

SAFETY DATA SHEET

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

Isooctane

Creation date	11. September 2019	Version	1.0
Revision date			

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

- 1.1. Product identifier**
- | | |
|----------------------|--|
| Substance / mixture | Isooctane |
| Chemical name | substance |
| CAS number | 2,2,4-trimethylpentane |
| Index number | 540-84-1 |
| EC (EINECS) number | 601-009-00-8 |
| Registration number | 208-759-1 |
| Other substance name | 01-2119457965-22-XXXX |
| | 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. |
| Chemical safety report | |
- 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**
- National Health Service (NHS) 111
National poisoning information centre Scotland, NHS 24: 111

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 Acute 1, H400
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. Very toxic to aquatic life with long lasting effects.

SAFETY DATA SHEET

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

Isooctane

Creation date 11. September 2019
Revision date Version 1.0

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 POISON CENTER.
P331 Do NOT induce vomiting.

Supplemental information

Only for professional users.

2.3. Other hazards

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 Aquatic Chronic 1, H410	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.

SAFETY DATA SHEET

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

Isooctane

Creation date	11. September 2019	Version	1.0
Revision date			

SECTION 4: First aid measures

4.1. Description of first aid measures

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

Take care of your own safety, do not let the affected person walk! Terminate the exposure immediately; move the affected person to fresh air. 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/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.

SAFETY DATA SHEET

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

Isooctane

Creation date	11. September 2019	Version	1.0
Revision date			

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 aerosols. Prevent contact with skin and eyes.

6.2. Environmental precautions

Do not allow to enter drains. 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 aerosols. Prevent contact with skin and eyes. No smoking. Use only non-sparking tools. 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 precautionary measures against static discharge. 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

none

8.2. Exposure controls

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. 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.

SAFETY DATA SHEET

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

Isooctane

Creation date	11. September 2019	Version	1.0
Revision date			

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

Appearance	
Physical state	liquid at 20°C
color	colourless
Odour	similar to gasoline
Odour threshold	data not available
pH	data not available
Melting point/freezing point	-107 °C
Initial boiling point and boiling range	99 °C
Flash point	-12 °C
Evaporation rate	data not available
Flammability (solid, gas)	data not available
Upper/lower flammability or explosive limits	
flammability limits	data not available
explosive limits	
bottom	1 %
upper	6 %
Vapour pressure	51 kPa at 20 °C
Vapour density	data not available
Relative density	0.7
Solubility(ies)	
solubility in water	0,56
solubility in fats	data not available
Partition coefficient: n-octanol/water	4.09
Auto-ignition temperature	data not available
Decomposition temperature	data not available
Viscosity	data not available
Explosive properties	data not available
Oxidising properties	It is not oxidising.

9.2. Other information

Density	data not available
ignition temperature	data 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.

SAFETY DATA SHEET

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

Isooctane

Creation date 11. September 2019
Revision date Version 1.0

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.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

No toxicological data is available for the substance.

Acute toxicity

Isooctane

Route of exposure	Parameter	Value	Time of exposure	Species	Sex
	LD50	>2500 mg/kg		Rat	
Inhalation (aerosols)	LC50	>2500 mg/kg		Rat	
Inhalation (vapor)	LC50	>24.2 mg/kg	4 hour	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

Based on available data the classification criteria are not met.

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.

SECTION 12: Ecological information

12.1. Toxicity

SAFETY DATA SHEET

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

Isooctane

Creation date 11. September 2019
Revision date Version 1.0

Acute toxicity

Very toxic to aquatic life with long lasting effects.

Isooctane

Parameter	Value	Time of exposure	Species	Environment
LC50	500 mg/l	96 hour	Fishes (Leuciscus idus)	

12.2. Persistence and degradability

Data 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. 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

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 available

14.6. Special precautions for user

Reference in the Sections 4 to 8.

14.7. Transport in bulk according to Annex II of Marpol and the IBC Code

not available

SAFETY DATA SHEET

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

Isooctane

Creation date 11. September 2019
Revision date Version 1.0

Additional information

Hazard identification No. **33** (Kemler Code)
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
Marine Pollutant No

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 of 16th December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No. 1907/2006, as amended.

15.2. Chemical safety assessment

not available

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.
P273 Avoid release to the environment.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER.
P331 Do NOT induce vomiting.
P243 Take action to prevent static discharges.

Other important information about human health protection

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

SAFETY DATA SHEET

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

Isooctane

Creation date	11. September 2019	Version	1.0
Revision date			

CAS	Chemical Abstracts Service
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substance and mixtures
DNEL	Derived no-effect level
EC	Identification code for each substance listed in EINECS
EC50	Concentration of a substance when it is affected 50% of the population
EINECS	European Inventory of Existing Commercial Chemical Substances
EmS	Emergency plan
EU	European Union
IATA	International Air Transport Association
IBC	International Code For The Construction And Equipment of Ships Carrying Dangerous Chemicals
IC50	Concentration causing 50% blockade
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods
INCI	International Nomenclature of Cosmetic Ingredients
ISO	International Organization for Standardization
IUPAC	International Union of Pure and Applied Chemistry
LC50	Lethal concentration of a substance in which it can be expected death of 50% of the population
LD50	Lethal dose of a substance in which it can be expected death of 50% of the population
LOAEC	Lowest observed adverse effect concentration
LOAEL	Lowest observed adverse effect level
log Kow	Octanol-water partition coefficient
MARPOL	International Convention for the Prevention of Pollution From Ships
NOAEC	No observed adverse effect concentration
NOAEL	No observed adverse effect level
NOEC	No observed effect concentration
NOEL	No observed effect level
OEL	Occupational Exposure Limits
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted no-effect concentration
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
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

SAFETY DATA SHEET

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

Isooctane

Creation date	11. September 2019	Version	1.0
Revision date			

Information about data sources used to compile the Safety Data Sheet

REGULATION (EC) No. 1907/2006 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL (REACH) as amended.
REGULATION (EC) No. 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL as amended. First aid principles after the exposure to the chemicals (Zásady pro poskytování první pomoci při expozici chemickým látkám, doc. MUDr. Daniela Pelclová, CSc., MUDr. Alexandr Fuchs, CSc., MUDr. Miroslava Hornyčová, CSc., MUDr. Zdeňka Trávníčková, CSc., Jiřina Fridrichovská, prom. chem.). Data from the manufacturer of the substance / mixture, if available - information from registration dossiers.

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.