

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 06.10.2017

Version 10.1

SECTION 1. Identification of the substance/mixture and of the company/undertaking**1.1 Product identifier**

Catalogue No.	100979
Product name	Isoamyl alcohol for analysis EMSURE® ACS, Reag. Ph Eur
REACH Registration Number	01-2119493725-26-XXXX
CAS-No.	123-51-3

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

Identified uses	Reagent for analysis In compliance with the conditions described in the annex to this safety data sheet.
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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.
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SECTION 2. Hazards identification**2.1 Classification of the substance or mixture****Classification (REGULATION (EC) No 1272/2008)**

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Product name Isoamyl alcohol for analysis EMSURE® ACS, Reag. Ph Eur

Flammable liquid, Category 3, H226

Acute toxicity, Category 4, Inhalation, H332

Specific target organ toxicity - single exposure, Category 3, Respiratory system, H335

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

H226 Flammable liquid and vapour.

H332 Harmful if inhaled.

H335 May cause respiratory irritation.

EUH066 Repeated exposure may cause skin dryness or cracking.

Precautionary statements

Prevention

P210 Keep away from heat.

Response

P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

Reduced labelling (≤ 125 ml)

Hazard pictograms



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Signal word

Warning

Index-No. 603-006-00-7

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	(CH ₃) ₂ CHCH ₂ CH ₂ OH	C ₅ H ₁₂ O (Hill)
Index-No.	603-006-00-7	
EC-No.	204-633-5	
Molar mass	88,15 g/mol	

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

Chemical name (Concentration)

CAS-No.	Registration number	Classification
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Isoamyl alcohol (<= 100 %)

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

123-51-3	01-2119493725-26-
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XXXX

Flammable liquid, Category 3, H226

Acute toxicity, Category 4, H332

Specific target organ toxicity - single exposure, Category 3, H335

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

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After inhalation: fresh air. If breathing stops: mouth-to-mouth breathing or artificial respiration.
Oxygen if necessary. Immediately call in physician.

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. 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

Dermatitis, Dizziness, Unconsciousness, Diarrhoea, Nausea, Vomiting, Headache, muscular
weakness, somnolence, confusion, Coma
irritant effects, Cough, Shortness of breath, Repeated exposure may cause skin dryness or
cracking.

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂), Foam, 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 at elevated temperatures.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

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Special protective equipment for firefighters

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

Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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. Risk of explosion.

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

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Observe label precautions.

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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. Preventive skin protection recommended. Wash hands after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

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

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Derived No Effect Level (DNEL)

Worker DNEL, longterm	Local and systemic effects	inhalation	73,16 mg/m ³
Worker DNEL, acute	Local and systemic effects	inhalation	292 mg/m ³
Consumer DNEL, longterm	Local and systemic effects	inhalation	15,4 mg/m ³
Consumer DNEL, acute	Local and systemic effects	inhalation	256,4 mg/m ³
Consumer DNEL, longterm	Systemic effects	oral	25 mg/kg Body weight

Predicted No Effect Concentration (PNEC)

PNEC Fresh water	0,255 mg/l
PNEC Marine water	0,0255 mg/l
PNEC Aquatic intermittent release	2,55 mg/l
PNEC Fresh water sediment	1,05 mg/kg
PNEC Marine sediment	0,105 mg/kg
PNEC Soil	0,061 mg/kg
PNEC Sewage treatment plant	37 mg/l

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.

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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:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 30 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 741 Dermatril® L (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 entrepreneur 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

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properly documented.

Environmental exposure controls

Do not let product enter drains.

Risk of explosion.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	malodorous
Odour Threshold	No information available.
pH	7 at 25 g/l 20 °C
Melting point	-147 °C Method: OECD Test Guideline 102
Boiling point/boiling range	130,7 °C at 1.013 hPa
Flash point	43,5 °C Method: closed cup
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.

