SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 08.06.2017 Version 11.16

SECTION 1. Identification of the substance/mixture and of the company/undertaking

1.1 Product identifier

Catalogue No.	820931
Product name	1-Octanol for synthesis
REACH Registration Number	01-2119486978-10-XXXX
CAS-No.	111-87-5

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses	Chemical for synthesis In compliance with the conditions described in the annex to this safety data sheet.

1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number

Please contact the regional company representation in your country.

SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Eye irritation, Category 2, H319

Chronic aquatic toxicity, Category 3, H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms

Signal word

Warning

Hazard statements

H319 Causes serious eye irritation.

H412 Harmful to aquatic life with long lasting effects.

Precautionary statements

Prevention

P273 Avoid release to the environment.

Response

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Reduced labelling (≤125 ml)

Hazard pictograms

Signal word

Warning

Hazard statements

H412 Harmful to aquatic life with long lasting effects.

CAS-No. 111-87-5

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	$CH_3(CH_2)_7OH$	$C_8H_{18}O$ (Hill)
EC-No.	203-917-6	
Molar mass	130,23 g/mol	

Hazardous components (REGULATION (EC) No 1272/2008)

Chemical name (Concentration)

CAS-No.	Registration number	Classification
1-octanol *(<= 100 %)*		
Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.		
111-87-5	01-2119486978-10-XXXX	Eye irritation, Category 2, H319 Chronic aquatic toxicity, Category 3, H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

3.2 Mixture

Not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

After inhalation: fresh air.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

4.2 Most important symptoms and effects, both acute and delayed

The following applies to aliphatic alcohols in general: effect when product is not handled and used properly: mucosal irritations; after absorption of large quantities: narcosis.
irritant effects, CNS disorders, somnolence, Vertigo, euphoria, agitation, spasms

4.3 Indication of any immediate medical attention and special treatment needed

Laxative: Sodium sulfate (1 tablespoon/1/4 l water).

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Foam, Carbon dioxide (CO2), Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Combustible.
Vapours are heavier than air and may spread along floors.
Forms explosive mixtures with air on intense heating.
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Special protective equipment for firefighters

In the event of fire, wear self-contained breathing apparatus.

Further information

Prevent fire extinguishing water from contaminating surface water or the ground water system.
Suppress (knock down) gases/vapours/mists with a water spray jet. Remove container from danger zone and cool with water.

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

Protective equipment see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Change contaminated clothing. Wash hands after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed.

Recommended storage temperature see product label.

7.3 Specific end use(s)

See exposure scenario in the Annex to this MSDS.

SECTION 8. Exposure controls/personal protection

8.1 Control parameters

Derived No Effect Level (DNEL)

Worker DNEL, acute	Systemic effects	dermal	125 mg/kg Body weight
Worker DNEL, acute	Systemic effects	inhalation	220 mg/m³
Worker DNEL, longterm	Systemic effects	dermal	125 mg/kg Body weight
Worker DNEL, longterm	Systemic effects	inhalation	220 mg/m³
Consumer DNEL, acute	Systemic effects	dermal	75 mg/kg Body weight
Consumer DNEL, acute	Systemic effects	inhalation	65 mg/m³
Consumer DNEL, acute	Systemic effects	oral	75 mg/kg Body weight
Consumer DNEL, longterm	Systemic effects	dermal	75 mg/kg Body weight
Consumer DNEL, longterm	Systemic effects	inhalation	65 mg/m³
Consumer DNEL, longterm	Systemic effects	oral	75 mg/kg Body weight

Predicted No Effect Concentration (PNEC)

PNEC Fresh water	0,2 mg/l
PNEC Marine water	0,02 mg/l
PNEC Sewage treatment plant	5,5 mg/l
PNEC Fresh water sediment	2,1 mg/kg
PNEC Marine sediment	0,21 mg/kg
PNEC Soil	1,6 mg/kg

8.2 Exposure controls

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Safety glasses

Hand protection

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,40 mm
Break through time:	> 480 min

splash contact:

Glove material:	polychloroprene
Glove thickness:	0,65 mm
Break through time:	> 240 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 730 Camatril® -Velours (full contact), KCL 720 Camapren® (splash contact).
The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.
This recommendation applies only to the product stated in the safety data sheet<(>,<)> supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment

Flame retardant antistatic protective clothing.

