

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 22.08.2018

Version 14.3

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

1.1 Product identifier

Catalogue No. 104727

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

REACH Registration Number 01-2119457965-22-XXXX

CAS-No. 540-84-1

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

Identified uses Reagent for analysis, Chemical production
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)

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

Flammable liquid, Category 2, H225

Skin irritation, Category 2, H315

Specific target organ toxicity - single exposure, Category 3, Central nervous system, H336

Aspiration hazard, Category 1, H304

Acute aquatic toxicity, Category 1, H400

Chronic aquatic toxicity, Category 1, H410

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

Danger

Hazard statements

H225 Highly flammable liquid and vapour.

H304 May be fatal if swallowed and enters airways.

H315 Causes skin irritation.

H336 May cause drowsiness or dizziness.

H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P240 Ground/bond container and receiving equipment.

P273 Avoid release to the environment.

Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

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P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

Storage

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Danger

Hazard statements

H304 May be fatal if swallowed and enters airways.

Precautionary statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

Index-No. 601-009-00-8

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	$\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_3$	C_8H_{18} (Hill)
Index-No.	601-009-00-8	
EC-No.	208-759-1	
Molar mass	114,23 g/mol	

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

Chemical name (Concentration)

CAS-No.	Registration number	Classification
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isooctane (<= 100 %)		
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Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

540-84-1	01-2119457965-22-	
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Flammable liquid, Category 2, H225

Skin irritation, Category 2, H315

Specific target organ toxicity - single exposure, Category 3, H336

Aspiration hazard, Category 1, H304

Acute aquatic toxicity, Category 1, H400

Chronic aquatic toxicity, Category 1, H410

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. 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. Call a physician immediately. Pulmonary failure possible after aspiration of vomit.

4.2 Most important symptoms and effects, both acute and delayed

irritant effects, Drowsiness, somnolence

It generally applies for aliphatic hydrocarbons with 6 - 18 carbon atoms that they may cause pneumonia, in some cases also pulmonary oedema, upon direct inhalation, i.e. in conditions that can occur only in very special circumstances (nebulizations, spraying, inhalation of aerosols and similar). After absorption of very large quantities: narcosis.

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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 ambient temperatures.

Pay attention to flashback.

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

5.3 Advice for firefighters

Special protective equipment for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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.

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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 carefully 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.

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

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

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face 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.

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SECTION 8. Exposure controls/personal protection

8.1 Control parameters

Derived No Effect Level (DNEL)

Worker DNEL, longterm	Systemic effects	inhalation	2035 mg/m ³
Worker DNEL, longterm	Systemic effects	dermal	773 mg/kg Body weight
Consumer DNEL, longterm	Systemic effects	inhalation	608 mg/m ³
Consumer DNEL, longterm	Systemic effects	dermal	699 mg/kg Body weight
Consumer DNEL, longterm	Systemic effects	oral	699 mg/kg Body weight

Predicted No Effect Concentration (PNEC)

PNEC Not applicable

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

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Break through time: > 480 min

splash contact:

Glove material: polychloroprene

Glove thickness: 0,65 mm

Break through time: > 120 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 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 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

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Colour	colourless
Odour	benzine-like
Odour Threshold	No information available.
pH	neutral
Melting point	-107 °C
Boiling point/boiling range	99 °C at 1.013 hPa
Flash point	-12 °C Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1 %(V)
Upper explosion limit	6 %(V)
Vapour pressure	51 hPa at 20 °C
Relative vapour density	3,9
Density	0,69 g/cm ³ at 20 °C
Relative density	No information available.

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Water solubility	0,56 mg/l at 25 °C
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Partition coefficient: n-octanol/water	log Pow: 4,09 (calculated) Potential bioaccumulation
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Auto-ignition temperature	No information available.
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Decomposition temperature	No information available.
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Viscosity, dynamic	0,50 mPa.s at 20 °C
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Explosive properties	Not classified as explosive.
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Oxidizing properties	none
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9.2 Other data

Ignition temperature	410 °C
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Saturated vapour concentration	239 g/m ³ at 20 °C
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SECTION 10. Stability and reactivity

10.1 Reactivity

Vapours may form explosive mixture with air.