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Lower explosion limit	1,2 %(V)
Upper explosion limit	8 %(V)
Vapour pressure	3 hPa at 20 °C
Relative vapour density	3,04
Density	0,81 g/cm ³ at 20 °C Method: DIN 53217
Relative density	No information available.
Water solubility	25 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 1,35 OECD Test Guideline 107 Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	Distillable in an undecomposed state at normal pressure.
Viscosity, dynamic	4,3 mPa.s at 20 °C
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

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Ignition temperature 335 °C
at 1.013 hPa
Method: DIN 51794

Saturated vapour concentration 11 g/m³
at 20 °C

Viscosity, kinematic 5,32 mm²/s
at 20 °C

SECTION 10. Stability and reactivity

10.1 Reactivity

Vapour/air-mixtures are explosive at intense warming.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

Risk of ignition or formation of inflammable gases or vapours with:

Fluorine, Strong oxidizing agents, Oxygen, Alkali metals, Alkaline earth metals, Acids,
Isocyanates, halogens, perchloric acid, lithium aluminium hydride, Acid anhydrides, perchlorates,
Aluminium, Sulphides

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

rubber

10.6 Hazardous decomposition products

no information available

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SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: > 5.000 mg/kg

(External MSDS)

Symptoms: Risk of aspiration upon vomiting., Aspiration may cause pulmonary oedema and pneumonitis.

Acute inhalation toxicity

Acute toxicity estimate: 11,1 mg/l; vapour

Expert judgement

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:., damage of respiratory tract, Inhalation may lead to the formation of oedemas in the respiratory tract.

Acute dermal toxicity

LD50 Rabbit: > 3.000 mg/kg

(External MSDS)

Skin irritation

Repeated exposure may cause skin dryness or cracking.

Dermatitis

Eye irritation

This information is not available.

Sensitisation

This information is not available.

Germ cell mutagenicity

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Genotoxicity in vitro

Ames test

Result: negative

(Lit.)

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

May cause respiratory irritation.

Target Organs: Respiratory system

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

Absorption via:

Gastrointestinal tract

After absorption of large quantities:

Headache, somnolence, lack of appetite, Nausea, Vomiting, Diarrhoea, Dizziness, muscular weakness, confusion, Unconsciousness, Coma

Possible damages:

Damage to:

Liver, Kidney, Lungs, Cardiac

Effect potentiated by: ethanol

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

LC50 *Oncorhynchus mykiss* (rainbow trout): 700 mg/l; 96 h
(IUCLID)

Toxicity to daphnia and other aquatic invertebrates

EC50 *Daphnia* (water flea): 260 mg/l; 48 h
(IUCLID)

Toxicity to algae

IC50 *Desmodesmus subspicatus* (green algae): 493 mg/l; 72 h
(IUCLID)

Toxicity to bacteria

EC50 *Pseudomonas putida*: 2.500 mg/l; 17 h
(IUCLID)

12.2 Persistence and degradability

Biodegradability

84 %; 27 d
OECD Test Guideline 301C
Readily biodegradable

Theoretical oxygen demand (ThOD)

2.740 mg/g

(Lit.)

Ratio BOD/COD

63 %
(IUCLID)

Ratio BOD/ThBOD

BOD5 55 %
(Lit.)

Ratio COD/ThBOD

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77 %

(Lit.)

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 1,35

OECD Test Guideline 107

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.

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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 UN number	UN 1105
14.2 Proper shipping name	PENTANOLS
14.3 Class	3
14.4 Packing group	III
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
Tunnel restriction code	D/E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number	UN 1105
14.2 Proper shipping name	PENTANOLS
14.3 Class	3
14.4 Packing group	III
14.5 Environmentally hazardous	--
14.6 Special precautions for user	no

Sea transport (IMDG)

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14.1 UN number UN 1105
14.2 Proper shipping name PENTANOLS
14.3 Class 3
14.4 Packing group III
14.5 Environmentally hazardous --
14.6 Special precautions for user yes
EmS F-E S-D

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 FLAMMABLE LIQUIDS
P5c
Quantity 1: 5.000 t
Quantity 2: 50.000 t

Occupational restrictions Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

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

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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 $\geq 0.1\%$ (w/w).

National legislation

Storage class 3

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.

H226 Flammable liquid and vapour.
H332 Harmful if inhaled.
H335 May cause respiratory irritation.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

Warning

Hazard statements

H226 Flammable liquid and vapour.

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H332 Harmful if inhaled.

H335 May cause respiratory irritation.

EUH066 Repeated exposure may cause skin dryness or cracking.

Precautionary statements

Prevention

P210 Keep away from heat.

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.