Respiratory protection
required when vapours/aerosols are generated.
Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds
The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Environmental exposure controls
Do not let product enter drains.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	characteristic
Odour Threshold	No information available.
pH	No information available.
pour point	ca. -16 - -14 °C at 1.013 hPa Method: ISO 3016
Boiling point/boiling range	195 °C at 1.013 hPa
Flash point	ca. 86 °C Method: DIN 51758

Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	0,8 %(V)
Upper explosion limit	No information available.
Vapour pressure	0,031 hPa at 20 °C
Relative vapour density	4,5
Density	0,83 g/cm3 at 20 °C
Relative density	No information available.
Water solubility	ca.0,43 g/l at 25 °C (External MSDS)
Partition coefficient: n-octanol/water	log Pow: 2,8 (experimental) (IUCLID) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	9,0 mPa.s at 20 °C
Explosive properties	Not classified as explosive.

Oxidizing properties	none

9.2 Other data

Ignition temperature	270 °C Method: DIN 51794
Viscosity, kinematic	ca.5,6 mm2/s at 40 °C Method: ASTM D 445

SECTION 10. Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Acid chlorides, Acid anhydrides, Oxidizing agents, acids, halogen compounds

Risk of explosion with:

perchloric acid, perchlorates

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

rubber, various plastics

10.6 Hazardous decomposition products

no information available

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: > 5.000 mg/kg

OECD Test Guideline 401

Symptoms: Nausea, Vomiting, Gastrointestinal discomfort, Risk of aspiration upon vomiting., Pulmonary failure possible after aspiration of vomit.

Acute inhalation toxicity

Symptoms: Possible damages:, mucosal irritations

Acute dermal toxicity

LD50 Rabbit: > 2.000 - 4.000 mg/kg

OECD Test Guideline 402

Skin irritation

human

Result: No irritation

Patch Test 24 Hrs.

Eye irritation

Rabbit

Result: Severe irritations

OECD Test Guideline 405

Causes serious eye irritation.

Sensitisation

Patch test:

Result: negative

Method: OECD Test Guideline 406

Germ cell mutagenicity

Genotoxicity in vivo

In vivo micronucleus test

Mouse

male and female

Oral

Bone marrow

Result: negative

Method: OECD Test Guideline 474

Genotoxicity in vitro

Ames test

Salmonella typhimurium

Result: negative

Method: OECD Test Guideline 471

In vitro mammalian cell gene mutation test

Mouse lymphoma test

Result: negative

Method: OECD Test Guideline 476

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

The following applies to aliphatic alcohols in general: effect when product is not handled and used properly: mucosal irritations; after absorption of large quantities: narcosis.
After absorption of large quantities:
CNS disorders, somnolence, Dizziness, euphoria, agitation, Convulsions
Other dangerous properties can not be excluded.
Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

flow-through test LC50 Pimephales promelas (fathead minnow): 13 mg/l; 96 h
Analytical monitoring: yes
OECD Test Guideline 203

Toxicity to algae

static test EC50 Desmodesmus subspicatus (green algae): 14 mg/l; 48 h
OECD Test Guideline 201

Toxicity to bacteria

EC50 activated sludge: 350 mg/l; 3 h
OECD Test Guideline 209

Toxicity to fish (Chronic toxicity)

flow-through test NOEC Pimephales promelas (fathead minnow): 1 - 10 mg/l; 7 d

(External MSDS)

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)

semi-static test NOEC Daphnia magna (Water flea): 1 mg/l; 21 d
Analytical monitoring: yes

OECD Test Guideline 211

12.2 Persistence and degradability

Biodegradability

92 %; 28 d; aerobic
OECD Test Guideline 310
Readily biodegradable

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 2,8

(experimental)

(IUCLID) Bioaccumulation is not expected.

