

**SAFETY DATA SHEET**

according to Regulation (EC) No. 1907/2006

Revision Date 22.08.2018

Version 1.4

**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 A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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  
For additional information on uses please refer to the Merck Chemicals portal ([www.merckgroup.com](http://www.merckgroup.com)).

**1.3 Details of the supplier of the safety data sheet**

Company Merck KGaA \* 64271 Darmstadt \* Germany \* Phone:+49 6151 72-0  
Responsible Department EHS Manager \*+61 (3) 8727 6300 \* Monday through Friday, 8:00am to 5:00pm (EST)  
Regional representation Merck Pty. Limited  
ABN 80 001 239 818  
Ground Floor, Building 1  
885 Mountain Highway  
Bayswater VIC 3153 Australia  
[www.merckmillipore.com](http://www.merckmillipore.com)

**1.4 Emergency telephone number** +61 (3) 8727 6300  
After hours: CHEMCALL +64 4 917 9888

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Poisons Information Centre: 13 1126

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## SECTION 2. Hazards identification

### 2.1 Classification of the substance or mixture

**Classification (REGULATION (EC) No 1272/2008)**

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*

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## 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.

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.

CAS-No. 540-84-1

## 2.3 Other hazards

None known.

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## SECTION 3. Composition/information on ingredients

### 3.1 Substance

Formula	$\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_3$	$\text{C}_8\text{H}_{18}$ (Hill)
EC-No.	208-759-1	

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Molar mass 114.23 g/mol

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

*Chemical name (Concentration)*

CAS-No. Registration number Classification

isooctane (<= 100 % )

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

540-84-1 \*)

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

\*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

### 3.2 Mixture

Not applicable

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## 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

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The Safety Data Sheets for catalogue items are available at [www.merckgroup.com](http://www.merckgroup.com)

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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.

#### 4.3 Indication of any immediate medical attention and special treatment needed

No information available.

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## SECTION 5. Firefighting measures

### 5.1 Extinguishing media

*Suitable extinguishing media*

Carbon dioxide (CO<sub>2</sub>), 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.

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## SECTION 6. Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

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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 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.

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## 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*

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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)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

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## SECTION 8. Exposure controls/personal protection

### 8.1 Control parameters

*isooctane (540-84-1)*

AU OEL	Short Term Exposure	375 ppm
	Limit (STEL):	1,750 mg/m <sup>3</sup>
	Time Weighted Average	300 ppm
	(TWA):	1,400 mg/m <sup>3</sup>

### 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

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Glove thickness: 0.40 mm  
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](http://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.

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## **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 <sup>3</sup> at 20 °C
Relative density	No information available.

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Water solubility 0.56 mg/l  
at 25 °C

Partition coefficient: n-  
octanol/water log Pow: 4.09  
(calculated)  
Potential bioaccumulation

Auto-ignition temperature No information available.

Decomposition temperature No information available.

Viscosity, dynamic 0.50 mPa.s  
at 20 °C

Explosive properties Not classified as explosive.

Oxidizing properties none

## 9.2 Other data

Ignition temperature 410 °C

Saturated vapour concentration 239 g/m<sup>3</sup>  
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

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## 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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## *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  $\geq 3$ ).

### 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·m<sup>3</sup>/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*

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## 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

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14.6 Special precautions for user no

## Sea transport (IMDG)

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  
EmS F-E S-E

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code  
Not relevant

## Other regulations

Hazchem Code 3YE

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## SECTION 15. Regulatory information

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

#### *National legislation*

Storage class 3  
Standard for the Uniform S5  
Scheduling of Medicines and Poisons - Poisons Schedule  
Number:

### 15.2 Chemical safety assessment

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

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## 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

P210 Keep away from heat/sparks/open flames/hot surfaces. No smoking.  
P240 Ground/bond container and receiving equipment.



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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](http://www.wikipedia.org).

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*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.*