

## SAFETY DATA SHEET

Version 6.6  
Revision Date 05/31/2021  
Print Date 01/15/2022

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 2-Methyl-4-isothiazolin-3-one

Product Number : 73569  
Brand : Sigma-Aldrich  
CAS-No. : 2682-20-4

**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 3), H301  
Acute toxicity, Inhalation (Category 2), H330  
Acute toxicity, Dermal (Category 3), H311  
Skin corrosion (Category 1B), H314  
Serious eye damage (Category 1), H318  
Skin sensitization (Sub-category 1A), 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)	
H301 + H311	Toxic if swallowed or in contact with skin.
H314	Causes severe skin burns and eye damage.
H317	May cause an allergic skin reaction.
H330	Fatal if inhaled.
H410	Very toxic to aquatic life with long lasting effects.
Precautionary statement(s)	
P260	Do not breathe 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.
P284	Wear respiratory protection.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. 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**  
Corrosive to the respiratory tract.

---

**SECTION 3: Composition/information on ingredients**

**3.1 Substances**

Synonyms	:	2-Methyl-3(2H)-isothiazolone
Formula	:	C <sub>4</sub> H <sub>5</sub> NOS
Molecular weight	:	115.15 g/mol
CAS-No.	:	2682-20-4
EC-No.	:	220-239-6

Component	Classification	Concentration
-----------	----------------	---------------

<b>2-Methyl-4-isothiazolin-3-one</b>		
	Acute Tox. 3; Acute Tox. 2; Acute Tox. 3; Skin Corr. 1B; Eye Dam. 1; Skin Sens. 1A; Aquatic Acute 1; Aquatic Chronic 1; H301, H330, H311, H314, H318, H317, H400, H410 Concentration limits: >= 0.0015 %: Skin Sens. 1A, H317; M-Factor - Aquatic Acute: 10 - Aquatic Chronic: 1	<= 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**

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible. 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

Water Foam Carbon dioxide (CO<sub>2</sub>) 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<sub>x</sub>)

Sulfur oxides

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

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: Avoid generation and inhalation of dusts in all circumstances. 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. 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 safe handling

Work under hood. Do not inhale substance/mixture.

#### 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. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

### **Storage stability**

Recommended storage temperature  
2 - 8 °C

Air sensitive. Store under inert gas.

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**

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.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC 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.

### **Body Protection**

Acid-resistant 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.

### **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: crystalline<br>Color: white   |
| b) Odor   | No data available   |
| c) Odor Threshold                               | No data available   |
| d) pH   | 2.58 at 50 g/l at 25 °C (77 °F) - OCSPP 830.7000  |
| e) Melting point/freezing point                 | Melting point/range: 46.7 - 48.3 °C (116.1 - 118.9 °F) - Regulation (EC) No. 440/2008, Annex, A.1 |
| f) Initial boiling point and boiling range      | > 130 °C > 266 °F at 16 hPa - Regulation (EC) No. 440/2008, Annex, A.2                            |
| g) Flash point                                  | ( )Not applicable   |
| h) Evaporation rate                             | No data available   |
| i) Flammability (solid, gas)                    | No data available   |
| j) Upper/lower flammability or explosive limits | No data available   |
| k) Vapor pressure                               | 0.0099 hPa at 20 °C (68 °F) - Regulation (EC) No. 440/2008, Annex, A.4                            |
| l) Vapor density                                | No data available   |
| m) Relative density                             | 1.39 at 20 °C (68 °F) - Regulation (EC) No. 440/2008, Annex, A.3                                  |
| n) Water solubility                             | soluble   |
| o) Partition coefficient: n-octanol/water       | log Pow: -0.34 at 30 °C (86 °F) - OECD Test Guideline 117 - Bioaccumulation is not expected.      |

- p) Autoignition temperature 396 °C (745 °F) at 1,012 hPa
- 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

- Surface tension 68.8 mN/m at 1g/l at 19.5 °C (67.1 °F) - OECD Test Guideline 115
- Dissociation constant > 2.81 at 21 °C (70 °F) - OECD Test Guideline 112

---

## SECTION 10: Stability and reactivity

### 10.1 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.

### 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 - male and female - 285.5 mg/kg  
(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - 0.11 mg/l  
(OECD Test Guideline 403)

LD50 Dermal - Rat - male and female - 242 mg/kg  
(OECD Test Guideline 402)

#### Skin corrosion/irritation

Skin - Rabbit

Result: Causes burns.

(OECD Test Guideline 404)

### **Serious eye damage/eye irritation**

Eyes - Rabbit

Remarks: Causes serious eye damage.

### **Respiratory or skin sensitization**

Buehler Test - Guinea pig

Result: positive

(OECD Test Guideline 406)

Local lymph node assay (LLNA) - Mouse

Result: positive

(OECD Test Guideline 429)

Maximization Test - Guinea pig

Result: positive

(OECD Test Guideline 406)

### **Germ cell mutagenicity**

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Human lymphocytes

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Test Type: unscheduled DNA synthesis assay

Species: Rat

Application Route: Oral

Method: OECD Test Guideline 486

### **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**

RTECS: NX8157080

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., 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	flow-through test LC50 - <i>Oncorhynchus mykiss</i> (rainbow trout) - 4.77 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	flow-through test EC50 - <i>Daphnia magna</i> (Water flea) - 0.85 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test EC50 - <i>Skeletonema costatum</i> - 0.069 mg/l - 96 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC50 - activated sludge - 41 mg/l - 3 h (OECD Test Guideline 209)

**12.2 Persistence and degradability**

Biodegradability Result: 55.8 % - Not readily biodegradable.  
(OECD Test Guideline 301B)  
Remarks: The 10 day time window criterion is not fulfilled.

**12.3 Bioaccumulative potential**

Bioaccumulation *Lepomis macrochirus* - 56 d  
(2-Methyl-4-isothiazolin-3-one)  
  
Bioconcentration factor (BCF): 5.75  
*Lepomis macrochirus* - 56 d  
(2-Methyl-4-isothiazolin-3-one)  
  
Bioconcentration factor (BCF): 48.1

**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](http://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: 2923 Class: 8 (6.1) Packing group: II  
Proper shipping name: Corrosive solids, toxic, n.o.s. (2-Methyl-4-isothiazolin-3-one)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

#### IMDG

UN number: 2923 Class: 8 (6.1) Packing group: II EMS-No: F-A, S-B  
Proper shipping name: CORROSIVE SOLID, TOXIC, N.O.S. (2-Methyl-4-isothiazolin-3-one)  
Marine pollutant : yes

#### IATA

UN number: 2923 Class: 8 (6.1) Packing group: II  
Proper shipping name: Corrosive solid, toxic, n.o.s. (2-Methyl-4-isothiazolin-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-Methyl-4-isothiazolin-3-one	CAS-No. 2682-20-4	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](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

Version: 6.6

Revision Date: 05/31/2021

Print Date: 01/15/2022