

SAFETY DATA SHEET

according to Regulation (EC) No 1907/2006 (REACH) as amended

Isooctane

| | | | |
|---------------|-----------------|---------|-----|
| Creation date | 13th June 2016 | Version | 6.0 |
| Revision date | 17th March 2023 | | |

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

- 1.1. Product identifier**
 Isooctane
 Substance / mixture: substance
 Chemical name: 2,2,4-trimethylpentane
 CAS number: 540-84-1
 Index number: 601-009-00-8
 EC (EINECS) number: 208-759-1
 Registration number: 01-2119457965-22-XXXX
 Other substance name: Isobutyltrimethylmethane, 2,2,4 - Trimethylpentane
- 1.2. Relevant identified uses of the substance or mixture and uses advised against**
Substance's intended use
 Chemical production, analytical chemistry, laboratory synthesis, industrial applications.
Substance uses advised against
 The product should not be used in ways other than those referred in Section 1.
- 1.3. Details of the supplier of the safety data sheet**
Supplier
 Name or trade name: Ing. Petr Švec - PENTA s.r.o.
 Address: Radiová 1122/1, Praha 10, 102 00
 Czech Republic
 Identification number (CRN): 02096013
 VAT Reg No: CZ02096013
 Phone: +420 226 060 681
 E-mail: info@pentachemicals.eu
 Web address: www.pentachemicals.eu
- Competent person responsible for the safety data sheet**
 Name: Ing. Petr Švec - PENTA s.r.o.
 E-mail: info@pentachemicals.eu
- 1.4. Emergency telephone number**
 European emergency number: 112

SECTION 2: Hazards identification

- 2.1. Classification of the substance or mixture**
Classification of the substance in accordance with Regulation (EC) No 1272/2008
 The substance is classified as dangerous.

Flam. Liq. 2, H225
 Asp. Tox. 1, H304
 Skin Irrit. 2, H315
 STOT SE 3, H336
 Aquatic Chronic 1, H410

Full text of all classifications and hazard statements is given in the section 16.

Most serious adverse physico-chemical effects

Highly flammable liquid and vapour.

Most serious adverse effects on human health and the environment

May be fatal if swallowed and enters airways. Causes skin irritation. May cause drowsiness or dizziness. Very toxic to aquatic life with long lasting effects.

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2.2. Label elements

Hazard pictogram



Signal word

Danger

Dangerous substance

2,2,4-trimethylpentane
(Index: 601-009-00-8; CAS: 540-84-1)

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

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P243 Take action to prevent static discharges.
P273 Avoid release to the environment.
P301+P310 IF SWALLOWED: Immediately call a doctor.
P331 Do NOT induce vomiting.

Supplemental information

Restricted to professional users.

2.3. Other hazards

The substance does not have endocrine disrupting properties in accordance with the criteria set out in Commission Delegated Regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605. Substance does not meet the criteria for PBT or vPvB in accordance with Annex XIII of Regulation (EC) No. 1907/2006 (REACH) as amended.

SECTION 3: Composition/information on ingredients

3.1. Substances

Chemical characterization

The substance specified below.

| Identification numbers | Substance name | Content in % weight | Classification according to Regulation (EC) No 1272/2008 | Note |
|--|---|---------------------|---|------|
| Index: 601-009-00-8 CAS: 540-84-1 EC: 208-759-1 Registration number: 01-2119457965-22-XXXX | substance main component 2,2,4-trimethylpentane | >99 | Flam. Liq. 2, H225 Asp. Tox. 1, H304 Skin Irrit. 2, H315 STOT SE 3, H336 Aquatic Acute 1, H400 (M=1) Aquatic Chronic 1, H410 (M=1) | 1 |

Notes

- 1 Note C: 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.

Full text of all classifications and hazard statements is given in the section 16.

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SECTION 4: First aid measures

4.1. Description of first aid measures

Do not perform artificial respiration without self-protection (e.g. a mask). Take care of your own safety. If any health problems are manifested or if in doubt, inform a doctor and show him information from this safety data sheet. If unconscious, put the person in the stabilized (recovery) position on his side with his head slightly bent backwards and make sure that airways are free; never induce vomiting. If the person vomits by himself, make sure that the vomit is not inhaled. In life threatening conditions first of all provide resuscitation of the affected person and ensure medical assistance. Respiratory arrest - provide artificial respiration immediately. Cardiac arrest - provide indirect cardiac massage immediately.

If inhaled

Terminate the exposure immediately; move the affected person to fresh air. Take care of your own safety, do not let the affected person walk! Beware of the contaminated clothes. Depending on the situation, call the medical rescue service and ensure medical treatment considering the frequent need of further observation for at least 24 hours.

