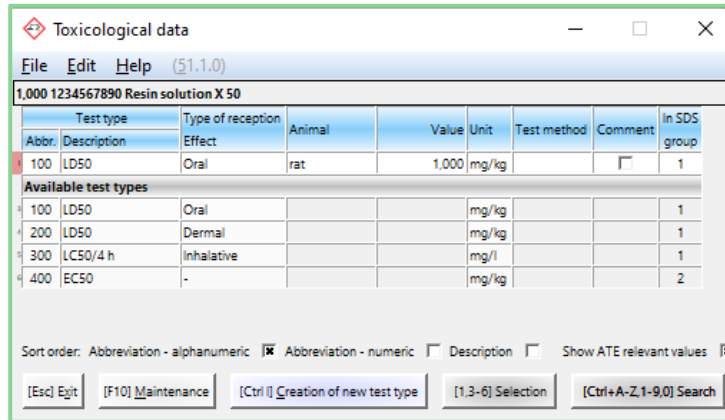
The **Ctrl L Substance Listings** screen shows the listing status of the various ingredients of your formulation.

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

File Edit Help (51.1.0)

1,000 1234567890 Resin solution X 50

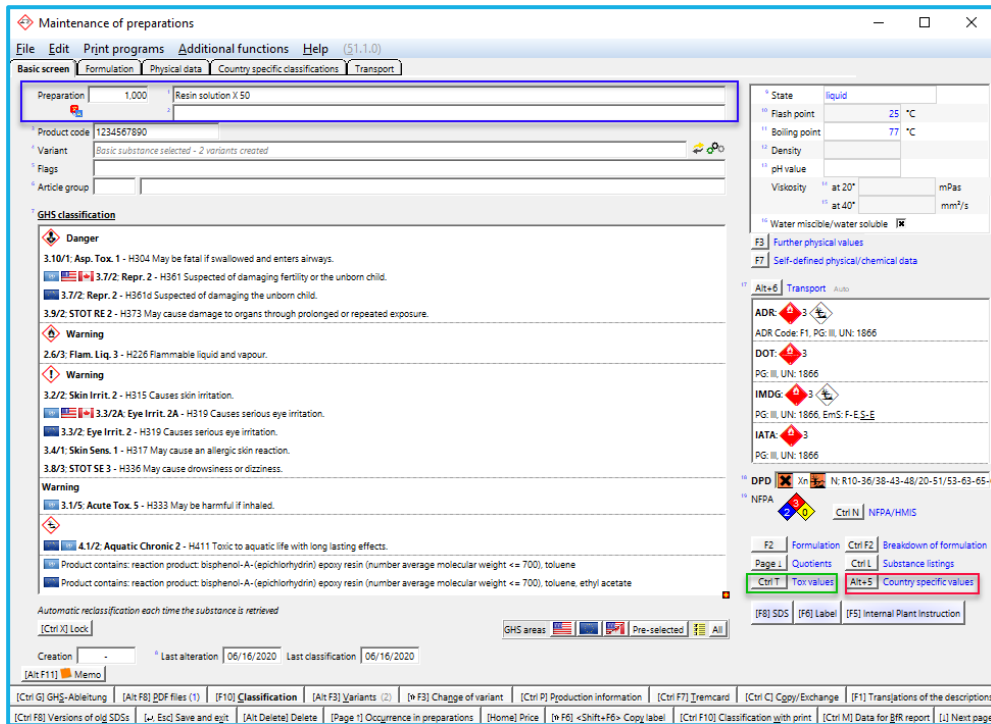
Abbr.	Description	Type of reception Effect	Animal	Value	Unit	Test method	Comment	In SDS group
100	LD50	Oral	rat	1,000	mg/kg			1

Available test types

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

File Edit Print programs Additional functions Help (51.1.0)

Basic screen Formulation Physical data Country specific classifications Transport

Preparation: 1,000 Resin solution X 50

Product code: 1234567890

Variant: Basic substance selected - 2 variants created

State: liquid

Flash point: 25 °C

Burning 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.
- 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.

ADR: F1, PG III, UN: 1866

DOT: 3

IMDG: 3

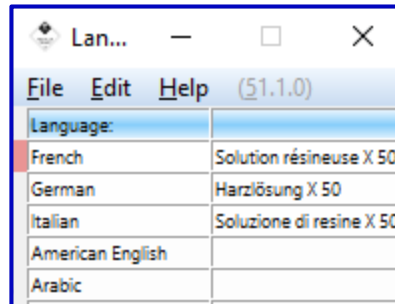
IATA: 3

DPD: Xn, N: R10-36/38-43-48/20-51/53-63-65-

NFPA: 0, 0, 0

Alt+5 Country specific values

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

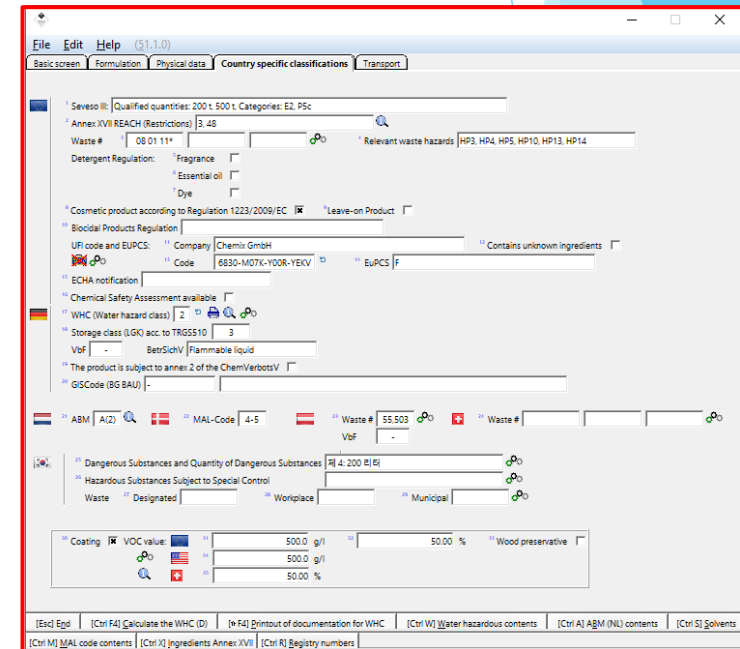


Lan...

File Edit Help (51.1.0)

Language:

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



Country specific classifications

File Edit Help (51.1.0)

Basic screen Formulation Physical data Country specific classifications Transport

Seveso III: Qualified quantities: 200 t, 500 t. Categories: E2, P5c

Annex XVII REACH (Restrictions): 3, 4, 8

Waste #: 08 01 11*

Detergent Regulation: Fragrance Essential oil Dye

Company: Chemix GmbH

Code: 6835-M07X-Y00R-YEUV

EuPCS: F

WHC (Water hazard class): 2

Storage class (LGO acc. to TRGS 510): 3

VdF: -

ABM: A21

Waste #: 55.503

Dangerous Substances and Quantity of Dangerous Substances: 4: 200 E[B]

Hazardous Substances Subject to Special Control: Waste Designated Workplace Municipal

VOC value: 500.0 g/l, 50.00 %

Coating VOC value: 500.0 g/l, 50.00 %

Wood preservative

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 a table of substances. The table has columns for Substance number, Description, Symbols, Percent, % in intermediate, and % in product. The substances listed are:

Substance number	Description	Symbols	Percent	% in intermediate	% in product
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		
25068-38-6	reaction product: bisphenol-A-(epichlorohydrin) 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 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 dialog box 'Breakdown of formul...' contains 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 keyboard shortcut menu includes the following options:

- [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

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