

SAFETY DATA SHEET

according to 1907/2006/EC, Article 3

Revision date: 30/03/2023

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

1.1 Product identifiers

Product name	Cetylpyridinium chloride monohydrate
Product Number	PSR37855
Brand	PureSynth research chemicals
CAS No.	6004-24-6

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

Identified uses : Purcert Standard

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

Acute toxicity, Oral (Category 4), H302 Acute toxicity,
Inhalation (Category 2), H330
Skin irritation (Category 2), H315
Serious eye damage (Category 1), H318
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
Short-term (acute) aquatic hazard (Category 1), H400

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram



Signal word Danger

Hazard statement(s)

H302	Harmful if swallowed.
H315	Causes skin irritation.
H318	Causes serious eye damage.
H330	Fatal if inhaled.
H335	May cause respiratory irritation.
H400	Very toxic to aquatic life.

Precautionary statement(s)

P273	Avoid release to the environment
P280	Wear protective gloves/ eye protection/ face protection.
P301 + P312	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.
P302 + P352	IF ON SKIN: Wash with plenty of water.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
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	none

2.3 Other hazards:

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

SECTION 3: Composition / information on ingredients

3.1 Substances

Common names & Synonyms	Mol. formula	CAS number
Hexadecylpyridinium chloride monohydrate	$C_{21}H_{38}ClN \cdot H_2O$	6004-24-6
Component	Classification	Concentration
Cetylpyridinium chloride	Acute Tox. 4; Acute Tox.2; Skin Irrit. 2; Eye Dam.1; STOT SE 3; Aquatic Acute 1; H302, H330, H315, H318, H335, H400 M-Factor - Aquatic Acute:100	<= 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	If breathed in, move person into fresh air. If not breathing, give artificial respiration.
In case of skin contact	Wash off with soap and plenty of water. Consult a physician.
In case of eye contact	Rinse thoroughly with plenty of water as precaution.
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: Firefighting measures

Extinguishing media	Water Foam Carbon dioxide (CO ₂) Dry powder
Suitable extinguishing media	

Special hazards arising from the substance or mixture	Carbon oxides Nitrogen oxides (NOx) Hydrogen chloride gas Combustible. Development of hazardous combustion gases or vapours possible in the event of fire.
Advice for firefighters	Wear self-contained breathing apparatus for firefighting if necessary Suppress (knock down) gases/vapors/mists with a water spray jet.
Further information	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	Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Avoid breathing dust. For personal protection see section 8.
Environmental precautions	Do not let product enter drains. Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.
Methods and materials for containment and cleaning up	
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. 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	Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons. Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials
Specific end use(s)	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). 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
Skin protection	
Body Protection	protective clothing
Respiratory protection	required when dusts 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 P3

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Appearance	Form: Crystal
	Colour: White
Odour	Characteristic
pH - Value	5.0 – 5.4 at 10 g/l at 20 °C
Density	No data available
Boiling Point	120 - 124 °C at 0.09 hPa
Melting Point	80 - 84 °C
Solubility in water	111 g/l at 20 °C
Flash point	Not applicable
Vapour pressure	No data available
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: 1.71 at 20 °C - (anhydrous substance), Bioaccumulation is not expected.
Viscosity	No data available
Explosive properties	No data available
Upper / lower flammability or explosive limits	No data available
Oxidizing properties	No data available

Other safety information: No data available

SECTION 10: Stability and reactivity

Reactivity	The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.
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	No data available
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 - female – 560.3 mg/kg LC50 Inhalation - Rat - male and female - 4 h - 0,054 – 0.51 mg/l LD50 Dermal - Rat - male and female - > 5,000 mg/kg Remarks: The value is given in analogy to the following substances: N-Cetylpyridinium chloride
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Skin corrosion/irritation	Skin - Rabbit Result: Irritations Remarks: The value is given in analogy to the following substances: N-Cetylpyridinium chloride
Serious eye damage/eye irritation	Eyes - Rabbit Result: Causes serious eye damage. Remarks: The value is given in analogy to the following substances: N-Cetylpyridinium chloride
Respiratory or skin sensitization	Buehler Test - Guinea pig Result: negative Remarks: The value is given in analogy to the following substances: N-Cetylpyridinium chloride Test Type: In vitro mammalian cell gene mutation test Test system: Mouse lymphoma test Metabolic activation: with and without metabolic activation Result: negative
Germ cell mutagenicity	Test Type: Ames test Test system: Salmonella typhimurium Metabolic activation: with and without metabolic activation Result: negative Remarks: The value is given in analogy to the following substances: N-Cetylpyridinium chloride
Carcinogenicity	No data available
Reproductive toxicity	No data available
Specific target organ toxicity - single exposure	May cause respiratory irritation. - Respiratory system
Specific target organ toxicity - repeated exposure	No data available
Aspiration hazard	No data available
Additional Information	No data available 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	

SECTION 12: Ecological information

Toxicity	static test LC50 - Oncorhynchus mykiss (rainbow trout) – 0.16 mg/l - 96 h
Toxicity to fish	Remarks: The value is given in analogy to the following substances: N-Cetylpyridinium chloride
Toxicity to daphnia and other aquatic invertebrates	semi-static test - Daphnia magna (Water flea) – 0.0041 mg/l - 48 h Remarks: The value is given in analogy to the following substances: N-Cetylpyridinium chloride
Toxicity to algae	static test EC50 - Pseudokirchneriella subcapitata (algae) – 0.0269 mg/l - 72 h Remarks: The value is given in analogy to the following substances: N-Cetylpyridinium chloride
Toxicity to bacteria	static test EC50 - activated sludge – 20.7 mg/l - 3 h Remarks: The value is given in analogy to the following substances: N-Cetylpyridinium chloride aerobic - Exposure time 28 d Result: 0 % - Not biodegradable.
Persistence and degradability	Remarks: The value is given in analogy to the following substances: N-Cetylpyridinium chloride
Bioaccumulative 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

Endocrine disrupting properties

either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (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.

Other adverse effects

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 uncleaned 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	2811	TOXIC SOLID, ORGANIC, N.O.S. (Cetylpyridinium chloride monohydrate)	6.1	II	Yes
IMDG	2811	TOXIC SOLID, ORGANIC, N.O.S. (Cetylpyridinium chloride monohydrate)	6.1	II	Yes
IATA	2811	Toxic solid, organic, n.o.s. (Cetylpyridinium chloride monohydrate)	6.1	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.