If on skin

Remove contaminated clothes. Wash the affected area with plenty of water, lukewarm if possible. Soap, soap solution or shampoo should be used if there is no skin injury. Provide medical treatment if skin irritation persists. Rinse skin with water or shower.

If in eyes

Rinse eyes immediately with a flow of running water, open the eyelids (also using force if needed); remove contact lenses immediately if worn by the affected person. Rinsing should continue at least for 10 minutes. Provide medical treatment, specialized if possible.

If swallowed

If the affected person vomits, make sure to prevent inhalation of the vomit (as there is a danger of lung damage after inhalation of these liquids in the airways also in infinitesimal amount). Ensure medical treatment considering the frequent need of further observation for at least 24 hours. Bring an original container with the label and the Safety Data Sheet of the given substance as appropriate.

4.2. Most important symptoms and effects, both acute and delayed

If inhaled

Cough, headache. May cause drowsiness or dizziness.

If on skin

Causes skin irritation.

If in eyes

Not expected.

If swallowed

Irritation, nausea.

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

Symptomatic treatment.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

Alcohol-resistant foam, carbon dioxide, powder, water spray jet, water mist.

Unsuitable extinguishing media

Water - full jet.

5.2. Special hazards arising from the substance or mixture

In the event of fire, carbon monoxide, carbon dioxide and other toxic gases may arise. Inhalation of hazardous degradation (pyrolysis) products may cause serious health damage.

5.3. Advice for firefighters

Self-Contained Breathing Apparatus (SCBA) with a chemical protection suit only where personal (close) contact is likely. Use a self-contained breathing apparatus and full-body protective clothing. Closed containers with the product near the fire should be cooled with water. Do not allow run-off of contaminated fire extinguishing material to enter drains or surface and ground water.

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SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Provide sufficient ventilation. The substance is flammable. Remove all ignition sources. Use personal protective equipment for work. Follow the instructions in the Sections 7 and 8. Do not inhale mist/vapours/spray. Prevent contact with skin and eyes.

6.2. Environmental precautions

Prevent contamination of the soil and entering surface or ground water.

6.3. Methods and material for containment and cleaning up

Spilled product should be covered with suitable (non-flammable) absorbing material (sand, diatomaceous earth, earth and other suitable absorption materials); to be contained in well closed containers and removed as per the Section 13. In the event of leakage of the substantial amount of the product, inform fire brigade and other competent bodies. After removal of the product, wash the contaminated site with plenty of water. Do not use solvents.

6.4. Reference to other sections

See the Section 7, 8 and 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Prevent formation of gases and vapours in flammable or explosive concentrations. The product should be used only in the areas where it is not in contact with open fire and other ignition sources. Use non-sparking tools. Use of antistatic clothes and footwear is recommended. Do not inhale mist/vapours/spray. Prevent contact with skin and eyes. No smoking. Wash hands and exposed parts of the body thoroughly after handling. Use only outdoors or in a well-ventilated area. Use personal protective equipment as per Section 8. Observe valid legal regulations on safety and health protection. Ground and bond container and receiving equipment. Use explosion-proof electrical/ventilating/lighting equipment. Take action to prevent static discharges. Avoid release to the environment.

7.2. Conditions for safe storage, including any incompatibilities

Store in tightly closed containers in cold, dry and well ventilated areas designated for this purpose. Do not expose to sunlight. Store locked up. Keep container tightly closed. Keep cool.

Storage class 3A - Flammable liquids (flash point below 55 °C)

The specific requirements or rules relating to the substance/mixture

Solvent vapours are heavier than air and accumulate especially near the floor where they may form an explosive mixture with the air.

7.3. Specific end use(s)

not available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

8.2. Exposure controls

Take off contaminated clothing and wash before reuse. Follow the usual measures intended for health protection at work and especially for good ventilation. This can be achieved only by local suction or efficient general ventilation. If exposure limits cannot be observed in this mode, suitable protection of airways must be used. Do not eat, drink and smoke during work. Wash your hands thoroughly with water and soap after work and before breaks for a meal and rest.

Eye/face protection

Protective goggles.

Skin protection

Hand protection: Protective gloves resistant to the product (nitrile rubber). When choosing appropriate thickness, material and permeability of the gloves, observe recommendations of their particular manufacturer. Observe other recommendations of the manufacturer. Other protection: protective workwear. Contaminated skin should be washed thoroughly.

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Respiratory protection

Mask with a filter against organic vapours in a poorly ventilated environment.

Thermal hazard

Not available.

