

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 Thymol Crystals
Product Number PSR39441
Brand PureSynth research chemicals
CAS No. 89-83-8

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

Identified uses : Laboratory chemicals, Manufacture of substances

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, Category 4	H302: Harmful if swallowed.
Skin corrosion, Sub-category 1B	H314: Causes severe skin burns and eye damage.
Serious eye damage, Category 1	H318: Causes serious eye damage.
Long-term (chronic) aquatic hazard, Category 2	H411: Toxic to aquatic life with long lasting effects.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram



Signal word

Danger

Hazard statement(s)

H302	Harmful if swallowed.
H314	Causes severe skin burns and eye damage.
H411	Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P260	Do not breathe dust.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.

P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
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.

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
2-Isopropyl-5-methylphenol, 5-Methyl-2-(1-methylethyl)phenol, 5-Methyl-2-isopropylphenol, IPMP	C ₁₀ H ₁₄ O	89-83-8
Component	Classification	Concentration
thymol	Acute toxicity estimate Acute oral toxicity: 980 mg/kg	>= 90 - <= 100

SECTION 4: First aid measures

Description of first aid measures

General advice	First aiders need to protect themselves. 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. 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: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.
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	
Suitable extinguishing media	Carbon dioxide (CO ₂) 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	Combustible. Carbon oxides Vapours are heavier than air and may spread along floors. Forms explosive mixtures with air on intense heating. Development of hazardous combustion gases or vapours possible in the event of fire.
Advice for fire-fighters	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	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: Avoid inhalation of dusts. 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.
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. Dispose of properly. Clean up affected area. Avoid generation of dusts.
Reference to other sections	For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling	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	Tightly closed. Dry. Storage class (TRGS 510): 8A: Combustible, corrosive 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	Ingredients with workplace control parameters
Exposure controls	
Appropriate engineering controls	No data available
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). Tightly fitting safety goggles
Hand protection	Material : Chloroprene Break through time : 480 min Glove thickness : 0.6 mm Protective index : Full contact Material : Nature latex/chloroprene Break through time : 60 min Glove thickness : 0.6 mm

Protective index : Splash contact

Remarks : Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it. If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Skin and Body Protection

Respiratory protection

protective clothing

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 P2

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.

SECTION 9: Physical and chemical properties

Appearance	Form: Powder or Crystals Colour: colourless to white to pale Yellow
Odour	No data available
pH - Value	No data available
Density	0.98 g/cm ³ (20 °C)
Boiling Point	231.8 °C (1003 hPa)
Melting Point	49.2 °C
Solubility in water	0.8 g/l (20 - 25 °C)
Flash point	116 °C(1013 hPa) Method: ISO 3679, closed cup
Vapour pressure	0.022 hPa (25 °C)
Auto -ignition temperature	285 °C
Vapour density	No data available
Flammability (solid, gas)	No data available
Evaporation rate	No data available
Partition coefficient: n- octanol / water	log Pow: 3.3 Bioaccumulation is not expected.
Viscosity	No data available
Explosive properties	Not classified as explosive.
Upper / lower flammability or explosive limits	No data available
Oxidizing properties	none

Other safety information: No data available

SECTION 10: Stability and reactivity

Reactivity	Forms explosive mixtures with air on intense heating. A range from approx. 15 Kelvin below the flash point is to be rated as critical. 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 bases strong oxidising agents
Condition to avoid	Strong heating.
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 - 980 mg/kg Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2) (ECHA) Acute toxicity estimate Oral - 980 mg/kg (Calculation method) Inhalation: No data available LD50 Dermal - Rat - male and female - > 2000 mg/kg
Skin corrosion/irritation	Skin - Rabbit Result: Causes burns. - 4 h (OECD Test Guideline 404) Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
Serious eye damage/eye irritation	Eyes - Rabbit Result: Irreversible effects on the eye - 24 h (OECD Test Guideline 405) Remarks: Causes serious eye damage.
Respiratory or skin sensitization	Open epicutaneous test - Guinea pig Result: negative Remarks: (ECHA)
Germ cell mutagenicity	Test Type: Ames test Test system: Escherichia coli/Salmonella typhimurium Metabolic activation: with and without metabolic activation Method: OECD Test Guideline 471 Result: negative Test Type: Mutagenicity (mammal cell test): chromosome aberration. Test system: Chinese hamster lung cells Metabolic activation: with and without metabolic activation Result: positive Remarks: (ECHA) Test Type: In vitro mammalian cell gene mutation test Test system: Chinese hamster lung cells Metabolic activation: with and without metabolic activation Method: OECD Test Guideline 476 Result: negative Test Type: In vivo micronucleus test Species: Rat Cell type: Bone marrow

	Application Route: Intraperitoneal injection
	Method: OECD Test Guideline 475
	Result: positive
Carcinogenicity	No data available
Reproductive toxicity	No data available
Specific target organ toxicity - single exposure	No data available
Specific target organ toxicity - repeated exposure	No data available
Aspiration hazard	No data available
Additional 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. Repeated dose toxicity - Rat - male and female - Oral - 43 Days - No observed adverse effect level - 8 mg/kg Remarks: (ECHA) Cough, Shortness of breath, Headache, Nausea, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. After absorption: Systemic effects: CNS disorders cardiovascular disorders Toxic effect on: Kidney Liver Effect potentiated by: ethanol Substances which occur in nature Other dangerous properties can not be excluded. Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information.

Toxicity

Toxicity to fish	LC50 (Pimephales promelas (fathead minnow)): 3.2 mg/l End point: mortality Exposure time: 96 h Test Type: static test Method: US-EPA
Toxicity to daphnia and other aquatic invertebrates	No data available
Toxicity to algae	ErC50 (Pseudokirchneriella subcapitata (green algae)): 14 mg/l Exposure time: 72 h Method: OECD Test Guideline 201 GLP: yes
Toxicity to Microorganism	EC50 (activated sludge): 40 mg/l Exposure time: 3 h Test Type: static test Method: OECD Test Guideline 209
Toxicity to fish (Chronic toxicity)	No data available
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)	NOEC: 2 mg/l End point: reproduction rate

Exposure time: 21 d
Species: Daphnia magna (Water flea)
Method: OECD Test Guideline 211
GLP: yes

Persistence and degradability

Biodegradability

Test Type: aerobic
Inoculum: activated sludge
Concentration: 0,8 mg/l
Result: Readily biodegradable.
Biodegradation: 83 %
Exposure time: 28 d
Method: Closed Bottle test
GLP: yes

Chemical Oxygen Demand (COD)

2690 mg/g

ThOD

Remarks: (IUCLID)

2760 mg/g

Remarks: (IUCLID)

Bioaccumulation

Bioaccumulation :
Species: Oryzias latipes
Exposure time: 6 Weeks
Concentration: ca. 1 µg/l
Bioconcentration factor (BCF): 48
Method: OECD Test Guideline 305C
Partition coefficient: n-octanol/water :
log Pow: 3.3
Remarks: Bioaccumulation is not expected.
No data available

Mobility in soil

Results of PBT and vPvB assessment

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.

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

No data available

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. 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	2430	ALKYLPHENOLS, SOLID, N.O.S.	8	III	no
IMDG	2430	ALKYLPHENOLS, SOLID, N.O.S. (thymol)	8	III	yes
IATA	2430	Alkylphenols, solid, n.o.s.	8	III	no

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

This material safety data sheet 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) : 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. E2 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.