

SAFETY DATA SHEET

according to 1907/2006/EC, Article 3

Version no. : 2.1
Prepared on : 30.03.2019
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SECTION 1: Identification of the substance/mixture and of the company/undertaking.

1.1 Product identifiers

Product name Heptane
Product Number PSR44646 / PSR44961 / PSR43078 / PSR2764 / PSR36662
Brand PureSynth research chemicals
CAS No. 142-82-5

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

Identified uses : Solvent for analytical purpose

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

Classification according to Regulation (EC) No 1272/2008

Flammable liquids (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
Short-term (acute) aquatic hazard (Category 1), H400
Long-term (chronic) aquatic hazard (Category 1), H410

2.2 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.
Response	
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

2.3 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.

Ecological information:

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.

Toxicological information:

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 3: Composition / information on ingredients

3.1 Substances

Common names & Synonyms	Mol. formula	CAS number
n-heptane	C ₇ H ₁₆	142-82-5
Component	Classification	Concentration
Heptane	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: 10	<= 100 %

SECTION 4: First aid measures

Description of first aid measures

General advice	Consult a physician. Show this 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.
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	Carbon dioxide (CO ₂) Foam Dry powder
Suitable extinguishing media	
Special hazards arising from the substance or mixture	Carbon oxides Flash back possible over considerable distance. Combustible. Pay attention to flashback. Vapors are heavier than air and may spread along floors.
Advice for fire-fighters	Development of hazardous combustion gases or vapors possible in the event of fire. 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, and consult an expert.
Environmental precautions	For personal protection see section 8. 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.
Reference to other sections	Dispose of properly. Clean up affected area. For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling	Avoid generation of vapors/aerosols Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge 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. Storage class (TRGS 510): 3:Flammable liquids
Specific end use(s)	Recommend storage temperature-ambient temperature. Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls / Personal protection

Control parameters	Components with workplace control parameters
Exposure controls	
Appropriate engineering controls	Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.
Personal protective equipment:	
Eye / face protection	Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Skin protection	Flame retardant antistatic protective clothing.
Body Protection	Flame retardant antistatic protective clothing.
Respiratory protection	required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system. Recommended Filter type: Filter type ABEK 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.
Control of environmental exposure	Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

Appearance	Form: Liquid Colour: Colourless
Odour	No data available
pH - Value	No data available
Density	No data available
Boiling Point	98.2 °C
Melting Point	-91 °C
Solubility in water	Insoluble
Flash point	-4 °C - c.c.
Vapour pressure	111 hPa at 37.7 °C 53.3 hPa at 20.0 °C
Auto -ignition temperature	223.0 °C
Vapour density	No data available
Flammability (solid, gas)	No data available
Evaporation rate	No data available
Partition coefficient: n- octanol / water	Log Pow: > 3 - Bioaccumulation is not expected.
Viscosity	Viscosity, kinematic: 0.64 mm ² /s at 20 °C
Explosive properties	Not classified as explosive.
Upper / lower flammability or explosive limits	Upper explosion limit: 7.0 %(V) Lower explosion limit: 1.1 %(V)
Oxidizing properties	No data available

Other safety information:

Molecular weight: 100.21 g/mol
Self-ignition: 223.0 °C

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	Risk of ignition or formation of inflammable gases or vapours with: Strong oxidizing agents phosphorus in the presence of: Chlorine
Condition to avoid	Warming
Incompatible materials	rubber, 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 Remarks: (in analogy to similar compounds) The value is given in analogy to the following substances: isooctane LC50 Inhalation - Rat - male and female - 4 h - > 29.29 mg/l LD50 Dermal - Rabbit - male and female - > 2.000 mg/kg Remarks: The value is given in analogy to the following substances: isooctane
Skin corrosion/irritation	Skin - Rabbit Result: Irritating to skin. - 24 h Remarks: The value is given in analogy to the following substances: isooctane 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 Remarks: The value is given in analogy to the following substances: isooctane
Respiratory or skin sensitization	Maximization Test - Guinea pig Result: negative
Germ cell mutagenicity	Test Type: Ames test Test system: Escherichia coli/Salmonella typhimurium Metabolic activation: with and without metabolic activation Result: negative Test Type: Chromosome aberration test in vitro Test system: rat hepatocytes Result: negative
Carcinogenicity	No data available
Reproductive toxicity	No data available
Specific target organ toxicity - single exposure	May cause drowsiness or dizziness.
Specific target organ toxicity - repeated exposure	No data available
Aspiration hazard	May be fatal if swallowed and enters airways. Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.
Additional Information	RTECS: MI7700000 Prolonged or repeated exposure to skin causes defatting and dermatitis. Central nervous system depression, narcosis, Damage to the lungs. To the best of our knowledge, the chemical, physical, and toxicological properties have not Been thoroughly investigated. Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

Toxicity

Toxicity to fish	LL50 (Rainbow darter (<i>Etheostoma caeruleum</i>)): > 13.4 mg/l Exposure time: 96 h Method: OECD Test Guideline 203
Toxicity to daphnia and other aquatic invertebrates	EC50 (<i>Daphnia magna</i> (Water flea)): 0.23 mg/l Exposure time: 21 d Test Type: static test Analytical monitoring: yes GLP: yes
Toxicity to algae/aquatic plants	EL50 (<i>Pseudokirchneriella subcapitata</i> (green algae)): 29 mg/l End point: Growth inhibition Exposure time: 72 h Method: OECD Test Guideline 201 GLP: yes

Persistence and degradability

Biodegradability

aerobic - Exposure time 10 d
Result: 70 % - Readily biodegradable.
Remarks: (ECHA)

Biochemical Oxygen Demand (BOD)

1.920 mg/g
Remarks: (IUCLID)

Theoretical oxygen demand

3.500 mg/g
Remarks: (Lit.)

Ratio BOD/ThBOD

55 %
Remarks: (Lit.)

Bio accumulative potential

Indication of bioaccumulation.

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.

Other adverse effects

Additional ecological information

Do not empty into drains.
Avoid release to the environment.

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.
Products	Handle uncleaned containers like the product itself.
Contaminated packaging	No data available

SECTION 14: Transport information

	UN no.	UN proper shipping name	Hazard Class(es)	Packaging group	Marine Pollutant
ADR / RID	1206	HEPTANES	3	II	Yes
IMDG	1206	HEPTANES	3	II	Yes
IATA	1206	Heptanes	3	II	No

SECTION 15: Regulatory information

15.1 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.

REACH - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles (Annex XVII)	Conditions of restriction for the following entries should be considered: Number on list 3 Number on list 40 Not applicable
REACH - Candidate List of Substances of Very High Concern for Authorisation (Article 59).	Not applicable
Regulation (EU) No 2024/590 on substances that deplete the ozone layer	Not applicable
Regulation (EU) 2019/1021 on persistent organic pollutants (recast)	Not applicable
REACH - List of substances subject to authorisation (Annex XIV)	Not applicable
Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.	E1 ENVIRONMENTAL HAZARDS

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out

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.