

SAFETY DATA SHEET

Version 6.12
Revision Date 09/06/2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : 1-Hydroxybenzotriazole hydrate

Product Number : 157260

Brand : Aldrich

Index-No. : 613-285-00-7

CAS-No. : 123333-53-9

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Eye irritation (Category 2A), H319

Short-term (acute) aquatic hazard (Category 3), H402

Long-term (chronic) aquatic hazard (Category 3), H412

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For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Warning

Hazard Statements

H319

Causes serious eye irritation.

H412

Harmful to aquatic life with long lasting effects.

Precautionary Statements

P264

Wash skin thoroughly after handling.

P273

Avoid release to the environment.

P280

Wear eye protection/ face protection.

P305 + P351 + P338

IF IN EYES: Rinse cautiously with water for several minutes.

Remove contact lenses, if present and easy to do. Continue rinsing.

P337 + P313

If eye irritation persists: Get medical advice/ attention.

P501

Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Desensitized explosive

Explosive when dry.

Risk of explosion if heated under confinement.

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : HOBt Hydrate

Formula : C₆H₅N₃O.xH₂O

Molecular weight : 135.12 g/mol

CAS-No. : 123333-53-9

EC-No. : 219-989-7

Index-No. : 613-285-00-7

Component	Classification	Concentration
1-hydroxybenzotriazole, monohydrate		
	Eye Irrit. 2A; Aquatic Acute 3; Aquatic Chronic 3; H319, H402, H412	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air.

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. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 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

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Combustible.

In the event of decomposition: danger of explosion!

Forms explosive mixtures with air on intense heating.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Avoid shock and friction.

Vapors are heavier than air and may spread along floors.

In the event of decomposition: danger of explosion!

Forms explosive mixtures with air on intense heating.

5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 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.

6.2 Environmental precautions

Do not let product enter drains.

6.3 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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition.

Hygiene measures

Change contaminated clothing. Wash hands after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed and away from sources of ignition and heat. Observe national regulations.

Storage class

Storage class (TRGS 510): 4.1A: Other explosive hazardous materials

7.3 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

8.1 Control parameters

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

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8.2 Exposure controls

Appropriate engineering controls

Change contaminated clothing. Wash hands after working with substance.

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

Handle with impervious gloves.

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 (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

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.

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.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---------------|-------------------|
| a) Appearance | Form: solid |
| b) Odor | No data available |

c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/ range: 155 - 158 °C (311 - 316 °F) - lit.
f) Initial boiling point and boiling range	No data available
g) Flash point	157 °C (315 °F)
h) Evaporation rate	No data available
i) Flammability (solid, gas)	The substance or mixture is a flammable solid with the category 2.
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Density	No data available
Relative density	No data available
n) Water solubility	soluble
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	Explosive when dry., Risk of explosion if heated under confinement.
t) Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.

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.

Forms explosive mixtures with air on intense heating. Risk of explosion if heated under confinement.

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.

10.2 Chemical stability

heat-sensitive

Sensitivity to light

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

Strong acids

nitrates

Copper

10.4 Conditions to avoid

Heating (explosive decomposition).

Keep away from open flames, hot surfaces and sources of ignition.

Strong heating.

10.5 Incompatible materials

No data available

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - female - > 2,000 mg/kg

(OECD Test Guideline 423)

Remarks: The value is given in analogy to the following substances: 1-hydroxybenzotriazole

Inhalation: No data available

LD50 Dermal - Rat - male and female - > 2,000 mg/kg

(OECD Test Guideline 402)

Remarks: The value is given in analogy to the following substances: 1-hydroxybenzotriazole

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

Eyes - in vitro test

Result: Causes serious eye irritation. - 6 h

(OECD Test Guideline 492)

Remarks: The value is given in analogy to the following substances: 1-hydroxybenzotriazole

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

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

11.2 Additional Information

Repeated dose toxicity - Rat - male - Oral - 28 d - NOAEL (No observed adverse effect level) - 250 mg/kg

Remarks: The value is given in analogy to the following substances: 1-hydroxybenzotriazole

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information**12.1 Toxicity**

Toxicity to fish	static test LC50 - Danio rerio (zebra fish) - > 100 mg/l - 96 h (OECD Test Guideline 203) Remarks: The value is given in analogy to the following substances: 1-hydroxybenzotriazole
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 75.5 mg/l - 48 h (OECD Test Guideline 202) Remarks: The value is given in analogy to the following substances: 1-hydroxybenzotriazole
Toxicity to algae	static test ErC50 - Desmodesmus subspicatus (green algae) - 87.3 mg/l - 72 h

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(OECD Test Guideline 201)

Remarks: The value is given in analogy to the following substances:
1-hydroxybenzotriazole

12.2 Persistence and degradability

Biodegradability

Result: 63.2 % - Inherently biodegradable.
(OECD Test Guideline 301D)

Remarks: The value is given in analogy to the following substances:
1-hydroxybenzotriazole

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

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. Explosive materials: transport and disposal only in sufficiently desensitised condition!

SECTION 14: Transport information

DOT (US)

UN number: 3474 Class: 4.1 Packing group: I
Proper shipping name: 1-Hydroxybenzotriazole, monohydrate
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 3474 Class: 4.1 Packing group: I EMS-No: F-B, S-J

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Proper shipping name: 1-HYDROXYBENZOTRIAZOLE MONOHYDRATE

IATA

UN number: 3474 Class: 4.1 Packing group: I
Proper shipping name: 1-Hydroxybenzotriazole monohydrate

SECTION 15: Regulatory information

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : Fire Hazard

SARA 313 : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

US State Regulations

Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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