Environmental exposure controls

Observe usual measures for protection of the environment, see Section 6.2. Collect spillage.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

| | |
|--|-----------------------------|
| Physical state | liquid |
| Colour | colourless |
| Odour | characteristic |
| Melting point/freezing point | -107 °C |
| Boiling point or initial boiling point and boiling range | 99 °C |
| Flammability | data not available |
| Lower and upper explosion limit | |
| bottom | 1 % |
| upper | 6 % |
| Flash point | -12 °C |
| Auto-ignition temperature | data not available |
| Decomposition temperature | data not available |
| pH | data not available |
| Kinematic viscosity | data not available |
| Solubility in water | 0,56 |
| Partition coefficient n-octanol/water (log value) | 4,09 |
| Vapour pressure | 51 kPa at 20 °C |
| Density and/or relative density | |
| Density | data not available |
| Relative density | 0,69 g/cm ³ 20°C |
| Relative vapour density | data not available |
| Particle characteristics | data not available |

9.2. Other information

not available

SECTION 10: Stability and reactivity

10.1. Reactivity

The substance is highly flammable.

10.2. Chemical stability

The product is stable under normal conditions.

10.3. Possibility of hazardous reactions

Unknown.

10.4. Conditions to avoid

The product is stable and no degradation occurs under normal use. Protect against flames, sparks, overheating and against frost.

10.5. Incompatible materials

Protect against strong acids, bases and oxidizing agents.

10.6. Hazardous decomposition products

Not developed under normal uses. Dangerous outcomes such as carbon monoxide and carbon dioxide are formed at high temperature and in fire.

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SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

No toxicological data is available for the substance.

Acute toxicity

Based on available data the classification criteria are not met.

Isooctane

| Route of exposure | Parameter | Value | Exposure time | Species | Sex |
|-----------------------|------------------|-------------|---------------|---------|-----|
| | LD ₅₀ | >2500 mg/kg | | Rat | |
| Inhalation (aerosols) | LC ₅₀ | >2500 mg/kg | | Rat | |
| Inhalation (vapor) | LC ₅₀ | >24.2 mg/kg | 4 hours | Rat | |

Skin corrosion/irritation

Causes skin irritation.

Serious eye damage/irritation

Based on available data the classification criteria are not met.

Respiratory or skin sensitisation

Based on available data the classification criteria are not met.

Germ cell mutagenicity**Carcinogenicity**

Based on available data the classification criteria are not met.

Reproductive toxicity

Based on available data the classification criteria are not met.

Toxicity for specific target organ - single exposure

May cause drowsiness or dizziness.

Toxicity for specific target organ - repeated exposure

Based on available data the classification criteria are not met.

Aspiration hazard

May be fatal if swallowed and enters airways.

11.2. Information on other hazards

The substance does not have endocrine disrupting properties in accordance with the criteria set out in Commission Delegated Regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605.

SECTION 12: Ecological information

12.1. Toxicity

Acute toxicity

Very toxic to aquatic life with long lasting effects.

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| Parameter | Value | Exposure time | Species | Environment |
|------------------|----------|---------------|-----------------------|-------------|
| LC ₅₀ | 500 mg/l | 96 hours | Fish (Leuciscus idus) | |

12.2. Persistence and degradability

not available

12.3. Bioaccumulative potential

Not available.

12.4. Mobility in soil

Not available.

12.5. Results of PBT and vPvB assessment

Product does not contain any substance meeting the criteria for PBT or vPvB in accordance with the Annex XIII of Regulation (EC) No 1907/2006 (REACH) as amended.

12.6. Endocrine disrupting properties

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This substance does not have endocrine disrupting properties with respect to non-target organisms as it does not meet the criteria set out in section B of Regulation (EU) No 2017/2100.

12.7. Other adverse effects

Not available.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Hazard of environmental contamination; dispose of the waste in accordance with the local and/or national regulations. Proceed in accordance with valid regulations on waste disposal. Any unused product and contaminated packaging should be put in labelled containers for waste collection and submitted for disposal to a person authorised for waste removal (a specialized company) that is entitled for such activity. Do not empty unused product in drainage systems. The product must not be disposed of with municipal waste. Empty containers may be used at waste incinerators to produce energy or deposited in a dump with appropriate classification. Perfectly cleaned containers can be submitted for recycling.

Waste management legislation

Directive 2008/98/EC of the European Parliament and of the Council of 19 November 2008 on waste, as amended. Decision 2000/532/EC establishing a list of wastes, as amended.

SECTION 14: Transport information

14.1. UN number or ID number

UN 1262

14.2. UN proper shipping name

OCTANES

14.3. Transport hazard class(es)

3 Flammable liquids

14.4. Packing group

II - substances presenting medium danger

14.5. Environmental hazards

not relevant

14.6. Special precautions for user

Reference in the Sections 4 to 8.

