SAFETY DATA SHEET

according to 1907/2006/EC, Article 3

Revision date: 30/09/2023

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

1.1 Product identifiers

Product name	2,2,4-Trimethylpentane
Product Number	PSR21882
Brand	PureSynth research chemicals
CAS No.	540-84-1

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

Identified uses : PurReagent

1.3 Details of the supplier of the safety data sheet

Company **PureSynth Research Chemicals GmbH.**

64683 Einhausen Marie-Curie-StraBe. 3, Germany

1.4 Emergency telephone number

Worldwide Helpline No.: 1800-8908-260

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Flammable liquids, (Category 2)	H225: Highly flammable liquid and vapour.
Skin irritation, (Category 2)	H315: Causes skin irritation.
Specific target organ toxicity - single exposure, (Category 3), Central nervous system	H336: May cause drowsiness or dizziness.
Aspiration hazard, (Category 1)	H304: May be fatal if swallowed and enters airways.
Short-term (acute) aquatic hazard, (Category 1)	H400: Very toxic to aquatic life.
Long-term (chronic) aquatic hazard, (Category 1)	H410: Very toxic to aquatic life with long lasting effects.

Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal word	Danger
Hazard statement(s)	
H225	Highly flammable liquid and vapor.
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 statement(s)	
P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233	Keep container tightly closed.
P273	Avoid release to the environment.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
P331	Do NOT induce vomiting.
Supplemental Hazard Statements	none

2.2 **Other hazards:** This substance/mixture contains no components considered to be either persistent, bio accumulative and toxic (PBT), or very persistent and very bio accumulative (vPvB) at levels of 0.1% or higher

SECTION 3: Composition / information on ingredients

3.1 Substances

Common names & Synonyms	**Mol. formula**	**CAS number**
Isooctane	C8H18	540-84-1
Component	**Classification**	**Concentration**
2,2,4-Trimethylpentane	Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 1; H225, H315, H336, H304, H400, H410 Concentration limits: >= 20 %: STOT SE 3, H336; M-Factor - Aquatic Acute: 1 - Aquatic Chronic: 1	<= 100 %

SECTION 4: First aid measures

Description of first aid measures

General advice	First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.
If inhaled	After inhalation: fresh air. Call in physician.
In case of skin contact	In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.
In case of eye contact	After eye contact: rinse out with plenty of water. Remove contact lenses.
If swallowed	After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately
Most important symptoms and effects, both acute and delayed	The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Indication of any immediate medical attention and special treatment needed	No data available

SECTION 5: Fire fighting measures

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.
Special hazards arising from the substance or mixture	Carbon oxides Flash back possible over considerable distance., Container explosion may occur under fire conditions. 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.
Advice for fire-fighters	Forms explosive mixtures with air at ambient temperatures. 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

Personal precautions, protective equipment and emergency procedures	Advice for non-emergency personnel: Do not breathe vapors, 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. For personal protection see section 8.
Environmental precautions	Do not let product enter drains. Risk of explosion.
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. Dispose of properly. Clean up affected area.
Reference to other sections	For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling	Work under hood. Do not inhale substance/mixture. Avoid generation of vapors/aerosols. 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. For precautions see section 2.2

Conditions for safe storage, including any incompatibilities	Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.
Specific end use(s)	Storage class (TRGS 510): 3: Flammable liquids Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls / Personal protection

Control parameters	Ingredients with workplace control parameters
Exposure controls	
Personal protective equipment:	
Eye / face protection	Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses
Skin protection	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 EN 16523-1 please contact the supplier of CE-approved gloves
Body Protection	Flame retardant antistatic protective clothing.
Respiratory protection	Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds
Control of environmental exposure	Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

