

SAFETY DATA SHEET

Version 8.6
Revision Date 03/31/2022
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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 : 725765
Brand : 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 : C₄H₅NOS

Molecular weight : 115.15 g/mol

CAS-No. : 2682-20-4

EC-No. : 220-239-6

Component	Classification	Concentration
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2-Methyl-4-isothiazolin-3-one		
	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 (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: 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.

Air sensitive. Store under inert gas.

Storage class

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

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: Powder with lumps
Color: dark yellow |
| 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) Density	1.39 g/cm ³ at 20 °C (68 °F)
Relative density	1.3920 °C - 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	none

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 - dust/mist

(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

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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 - Oncorhynchus mykiss (rainbow trout) - 4.77 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	flow-through test EC50 - Daphnia magna (Water flea) - 0.85 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test EC50 - Skeletonema costatum - 0.069 mg/l - 96 h (OECD Test Guideline 201)

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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 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. 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: 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.

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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