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:

Strong oxidizing agents

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10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

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: > 2.500 mg/kg

(IUCLID)

Acute inhalation toxicity

LC50 Rat: 37,5 mg/l; 4 h

(IUCLID)

Symptoms: mucosal irritations

Acute dermal toxicity

This information is not available.

Skin irritation

Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

Causes skin irritation.

Eye irritation

Possible damages:

slight irritation

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

Sensitisation

This information is not available.

Germ cell mutagenicity

Genotoxicity in vitro

Mutagenicity (mammal cell test):

Result: negative

(IUCLID)

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 drowsiness or dizziness.

Target Organs: Central nervous system

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary oedema and pneumonitis.

11.2 Further information

It generally applies for aliphatic hydrocarbons with 6 - 18 carbon atoms that they may cause pneumonia, in some cases also pulmonary oedema, upon direct inhalation, i.e. in conditions that can occur only in very special circumstances (nebulizations, spraying, inhalation of aerosols and similar). After absorption of very large quantities: narcosis.

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

LC0 Leuciscus idus (Golden orfe): 500 mg/l; 48 h

(External MSDS)

Toxicity to bacteria

EC0 Pseudomonas putida: 10.000 mg/l

(IUCLID)

12.2 Persistence and degradability

No information available.

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 4,09

(calculated)

Potential bioaccumulation

12.4 Mobility in soil

Distribution among environmental compartments

log Koc: 4,35

(HSDB) High mobility of the substance in soil is not expected (log koc ≥ 3).

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

Henry constant

305000 Pa·m³/mol

(HSDB) Distribution preferentially in air.

Additional ecological information

Biological effects:

Endangers drinking-water supplies if allowed to enter soil and/or waters in large quantities.

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 1262
14.2 Proper shipping name	OCTANES
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	yes
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 1262
14.2 Proper shipping name	OCTANES
14.3 Class	3
14.4 Packing group	II
14.5 Environmentally hazardous	yes
14.6 Special precautions for user	no

Sea transport (IMDG)

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

14.1 UN number UN 1262

14.2 Proper shipping name OCTANES

14.3 Class 3

14.4 Packing group II

14.5 Environmentally hazardous yes

14.6 Special precautions for yes

user

EmS F-E S-E

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

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 3

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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.

H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H336	May cause drowsiness or dizziness.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

Danger

Hazard statements

H225 Highly flammable liquid and vapour.
H304 May be fatal if swallowed and enters airways.
H315 Causes skin irritation.
H336 May cause drowsiness or dizziness.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

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P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P240 Ground/bond container and receiving equipment.

P273 Avoid release to the environment.

Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P313 Get medical advice/ attention.

Storage

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

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, Chemical production)

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

- 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
- SpERC* SpERC ESVOC 1
- ESVOC 1*

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SpERC SpERC ESVOC 3
ESVOC 3
SpERC SpERC ESVOC 4
ESVOC 4
SpERC SpERC ESVOC 38
ESVOC 38

2. Contributing scenarios: Operational conditions and risk management measures

2.1 Contributing scenario controlling environmental exposure for: ERC1, SpERC ESVOC 1

Amount used

Daily amount per site (Msafe) 3.000 t

Environment factors not influenced by risk management

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 0,003 %
Emission or Release Factor: Soil 0,01 %

Technical conditions and measures / Organizational measures

Air Use of air emission abatement equipments.
Effectiveness (of a measure): 90 %

Conditions and measures related to municipal sewage treatment plant

Flow rate of sewage treatment 10.000 m³/d
plant effluent
Percentage removed from waste 96,3 %
water
Sludge Treatment Sewage sludge should not be applied to natural soils. Sewage
sludge should be incinerated.

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2.2 Contributing scenario controlling environmental exposure for: ERC2, SpERC ESVOC 4

Amount used

Daily amount per site (Msafe) 900 t

Environment factors not influenced by risk management

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 0,002 %

Emission or Release Factor: Soil 0,01 %

Conditions and measures related to municipal sewage treatment plant

Flow rate of sewage treatment 2.000 m3/d
plant effluent

Percentage removed from waste 96,3 %
water

Sludge Treatment Sewage sludge should not be applied to natural soils. Sewage
sludge should be incinerated.