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

12.6 Other adverse effects

Discharge into the environment must be avoided.

SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

14.1 - 14.6	Not classified as dangerous in the meaning of transport regulations.

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 - 14.6	Not classified as dangerous in the meaning of transport regulations.

Sea transport (IMDG)

14.1 - 14.6 Not classified as dangerous in the meaning of transport regulations.

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

SECTION 15. Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

EU regulations

Major Accident Hazard	SEVESO III
Legislation	Not applicable
Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work.
Regulation (EC) No 1005/2009 on substances that deplete the ozone layer	not regulated
Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC	not regulated
Substances of very high concern (SVHC)	This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of ≥ 0.1 % (w/w).

National legislation

Storage class	10 - 13

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out.

SECTION 16. Other information

Full text of H-Statements referred to under sections 2 and 3.

H319	Causes serious eye irritation.
H412	Harmful to aquatic life with long lasting effects.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms

Signal word

Warning

Hazard statements

H227 Combustible liquid.

H319 Causes serious eye irritation.

H412 Harmful to aquatic life with long lasting effects.

Precautionary statements

Prevention

P273 Avoid release to the environment.

Response

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.

EXPOSURE SCENARIO 1 (Industrial use)

1. Industrial use Chemical for synthesis)

Sectors of end-use

SU 3	Industrial uses: Uses of substances as such or in preparations at industrial sites
SU9	Manufacture of fine chemicals
SU 10	Formulation [mixing] of preparations and/ or re-packaging (excluding alloys)

Chemical product category

PC19	Intermediate
PC21	Laboratory chemicals

Process categories

PROC1	Use in closed process, no likelihood of exposure
PROC2	Use in closed, continuous process with occasional controlled exposure
PROC3	Use in closed batch process (synthesis or formulation)
PROC4	Use in batch and other process (synthesis) where opportunity for exposure arises
PROC5	Mixing or blending in batch processes for formulation of preparations and articles (multistage and/ or significant contact)
PROC8a	Transfer of substance or preparation (charging/ discharging) from/ to vessels/ large containers at non-dedicated facilities
PROC8b	Transfer of substance or preparation (charging/ discharging) from/ to vessels/ large containers at dedicated facilities
PROC9	Transfer of substance or preparation into small containers (dedicated filling line, including weighing)
PROC10	Roller application or brushing
PROC15	Use as laboratory reagent

Environmental Release Categories

ERC1	Manufacture of substances
ERC2	Formulation of preparations
ERC4	Industrial use of processing aids in processes and products, not becoming part of articles
ERC6a	Industrial use resulting in manufacture of another substance (use of intermediates)
ERC6b	Industrial use of reactive processing aids

2. Contributing scenarios: Operational conditions and risk management measures

2.1 Contributing scenario controlling environmental exposure for: ERC1

Amount used

Annual amount per site	105000 t
Daily amount per site (Msafe)	350 t

Environment factors not influenced by risk management

Flow rate	18.000 m3/d
Dilution Factor (River)	10
Dilution Factor (Coastal Areas)	100

Other given operational conditions affecting environmental exposure

Number of emission days per year	300
Emission or Release Factor: Air	5 %
Emission or Release Factor: Water	0,01 %
Emission or Release Factor: Soil	0,01 %

Technical conditions and measures / Organizational measures

Water	Ensure all waste water is collected and treated via a WWTP.

Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant	Municipal sewage treatment plant
Flow rate of sewage treatment plant effluent	2.000 m3/d
Percentage removed from waste water	96,5 %

Conditions and measures related to external treatment of waste for disposal

Waste treatment	Aqueous waste to be treated in on-site or municipal secondary biological treatment plants prior to discharge.

