

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	3-Pentanone
Product Number	PSR28335
Brand	PureSynth research chemicals
CAS No.	96-22-0

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

Identified uses : PurCert Standard for GC

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

Eye irritation (Category 2), H319

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

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram



Signal word

Danger

Hazard statement(s)

H225	Highly flammable liquid and vapor.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H336	May cause drowsiness or dizziness.

Precautionary statement(s)

P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233	Keep container tightly closed.
P240	Ground and bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use non-sparking tools.

P305 + P351 + P338

IF IN EYES: Rinse cautiously with water for several minutes.
Remove contact lenses, if present and easy to do. Continue rinsing.

Supplemental Hazard
Statements

EUH066

Repeated exposure may cause skin dryness or cracking.

- 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
Diethyl ketone	C ₅ H ₁₀ O	96-22-0
Component	Classification	Concentration
pentan-3-one	Flam. Liq. 2; Eye Irrit. 2; STOT SE 3; H225, H319, H336, H335	<= 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. Call in ophthalmologist. Remove contact lenses.
If swallowed	After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.
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	
Unsuitable extinguishing media	For this substance/mixture no limitations of extinguishing agents are given.
	Carbon oxides
Special hazards arising from the substance or mixture	Combustible.
	Pay attention to flashback.
	Vapors 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. In the event of fire, wear self-contained breathing apparatus.
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. 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 vapours/aerosols. 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. 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 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
Skin protection	
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	Form : Liquid
Odour	Colour : Colourless acetone-like
pH - Value	No data available
Density	0.813 g/cm ³ at 25 °C
Boiling Point	101.5 °C
Melting Point	-42 °C
Solubility in water	45.6 g/l at 25 °C
Flash point	7 °C - DIN 51755 Part 1
Vapour pressure	34.45 hPa at 19.2 °C
Auto -ignition temperature	455 °C
Vapour density	No data available
Flammability (solid, gas)	No data available
Evaporation rate	No data available
Partition coefficient: n- octanol / water	Pow: 7.04; log Pow: 0.85
Viscosity	Viscosity, kinematic: 0.444 mm ² /s at 25 °C Viscosity, dynamic: No data available
Explosive properties	No data available
Upper / lower flammability or explosive limits	Upper explosion limit: 7.7 %(V) Lower explosion limit: 1.6 %(V)
Oxidizing properties	No data available

Other safety information: No data available

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). Exothermic reaction with: Amines amides
Possibility of hazardous reactions	strong reducing agents Oxidizing agents hydrogen peroxide metallic hydroxides
Condition to avoid	Warming
Incompatible materials	No data available
Hazardous decomposition products	In the event of fire: see section 5

SECTION 11: Toxicological information

Acute toxicity	LD50 Oral - Rat - male and female - 2.900 mg/kg Inhalation: No data available LD50 Dermal - Rabbit - male - 16.200 mg/kg
Skin corrosion/irritation	No data available
Serious eye damage/eye irritation	Eyes - Rat Result: Eye irritation
Respiratory or skin sensitization	No data available
Germ cell mutagenicity	No data available
Carcinogenicity	No data available
Reproductive toxicity	No data available
Specific target organ toxicity - single exposure	May cause respiratory irritation. - Respiratory system May cause drowsiness or dizziness. - Central nervous system
Specific target organ toxicity - repeated exposure	No data available
Aspiration hazard	No data available
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	flow-through test LC50 - Pimephales promelas (fathead minnow) - 1.540 mg/l - 96 h
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia - > 500 mg/l - 48 h
Toxicity to algae	static test ErC50 - Desmodesmus subspicatus (green algae) - > 500 mg/l - 72 h
Toxicity to bacteria	static test EC50 - Pseudomonas putida - ca. 10.000 mg/l - 17 h
Persistence and degradability	Readily biodegradable
Biochemical Oxygen Demand (BOD)	1.310 mg/g
Chemical Oxygen Demand (COD)	2.246 mg/g
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. 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.
Endocrine disrupting properties	
Other adverse effects	No data available

SECTION 13: Disposal considerations

Waste treatment methods	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.
Products	
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	1156	DIETHYL KETONE	3	II	No
IMDG	1156	DIETHYL KETONE	3	II	No
IATA	1156	Diethyl ketone	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

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.