2.3 Contributing scenario controlling environmental exposure for: ERC4, SpERC ESVOC 3

Amount used

Daily amount per site (Msafe) 89 t

Environment factors not influenced by risk management

Dilution Factor (River) 10

Dilution Factor (Coastal Areas) 100

Other given operational conditions affecting environmental exposure

Number of emission days per year 300

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Emission or Release Factor: Air	0,1 %
Emission or Release Factor: Water	0,0001 %
Emission or Release Factor: Soil	0,001 %

Technical conditions and measures / Organizational measures

Air	Use of air emission abatement equipments. Effectiveness (of a measure): 90 %
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Conditions and measures related to municipal sewage treatment plant

Flow rate of sewage treatment plant effluent	2.000 m3/d
Percentage removed from waste water	96,3 %
Sludge Treatment	Sewage sludge should not be applied to natural soils. Sewage sludge should be incinerated.

2.4 Contributing scenario controlling environmental exposure for: ERC4, SpERC ESVOC 4

Amount used

Daily amount per site (Msafe)	260 t
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Environment factors not influenced by risk management

Dilution Factor (River)	10
Dilution Factor (Coastal Areas)	100

Other given operational conditions affecting environmental exposure

Number of emission days per year	20
Emission or Release Factor: Air	98 %
Emission or Release Factor: Water	0,007 %
Emission or Release Factor: Soil	0 %

Technical conditions and measures / Organizational measures

Air	Use of air emission abatement equipments. Effectiveness (of a measure): 90 %
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Conditions and measures related to municipal sewage treatment plant

Flow rate of sewage treatment 2.000 m³/d

plant effluent

Percentage removed from waste 96,3 %

water

Sludge Treatment Sewage sludge should not be applied to natural soils. Sewage sludge should be incinerated.

2.5 Contributing scenario controlling environmental exposure for: ERC2, ERC4, SpERC ESVOC 38

Amount used

Daily amount per site (Msafe) 900 kg

Environment factors not influenced by risk management

Dilution Factor (River) 10

Dilution Factor (Coastal Areas) 100

Other given operational conditions affecting environmental exposure

Number of emission days per year 20

Emission or Release Factor: Air 2,5 %

Emission or Release Factor: Water 2 %

Emission or Release Factor: Soil 0,1 %

Conditions and measures related to municipal sewage treatment plant

Flow rate of sewage treatment 2.000 m³/d

plant effluent

Percentage removed from waste 96,3 %

water

Sludge Treatment Sewage sludge should not be applied to natural soils. Sewage sludge should be incinerated.

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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) High volatile liquid

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)

Organisational measures to prevent /limit releases, dispersion and exposure

Covers daily exposures up to 8 hours.

Additional good practice advice beyond the REACH Chemical Safety Assessment

Additional good practice advice Wear suitable gloves tested to EN374.

3. Exposure estimation and reference to its source

Environment

CS	Use descriptor	Msafe	Compartment	RCR	Exposure Assessment Method
2.1	ERC1	3000 t/day	Fresh water sediment	1	Petrorisk
2.2	ERC2	900 t/day	Fresh water sediment	1	Petrorisk
2.3	SpERC ESVOC 3	89 t/day	Fresh water	1	Petrorisk
2.4	SpERC ESVOC 4	260 t/day	Fresh water sediment	1	Petrorisk
2.5	SpERC ESVOC 38	900 kg/day	Fresh water sediment	1	Petrorisk