2.2 Contributing scenario controlling environmental exposure for: ERC2

Amount used

Annual amount per site	3500 t
Daily amount per site (Msafe)	11,6 t

Environment factors not influenced by risk management

Flow rate	18.000 m3/d
Dilution Factor (River)	10
Dilution Factor (Coastal Areas)	100

Other given operational conditions affecting environmental exposure

Number of emission days per year	300
Emission or Release Factor: Air	2,5 %
Emission or Release Factor: Water	0,3 %
Emission or Release Factor: Soil	0,01 %

Technical conditions and measures / Organizational measures

Water	Ensure all waste water is collected and treated via a WWTP.

Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant	Municipal sewage treatment plant
Flow rate of sewage treatment plant effluent	2.000 m3/d
Percentage removed from waste water	96,5 %

Conditions and measures related to external treatment of waste for disposal

Waste treatment	Aqueous waste to be treated in on-site or municipal secondary biological treatment plants prior to discharge.

2.3 Contributing scenario controlling environmental exposure for: ERC4

Amount used

Annual amount per site	352 t
Daily amount per site (Msafe)	1.176 kg

Environment factors not influenced by risk management

Flow rate	18.000 m3/d
Dilution Factor (River)	10
Dilution Factor (Coastal Areas)	100

Other given operational conditions affecting environmental exposure

Number of emission days per year	300
Emission or Release Factor: Air	100 %
Emission or Release Factor: Water	3 %
Emission or Release Factor: Soil	5 %

Technical conditions and measures / Organizational measures

Water	Ensure all waste water is collected and treated via a WWTP.

Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant	Municipal sewage treatment plant
Flow rate of sewage treatment plant effluent	2.000 m3/d
Percentage removed from waste water	96,5 %

Conditions and measures related to external treatment of waste for disposal

Waste treatment	Aqueous waste to be treated in on-site or municipal secondary biological treatment plants prior to discharge.

2.4 Contributing scenario controlling environmental exposure for: ERC6a

Amount used

Annual amount per site	1510 t
Daily amount per site (Msafe)	5 t

Environment factors not influenced by risk management

Flow rate	18.000 m3/d
Dilution Factor (River)	10
Dilution Factor (Coastal Areas)	100

Other given operational conditions affecting environmental exposure

Number of emission days per year	300
Emission or Release Factor: Air	5 %
Emission or Release Factor: Water	0,7 %
Emission or Release Factor: Soil	0,1 %

Technical conditions and measures / Organizational measures

Water	Ensure all waste water is collected and treated via a WWTP.

Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant	Municipal sewage treatment plant
Flow rate of sewage treatment plant effluent	2.000 m3/d
Percentage removed from waste water	96,5 %

Conditions and measures related to external treatment of waste for disposal

Waste treatment	Aqueous waste to be treated in on-site or municipal secondary biological treatment plants prior to discharge.

2.5 Contributing scenario controlling environmental exposure for: ERC6b

Amount used

Annual amount per site	1058 t
Daily amount per site (Msafe)	3,5 t

Environment factors not influenced by risk management

Flow rate	18.000 m3/d
Dilution Factor (River)	10
Dilution Factor (Coastal Areas)	100

Other given operational conditions affecting environmental exposure

Number of emission days per year	300
Emission or Release Factor: Air	0,1 %
Emission or Release Factor: Water	1 %
Emission or Release Factor: Soil	0,02 %

Technical conditions and measures / Organizational measures

Water	Ensure all waste water is collected and treated via a WWTP.

Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant	Municipal sewage treatment plant
Flow rate of sewage treatment plant effluent	2.000 m3/d
Percentage removed from waste water	96,5 %

Conditions and measures related to external treatment of waste for disposal

Waste treatment	Aqueous waste to be treated in on-site or municipal secondary biological treatment plants prior to discharge.

