

SAFETY DATA SHEET

Version 6.2
Revision Date 06/17/2021
Print Date 06/19/2021

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

1.1 Product identifiers

Product name : 2-Octyl-4-isothiazolin-3-one
Product Number : 46078
Brand : Sigma
Index-No. : 613-112-00-5
CAS-No. : 26530-20-1

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

Identified uses : Laboratory chemicals, Synthesis of substances

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)

Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Skin corrosion (Category 1B), H314
Serious eye damage (Category 1), H318
Skin sensitization (Category 1), H317
Short-term (acute) aquatic hazard (Category 1), H400
Long-term (chronic) aquatic hazard (Category 1), H410

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

Danger

Hazard statement(s)

H302 Harmful if swallowed.
H311 + H331 Toxic in contact with skin or if inhaled.
H314 Causes severe skin burns and eye damage.
H317 May cause an allergic skin reaction.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P261 Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P271 Use only outdoors or in a well-ventilated area.
P272 Contaminated work clothing must not be allowed out of the workplace.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
P362 Take off contaminated clothing and wash before reuse.
P391 Collect spillage.
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
P405 Store locked up.
P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms : 2-Octyl-3(2H)-isothiazolone
Octhilinone

Formula : C₁₁H₁₉NOS

Molecular weight : 213.34 g/mol

CAS-No. : 26530-20-1

EC-No. : 247-761-7

Index-No. : 613-112-00-5

Component	Classification	Concentration
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2-Octyl-2H-isothiazol-3-one		
	Acute Tox. 4; Acute Tox. 3; Skin Corr. 1B; Eye Dam. 1; Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 1; H302, H331, H311, H314, H318, H317, H400, H410 Concentration limits: >= 0.05 %: Skin Sens. 1, H317; M-Factor - Aquatic Acute: 10 - Aquatic Chronic: 10	<= 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

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately 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.

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

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)

Sulfur oxides

Combustible.

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

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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: 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.

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 carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. 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

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.

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face 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). Tightly fitting safety goggles

Skin protection

required

Body Protection

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.

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: liquid |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | No data available |
| f) Initial boiling point and boiling range | No data available |
| g) Flash point | ()No data available |
| h) Evaporation rate | No data available |
| i) Flammability (solid, | No data available |

- gas)
- | | |
|---|-------------------|
| j) Upper/lower flammability or explosive limits | No data available |
| k) Vapor pressure | No data available |
| l) Vapor density | No data available |
| m) Relative density | No data available |
| n) Water solubility | No data available |
| o) Partition coefficient: n-octanol/water | log Pow: 5 |
| p) Autoignition temperature | No data available |
| q) Decomposition temperature | No data available |
| r) Viscosity | No data available |
| s) Explosive properties | No data available |
| t) Oxidizing properties | No data available |

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

Strong oxidizing agents

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 - 550 mg/kg

Inhalation: No data available

LD50 Dermal - Rabbit - 690 mg/kg

No data available

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Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Eye irritation

(Draize Test)

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

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

RTECS: NX8156900

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

SECTION 12: Ecological information**12.1 Toxicity**

No data available

Toxicity to fish LC50 - Pimephales promelas (fathead minnow) - 0.14 mg/l - 96.0 h

Toxicity to daphnia and other aquatic invertebrates EC50 - Daphnia magna (Water flea) - 0.18 mg/l - 48 h

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

Bioaccumulation Lepomis macrochirus - 67 d
- 50 µg/l(2-Octyl-2H-isothiazol-3-one)

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Bioconcentration factor (BCF): 165

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 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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)

UN number: 2922 Class: 8 (6.1) Packing group: II
Proper shipping name: Corrosive liquids, toxic, n.o.s. (2-Octyl-2H-isothiazol-3-one)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 2922 Class: 8 (6.1) Packing group: II EMS-No: F-A, S-B
Proper shipping name: CORROSIVE LIQUID, TOXIC, N.O.S. (2-Octyl-2H-isothiazol-3-one)

IATA

UN number: 2922 Class: 8 (6.1) Packing group: II
Proper shipping name: Corrosive liquid, toxic, n.o.s. (2-Octyl-2H-isothiazol-3-one)

SECTION 15: Regulatory information

SARA 302 Components

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

SARA 313 Components

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.

SARA 311/312 Hazards

Acute Health Hazard

Massachusetts Right To Know Components

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

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

Pennsylvania Right To Know Components

2-Octyl-2H-isothiazol-3-one

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New Jersey Right To Know Components

2-Octyl-2H-isothiazol-3-one

CAS-No.
26530-20-1

Revision Date

SECTION 16: Other information

Further information

The above information 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. 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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