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EXPOSURE SCENARIO 1 (Industrial use)

1. Industrial use Reagent for analysis)

Sectors of end-use

- SU 3* Industrial uses: Uses of substances as such or in preparations at industrial sites
- SU 9* Manufacture of fine chemicals
- SU 10* Formulation [mixing] of preparations and/ or re-packaging (excluding alloys)

Chemical product category

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

2. Contributing scenarios: Operational conditions and risk management measures

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2.1 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)	Medium volatile liquid
Process Temperature	< 78 °C

Frequency and duration of use

Frequency of use	8 hours/day
Frequency of use	5 days/week

Other operational conditions affecting workers exposure

Outdoor / Indoor	Indoor without local exhaust ventilation (LEV)
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Organisational measures to prevent /limit releases, dispersion and exposure

Covers daily exposures up to 8 hours.

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

A chemical safety assessment was performed according REACH Article 14(3), Annex I, sections 3 (Environmental Hazard Assessment) and 4 (PBT/vPvB Assessment). As no hazard was identified, an exposure assessment and risk characterisation is not necessary (REACH Annex I section 5.0).

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Workers

CS	Use descriptor	Exposure duration, route, effect	RCR	Exposure Assessment Method
2.1	PROC1	longterm, inhalative, local	< 0,01	ECETOC TRA 2
		longterm, inhalative, systemic	< 0,01	ECETOC TRA 2
2.1	PROC2	longterm, inhalative, local	0,05	ECETOC TRA 2
		longterm, inhalative, systemic	0,05	ECETOC TRA 2
2.1	PROC3	longterm, inhalative, local	0,15	ECETOC TRA 2
		longterm, inhalative, systemic	0,15	ECETOC TRA 2
2.1	PROC4	longterm, inhalative, local	0,25	ECETOC TRA 2
		longterm, inhalative, systemic	0,25	ECETOC TRA 2
2.1	PROC5	longterm, inhalative, local	0,25	ECETOC TRA 2
		longterm, inhalative, systemic	0,25	ECETOC TRA 2
2.1	PROC8a	longterm, inhalative, local	0,50	ECETOC TRA 2
		longterm, inhalative, systemic	0,50	ECETOC TRA 2
2.1	PROC8b	longterm, inhalative, local	0,25	ECETOC TRA 2
		longterm, inhalative, systemic	0,25	ECETOC TRA 2
2.1	PROC9	longterm, inhalative, local	0,25	ECETOC TRA 2
		longterm, inhalative, systemic	0,25	ECETOC TRA 2
2.1	PROC10	longterm, inhalative, local	0,50	ECETOC TRA 2
		longterm, inhalative, systemic	0,50	ECETOC TRA 2
2.1	PROC15	longterm, inhalative, local	0,25	ECETOC TRA 2
		longterm, inhalative, systemic	0,25	ECETOC TRA 2

The default parameters and -efficiencies of the applied exposure assessment model were used for the calculation (unless stated differently).

For (other) local effects risk management measures are based on qualitative risk characterisation.

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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).

For scaling of worker exposure assessments performed with ECETOC TRA, please consult the Merck tool SciDeEx® at www.merckmillipore.com/scideex.

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EXPOSURE SCENARIO 2 (Professional use)

1. Professional use Reagent for analysis)

Sectors of end-use

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

Chemical product category

PC 21 Laboratory chemicals

Process categories

PROC 15 Use as laboratory reagent

Environmental Release Categories

ERC 2 Formulation of preparations

ERC 6a Industrial use resulting in manufacture of another substance (use of intermediates)

2. Contributing scenarios: Operational conditions and risk management measures

2.1 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)	Medium volatile liquid
Process Temperature	< 78 °C

Frequency and duration of use

Frequency of use	8 hours/day
Frequency of use	5 days/week

Other operational conditions affecting workers exposure

Outdoor / Indoor	Indoor without local exhaust ventilation (LEV)
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Organisational measures to prevent /limit releases, dispersion and exposure

Covers daily exposures up to 8 hours.

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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

A chemical safety assessment was performed according REACH Article 14(3), Annex I, sections 3 (Environmental Hazard Assessment) and 4 (PBT/vPvB Assessment). As no hazard was identified, an exposure assessment and risk characterisation is not necessary (REACH Annex I section 5.0).

Workers

CS	Use descriptor	Exposure duration, route, effect	RCR	Exposure Assessment Method
2.1	PROC15	longterm, inhalative, local	0,25	ECETOC TRA 2
		longterm, inhalative, systemic	0,25	ECETOC TRA 2

The default parameters and -efficiencies of the applied exposure assessment model were used for the calculation (unless stated differently).

For (other) local effects risk management measures are based on qualitative risk characterisation.

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