14.7. Maritime transport in bulk according to IMO instruments

not relevant

Additional information

Hazard identification No.

33

UN number

1262

Classification code

F1

Safety signs

3+hazardous for the environment



Air transport - ICAO/IATA

Packaging instructions passenger

353

Cargo packaging instructions

364

Marine transport - IMDG

EmS (emergency plan)

F-E, S-E

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SECTION 15: Regulatory information

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

Regulation (EC) No. 1907/2006 of the European Parliament and of the Council of 18th December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing the European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No. 793/93 and Commission Regulation (EC) No. 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC, as amended. REGULATION (EC) No. 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL as amended. Commission Regulation (EU) 2020/878 of 18 June 2020 amending Annex II to Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH).

15.2. Chemical safety assessment

No chemical safety assessment has been performed for this substance.

No chemical safety assessment has been performed for this substance.

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No chemical safety assessment has been performed for this substance.

SECTION 16: Other information

A list of standard risk phrases used in the safety data sheet

| | |
|------|---|
| 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. |

Guidelines for safe handling used in the safety data sheet

| | |
|-----------|---|
| P210 | Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. |
| P243 | Take action to prevent static discharges. |
| P273 | Avoid release to the environment. |
| P301+P310 | IF SWALLOWED: Immediately call a doctor. |
| P331 | Do NOT induce vomiting. |

Other important information about human health protection

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The product must not be - unless specifically approved by the manufacturer/importer - used for purposes other than as per the Section 1. The user is responsible for adherence to all related health protection regulations.

Key to abbreviations and acronyms used in the safety data sheet

| | |
|---------------------|---|
| ADR | European agreement concerning the international carriage of dangerous goods by road |
| BCF | Bioconcentration Factor |
| CAS | Chemical Abstracts Service |
| CLP | Regulation (EC) No 1272/2008 on classification, labelling and packaging of substance and mixtures |
| EC | Identification code for each substance listed in EINECS |
| EINECS | European Inventory of Existing Commercial Chemical Substances |
| EmS | Emergency plan |
| EU | European Union |
| EuPCS | European Product Categorisation System |
| IATA | International Air Transport Association |
| IBC | International Code For The Construction And Equipment of Ships Carrying Dangerous Chemicals |
| ICAO | International Civil Aviation Organization |
| IMDG | International Maritime Dangerous Goods |
| IMO | International Maritime Organization |
| INCI | International Nomenclature of Cosmetic Ingredients |
| ISO | International Organization for Standardization |
| IUPAC | International Union of Pure and Applied Chemistry |
| LC ₅₀ | Lethal concentration of a substance in which it can be expected death of 50% of the population |
| LD ₅₀ | Lethal dose of a substance in which it can be expected death of 50% of the population |
| log K _{ow} | Octanol-water partition coefficient |
| OEL | Occupational Exposure Limits |
| PBT | Persistent, Bioaccumulative and Toxic |
| ppm | Parts per million |
| REACH | Registration, Evaluation, Authorisation and Restriction of Chemicals |
| RID | Agreement on the transport of dangerous goods by rail |
| UN | Four-figure identification number of the substance or article taken from the UN Model Regulations |
| UVCB | Substances of unknown or variable composition, complex reaction products or biological materials |
| VOC | Volatile organic compounds |
| vPvB | Very Persistent and very Bioaccumulative |
| Aquatic Acute | Hazardous to the aquatic environment |
| Aquatic Chronic | Hazardous to the aquatic environment (chronic) |
| Asp. Tox. | Aspiration hazard |
| Flam. Liq. | Flammable liquid |
| Skin Irrit. | Skin irritation |
| STOT SE | Specific target organ toxicity - single exposure |

Training guidelines

Inform the personnel about the recommended ways of use, mandatory protective equipment, first aid and prohibited ways of handling the product.

Recommended restrictions of use

not available

Information about data sources used to compile the Safety Data Sheet

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REGULATION (EC) No. 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL as amended. Data from the manufacturer of the substance / mixture, if available - information from registration dossiers.

The changes (which information has been added, deleted or modified)

The version 6.0 replaces the SDS version from 22 February 2023. Changes were made in sections 1, 2, 12, 13, 15 and 16.

More information

Classification procedure - calculation method.

Statement

The safety data sheet provides information aimed at ensuring safety and health protection at work and environmental protection. The provided information corresponds to the current status of knowledge and experience and complies with valid legal regulations. The information should not be understood as guaranteeing the suitability and usability of the product for a particular application.