

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 15.06.2018

Version 10.16

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

Catalogue No. 107177

Product name n-Pentane for analysis EMSURE®

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. 109-66-0

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).

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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Flammable liquid, Category 2, H225

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

Aspiration hazard, Category 1, H304

Chronic aquatic toxicity, Category 2, H411

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.

H336 May cause drowsiness or dizziness.

H411 Toxic to aquatic life with long lasting effects.

EUH066 Repeated exposure may cause skin dryness or cracking.

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.

Storage

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

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Some organic substances may be marketed either in a specific isomeric form or as a mixture of several isomers. In this case the supplier must state on the label whether the substance is a specific isomer or a mixture of isomers.

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.

Some organic substances may be marketed either in a specific isomeric form or as a mixture of several isomers. In this case the supplier must state on the label whether the substance is a specific isomer or a mixture of isomers.

Index-No. 601-006-00-1

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula	CH ₃ (CH ₂) ₃ CH ₃	C ₅ H ₁₂ (Hill)
Index-No.	601-006-00-1	
EC-No.	203-692-4	
Molar mass	72,15 g/mol	

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

Chemical name (Concentration)

CAS-No. Registration number Classification

pentane (<= 100 %)

109-66-0 *)

Flammable liquid, Category 2, H225

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

Aspiration hazard, Category 1, H304

Chronic aquatic toxicity, Category 2, H411

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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.

Do not give milk. No digestible oils.

Subsequently administer: activated charcoal (20 - 40 g in 10% slurry).

4.2 Most important symptoms and effects, both acute and delayed

irritant effects, respiratory arrest, narcosis, Convulsions

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somnolence, Drowsiness, 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.

Pay attention to flashback.

Vapours are heavier than air and may spread along floors.

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

Forms explosive mixtures with air at ambient temperatures.

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

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)

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

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:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 10 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.

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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 AX (EN 371)

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
Colour	colourless
Odour	benzine-like
Odour Threshold	No information available.
pH	No information available.
Melting point	ca. -130 °C

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Boiling point/boiling range	ca. 36 °C at 1.013 hPa
Flash point	-48 °C Method: c.c. (refers to pure substance)
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1,4 %(V)
Upper explosion limit	8 %(V)
Vapour pressure	ca.570 hPa at 20 °C
Relative vapour density	2,49 (refers to pure substance)
Density	ca.0,63 g/cm ³ at 20 °C
Relative density	No information available.
Water solubility	ca.0,4 g/l at 16 °C
Partition coefficient: n-octanol/water	log Pow: 3,39 (calculated) (Lit.) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.

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Decomposition temperature No information available.
Viscosity, dynamic No information available.
Explosive properties Not classified as explosive.
Oxidizing properties none

9.2 Other data

Ignition temperature 285 °C

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:

Nitric acid, Strong oxidizing agents, halogens

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

rubber, 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: > 2.000 mg/kg

OECD Test Guideline 401

Acute inhalation toxicity

LC50 Rat: > 20 mg/l; 4 h ; vapour

(ECHA)

Symptoms: mucosal irritations, narcosis, Inhalation may lead to the formation of oedemas in the respiratory tract.

Acute dermal toxicity

This information is not available.

Skin irritation

Rabbit

Result: No skin irritation

OECD Test Guideline 404

Repeated exposure may cause skin dryness or cracking.

Eye irritation

Rabbit

Result: No eye irritation

OECD Test Guideline 405

Sensitisation

Buehler Test Guinea pig

Result: negative

Method: OECD Test Guideline 406

Germ cell mutagenicity

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Genotoxicity in vivo

In vivo micronucleus test

Rat

male and female

inhalation (vapour)

Bone marrow

Result: negative

Method: OECD Test Guideline 474

Genotoxicity in vitro

Mutagenicity (mammal cell test): chromosome aberration.

Result: negative

Method: OECD Test Guideline 473

Ames test

Salmonella typhimurium

Result: negative

Method: OECD Test Guideline 471

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.

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11.2 Further information

After uptake:

Convulsions, respiratory arrest

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

static test LC50 *Oncorhynchus mykiss* (rainbow trout): 4,26 mg/l; 96 h

Analytical monitoring: yes

OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates

static test EC50 *Daphnia magna* (Water flea): 2,7 mg/l; 48 h

Analytical monitoring: yes

(ECHA)

Toxicity to algae

static test ErC50 *Selenastrum capricornutum* (green algae): 10,7 mg/l; 72 h

Analytical monitoring: yes

OECD Test Guideline 201

static test NOEC *Selenastrum capricornutum* (green algae): 7,51 mg/l; 72 h

Analytical monitoring: yes

OECD Test Guideline 201

12.2 Persistence and degradability

Biodegradability

87 %; 28 d; aerobic

OECD Test Guideline 301F

Readily biodegradable

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 3,39

(calculated)

(Lit.) Bioaccumulation is not expected.

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12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6 Other adverse effects

Surface tension

ca. 15,49 mN/m

at 25 °C

Additional ecological information

Biological effects:

Endangers drinking-water supplies if allowed to enter soil or water.

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.

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SECTION 14. Transport information

Land transport (ADR/RID)

14.1 UN number	UN 1265
14.2 Proper shipping name	PENTANES
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 1265
14.2 Proper shipping name	PENTANES
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 n-Pentane for analysis EMSURE®

14.1 UN number UN 1265

14.2 Proper shipping name PENTANES

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-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 ENVIRONMENTAL HAZARDS

E2

Quantity 1: 200 t

Quantity 2: 500 t

SEVESO III

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.

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

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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

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.
H336 May cause drowsiness or dizziness.
H411 Toxic to aquatic life with long lasting effects.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



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Signal word

Danger

Hazard statements

H225 Highly flammable liquid and vapour.

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H336 May cause drowsiness or dizziness.

H411 Toxic to aquatic life with long lasting effects.

EUH066 Repeated exposure may cause skin dryness or cracking.

Precautionary statements

Prevention

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.

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.