Appearance	Colourless liquid
Odour	No data available
pH - Value	No data available
Density	0.692 g/mL at 25 °C
Boiling Point	98 - 99 °C
Melting Point	-107 °C
Solubility in water	insoluble
Flash point	-12 °C - closed cup
Vapour pressure	55 hPa at 21 °C 120 hPa at 37.80 °C
Auto -ignition temperature	No data available
Vapour density	No data available
Flammability (solid, gas)	No data available
Evaporation rate	No data available
Partition coefficient: n- octanol / water	log Pow: 4.6 - Bioaccumulation is not expected.
Viscosity	No data available
Explosive properties	Not classified as explosive.
Upper / lower flammability or explosive limits	Upper explosion limit: 6.0 %(V) Lower explosion limit: 1.0 %(V)
Oxidizing properties	none

Other safety information: Relative vapor density : 3.94 - (Air = 1.0)

SECTION 10: Stability and reactivity

Reactivity	Vapors may form explosive mixture with air.
Chemical stability	The product is chemically stable under standard ambient conditions (room temperature).
Possibility of hazardous reactions	Violent reactions possible with: Strong oxidizing agents
Condition to avoid	Warming
Incompatible materials	various plastics
Hazardous decomposition products	In the event of fire: see section 5

SECTION 11: Toxicological information

Acute toxicity	LD50 Oral - Rat - male and female - > 5.000 mg/kg LC50 Inhalation - Rat - male and female - 4 h - > 33.52 mg/l – vapor Symptoms: mucosal irritations LD50 Dermal - Rabbit - male and female - > 2.000 mg/kg
Skin corrosion/irritation	LD50 Dermal - Rabbit - male and female - > 2.000 mg/kg Remarks: Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.
Serious eye damage/eye irritation	Eyes - Rabbit Result: No eye irritation
Respiratory or skin sensitization	Maximization Test - Guinea pig Result: negative
Germ cell mutagenicity	Test Type: Ames test Test system: TA98 Metabolic activation: with and without metabolic activation Result: negative Test Type: In vitro mammalian cell gene mutation test Test system: human lymphoblastoid cells Metabolic activation: with and without metabolic activation Result: negative Test Type: unscheduled DNA synthesis assay Species: Rat Cell type: Liver cells Application Route: Oral Result: negative
Carcinogenicity	No data available
Reproductive toxicity	No data available
Specific target organ toxicity - single exposure	May cause drowsiness or dizziness. - Central nervous system
Specific target organ toxicity - repeated exposure	No data available
Aspiration hazard	Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis
Additional Information	
Endocrine disrupting properties	
Assessment	The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher

SECTION 12: Ecological information

Toxicity	
Toxicity to fish	semi-static test LC50 - Oncorhynchus mykiss (rainbow trout) – 0.11 mg/l - 96 h
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) – 0.4 mg/l - 48 h
Toxicity to bacteria	EC0 - Pseudomonas putida – 10,000 mg/l
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	static test EC50 - Daphnia magna (Water flea) – 0.23 mg/l - 21 d
Persistence and degradability	aerobic - Exposure time 28 d Result: 51.3 % - Inherently biodegradable.
Bio accumulative potential	No data available
Mobility in soil	No data available
Results of PBT and vPvB assessment	This substance/mixture contains no components considered to be either persistent, bio accumulative and toxic (PBT), or very persistent and very bio accumulative (vPvB) at Levels of 0.1% or higher.
Endocrine disrupting properties	The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.
Other adverse effects	Endangers drinking-water supplies if allowed to enter soil and/or waters in large quantities. Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

Waste treatment methods Products	Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleansed containers like the product itself.
Contaminated packaging	Dispose of as unused product.

SECTION 14: Transport information

	UN no.	UN proper shipping name	Hazard Class(es)	Packaging group	Marine Pollutant
ADR / RID	1262	OCTANES	3	II	Yes
IMDG	1262	OCTANES	3	II	Yes
IATA	1262	Octanes	3	II	No

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture
This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.

Chemical safety assessment
A Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

The information in this SDS is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. The user must be determined suitability of this information for his application.