2.6 Contributing scenario controlling worker exposure for: PROC1, PROC2, PROC3, PROC4, PROC5, PROC8a, PROC8b, PROC9, PROC10, PROC15

Product characteristics

Concentration of the Substance in Mixture/Article	Covers the percentage of the substance in the product up to 100 %.
Physical Form (at time of use)	Low volatile liquid
Process Temperature	< 86 °C

Frequency and duration of use

Frequency of use	8 hours/day

Other operational conditions affecting workers exposure

Outdoor / Indoor	Indoor without local exhaust ventilation (LEV)

Conditions and measures related to personal protection, hygiene and health evaluation

Wear suitable gloves (tested to EN374) and eye protection.

2.7 Contributing scenario controlling worker exposure for: PROC10

Product characteristics

Concentration of the Substance in Mixture/Article	Covers the percentage of the substance in the product up to 100 %.
Physical Form (at time of use)	Low volatile liquid
Process Temperature	< 86 °C

Frequency and duration of use

Frequency of use	8 hours/day

Other operational conditions affecting workers exposure

Outdoor / Indoor	Indoor without local exhaust ventilation (LEV)

Conditions and measures related to personal protection, hygiene and health evaluation

Wear suitable gloves (tested to EN374) and eye protection. During spraying, wear suitable respiratory equipment.

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3. Exposure estimation and reference to its source

Environment

CS	Use descriptor	Msafe	Compartment	RCR	Exposure Assessment Method
2.1	ERC1	350 t/day	Fresh water sediment	0,99	EUSES
2.2	ERC2	11,6 t/day	Fresh water sediment	0,99	EUSES
2.3	ERC4	1176 kg/day	Fresh water sediment	1	EUSES
2.4	ERC6a	5 t/day	Fresh water sediment	1	EUSES
2.5	ERC6a	3,5 t/day	Fresh water sediment	1	EUSES

The default parameters and -efficiencies of the applied exposure assessment model were used for the calculation (unless stated differently).
For (other) acute and local effects risk management measures are based on qualitative risk characterisation.

4. Guidance to Downstream User to evaluate whether he works inside the boundaries set by the Exposure Scenario

Please refer to the following documents: ECHA Guidance on information requirements and chemical safety assessment Chapter R.12: Use descriptor system; ECHA Guidance for downstream users; ECHA Guidance on information requirements and chemical safety assessment Part D: Exposure Scenario Building, Part E: Risk Characterisation and Part G: Extending the SDS; VCI/Cefic REACH Practical Guides on Exposure Assessment and Communications in the Supply Chain; CEFIC Guidance Specific Environmental Release Categories (SPERCs).

EXPOSURE SCENARIO 2 (Professional use)

1. Professional use Chemical for synthesis)

Sectors of end-use

SU 22 Professional uses: Public domain (administration, education, entertainment, services, craftsmen)

Chemical product category

PC21 Laboratory chemicals

Process categories

PROC15 Use as laboratory reagent

Environmental Release Categories

ERC2 Formulation of preparations

ERC6a Industrial use resulting in manufacture of another substance (use of intermediates)

ERC6b Industrial use of reactive processing aids

2. Contributing scenarios: Operational conditions and risk management measures

2.1 Contributing scenario controlling environmental exposure for: ERC2

Amount used

Annual amount per site	3500 t
Daily amount per site (Msafe)	11,6 t

Environment factors not influenced by risk management

Flow rate	18.000 m3/d
Dilution Factor (River)	10
Dilution Factor (Coastal Areas)	100

Other given operational conditions affecting environmental exposure

Number of emission days per year	300
Emission or Release Factor: Air	2,5 %
Emission or Release Factor: Water	0,3 %
Emission or Release Factor: Soil	0,01 %

Technical conditions and measures / Organizational measures

Water	Ensure all waste water is collected and treated via a WWTP.

Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant	Municipal sewage treatment plant
Flow rate of sewage treatment plant effluent	2.000 m3/d
Percentage removed from waste water	96,5 %

Conditions and measures related to external treatment of waste for disposal

Waste treatment	Aqueous waste to be treated in on-site or municipal secondary biological treatment plants prior to discharge.

2.2 Contributing scenario controlling environmental exposure for: ERC6a

Amount used

Annual amount per site	1510 t
Daily amount per site (Msafe)	5 t

Environment factors not influenced by risk management

Flow rate	18.000 m3/d
Dilution Factor (River)	10
Dilution Factor (Coastal Areas)	100

Other given operational conditions affecting environmental exposure

Number of emission days per year	300
Emission or Release Factor: Air	5 %
Emission or Release Factor: Water	0,7 %
Emission or Release Factor: Soil	0,1 %

Technical conditions and measures / Organizational measures

Water	Ensure all waste water is collected and treated via a WWTP.

Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant	Municipal sewage treatment plant
Flow rate of sewage treatment plant effluent	2.000 m3/d
Percentage removed from waste water	96,5 %

Conditions and measures related to external treatment of waste for disposal

Waste treatment	Aqueous waste to be treated in on-site or municipal secondary biological treatment plants prior to discharge.

2.3 Contributing scenario controlling environmental exposure for: ERC6b

Amount used

Annual amount per site	1058 t
Daily amount per site (Msafe)	3,5 t

Environment factors not influenced by risk management

Flow rate	18.000 m3/d
Dilution Factor (River)	10
Dilution Factor (Coastal Areas)	100

Other given operational conditions affecting environmental exposure

Number of emission days per year	300
Emission or Release Factor: Air	0,1 %
Emission or Release Factor: Water	1 %
Emission or Release Factor: Soil	0,02 %

Technical conditions and measures / Organizational measures

Water	Ensure all waste water is collected and treated via a WWTP.

Conditions and measures related to municipal sewage treatment plant

Type of Sewage Treatment Plant	Municipal sewage treatment plant

Flow rate of sewage treatment plant effluent	2.000 m3/d
Percentage removed from waste water	96,5 %

Conditions and measures related to external treatment of waste for disposal

Waste treatment	Aqueous waste to be treated in on-site or municipal secondary biological treatment plants prior to discharge.

2.4 Contributing scenario controlling worker exposure for: PROC15

Product characteristics

Concentration of the Substance in Mixture/Article	Covers the percentage of the substance in the product up to 100 %.
Physical Form (at time of use)	Low volatile liquid
Process Temperature	< 86 °C

Frequency and duration of use

Frequency of use	8 hours/day

Other operational conditions affecting workers exposure

Outdoor / Indoor	Indoor without local exhaust ventilation (LEV)

Conditions and measures related to personal protection, hygiene and health evaluation

Wear suitable gloves (tested to EN374) and eye protection.

3. Exposure estimation and reference to its source

Environment

CS	Use descriptor	Msafe	Compartment	RCR	Exposure Assessment Method
2.1	ERC2	11,6 t/day	Fresh water sediment	0,99	EUSES
2.2	ERC6a	5 t/day	Fresh water sediment	1	EUSES
2.3	ERC6a	3,5 t/day	Fresh water sediment	1	EUSES

The default parameters and -efficiencies of the applied exposure assessment model were used for the calculation (unless stated differently).
For (other) acute and local effects risk management measures are based on qualitative risk characterisation.

4. Guidance to Downstream User to evaluate whether he works inside the boundaries set by the Exposure Scenario

Please refer to the following documents: ECHA Guidance on information requirements and chemical safety assessment Chapter R.12: Use descriptor system; ECHA Guidance for downstream users; ECHA Guidance on information requirements and chemical safety assessment Part D: Exposure Scenario Building, Part E: Risk Characterisation and Part G: Extending the SDS; VCI/Cefic REACH Practical Guides on Exposure Assessment and Communications in the Supply Chain; CEFIC Guidance Specific Environmental Release Categories (SPERCs).