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Workers

CS	Use descriptor	Exposure duration, route, effect	RCR	Exposure Assessment Method
2.6	PROC1	longterm, inhalative, systemic	< 0,001	ECETOC TRA
		longterm, dermal, systemic	< 0,001	ECETOC TRA
		longterm, combined, systemic	< 0,001	
2.6	PROC2	longterm, inhalative, systemic	0,117	ECETOC TRA
		longterm, dermal, systemic	0,002	ECETOC TRA
		longterm, combined, systemic	0,12	
2.6	PROC3	longterm, inhalative, systemic	0,233	ECETOC TRA
		longterm, dermal, systemic	< 0,001	ECETOC TRA
		longterm, combined, systemic	0,234	
2.6	PROC4	longterm, inhalative, systemic	0,233	ECETOC TRA
		longterm, dermal, systemic	0,009	ECETOC TRA
		longterm, combined, systemic	0,242	
2.6	PROC5	longterm, inhalative, systemic	0,583	ECETOC TRA
		longterm, dermal, systemic	0,018	ECETOC TRA
		longterm, combined, systemic	0,6	
2.6	PROC8a	longterm, inhalative, systemic	0,583	ECETOC TRA
		longterm, dermal, systemic	0,018	ECETOC TRA
		longterm, combined, systemic	0,6	
2.6	PROC8b	longterm, inhalative, systemic	0,35	ECETOC TRA
		longterm, dermal, systemic	0,009	ECETOC TRA
		longterm, combined, systemic	0,242	
2.6	PROC9	longterm, inhalative, systemic	0,466	ECETOC TRA
		longterm, dermal, systemic	0,009	ECETOC TRA
		longterm, combined, systemic	0,475	
2.6	PROC10	longterm, inhalative, systemic	0,583	ECETOC TRA
		longterm, dermal, systemic	0,035	ECETOC TRA
		longterm, combined, systemic	0,618	
2.6	PROC15	longterm, inhalative, systemic	0,117	ECETOC TRA
		longterm, dermal, systemic	< 0,001	ECETOC TRA
		longterm, combined, systemic	0,117	

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

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No. 104727

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

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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, Chemical production)

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 8a Wide dispersive indoor use of processing aids in open systems

ERC 8d Wide dispersive outdoor use of processing aids in open systems

SpERC SpERC ESVOC 6

ESVOC 6

SpERC SpERC ESVOC 39

ESVOC 39

2. Contributing scenarios: Operational conditions and risk management measures

2.1 Contributing scenario controlling environmental exposure for: ERC8a, ERC8d, SpERC ESVOC 6

Amount used

Daily amount per site (Msafe) 980 kg

Environment factors not influenced by risk management

Dilution Factor (River) 10

Dilution Factor (Coastal Areas) 100

Other given operational conditions affecting environmental exposure

Number of emission days per year 365

Emission or Release Factor: Air 98 %

Emission or Release Factor: Water 1 %

Emission or Release Factor: Soil 1 %

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Technical conditions and measures / Organizational measures

Air	Use of air emission abatement equipments.
	Effectiveness (of a measure): 90 %

Conditions and measures related to municipal sewage treatment plant

Flow rate of sewage treatment plant effluent	2.000 m ³ /d
Percentage removed from waste water	96,3 %
Sludge Treatment	Sewage sludge should not be applied to natural soils. Sewage sludge should be incinerated.

2.2 Contributing scenario controlling environmental exposure for: ERC8a, SpERC ESVOC 39

Amount used

Daily amount per site (Msafe)	13 kg
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Environment factors not influenced by risk management

Dilution Factor (River)	10
Dilution Factor (Coastal Areas)	100

Other given operational conditions affecting environmental exposure

Number of emission days per year	365
Emission or Release Factor: Air	50 %
Emission or Release Factor: Water	50 %
Emission or Release Factor: Soil	0 %

Conditions and measures related to municipal sewage treatment plant

Flow rate of sewage treatment plant effluent	2.000 m ³ /d
Percentage removed from waste water	96,3 %
Sludge Treatment	Sewage sludge should not be applied to natural soils. Sewage

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sludge should be incinerated.

2.3 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)	High volatile liquid

Frequency and duration of use

Frequency of use	8 hours/day
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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.

Additional good practice advice beyond the REACH Chemical Safety Assessment

Additional good practice advice	Wear suitable gloves tested to EN374.
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3. Exposure estimation and reference to its source

Environment

CS	Use descriptor	Msafe	Compartment	RCR	Exposure Assessment Method
2.1	SpERC ESVOC 6	980 kg/day	Fresh water sediment	1	Petrorisk
2.2	SpERC ESVOC 39	13 kg/day	Fresh water	1	Petrorisk

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Workers

CS	Use descriptor	Exposure duration, route, effect	RCR	Exposure Assessment Method
2.3	PROC15	longterm, inhalative, systemic	0,117	ECETOC TRA
		longterm, dermal, systemic	< 0,001	ECETOC TRA
		longterm, combined, systemic	0,117	

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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).

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