Chemical Safety Data Sheet MSDS / SDS

2-Methyl-4-isothiazolin-3-one

Revision Date:2026-10-24 Revision Number:1

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

Product identifier

Product name	: 2-Methyl-4-isothiazolin-3-one
CBnumber	: CB0193926
CAS	: 2682-20-4
EINECS Number	: 220-239-6
Synonyms	: methylisothiazolinone,2-methyl-4-isothiazolin-3-one

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

Relevant identified uses	: For R&D use only. Not for medicinal, household or other use.
Uses advised against	: none

Company Identification

Company	: Chemicalbook
Address	: Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone	: 010-86108875

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word Danger

Precautionary statements

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P273 Avoid release to the environment.

P280 Wear protective gloves/protective clothing/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. Continuerinsing.

P310 Immediately call a POISON CENTER or doctor/physician.

Hazard statements

H302 Harmful if swallowed

H314 Causes severe skin burns and eye damage

H317 May cause an allergic skin reaction

H331 Toxic if inhaled

H335 May cause respiratory irritation

H400 Very toxic to aquatic life

SECTION 3: Composition/information on ingredients

Substance

Product name	: 2-Methyl-4-isothiazolin-3-one
Synonyms	: methylisothiazolinone,2-methyl-4-isothiazolin-3-one
CAS	: 2682-20-4
EC number	: 220-239-6
MF	: C4H5NOS
MW	: 115.15

SECTION 4: First aid measures

Description of first aid measures

General advice

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

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

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

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special hazards arising from the substance or mixture

Carbon oxides Nitrogen oxides (NOx) Sulfur oxides Combustible.

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

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.

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

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.

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

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.

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.

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 parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

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.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Body Protection

Acid-resistant protective clothing

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	dark yellow Powder with lumps
Odour	No data available
Odour Threshold	No data available
pH	2,58 at 50 g/l at 25 °C - OCSPP 830.7000
Melting point/freezing point	Melting point/range: 46,7 - 48,3 °C - Regulation (EC) No. 440/2008, Annex, A.1
Initial boiling point and boiling range	>130 °C at 16 hPa - Regulation (EC) No. 440/2008, Annex, A.2
Flash point	Not applicable
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	0,0099 hPa at 20 °C - Regulation (EC) No. 440/2008, Annex, A.4
Vapour density	No data available
Relative density	1,39 g/cm3 at 20 °C 1,39 at 20 °C - Regulation (EC) No. 440/2008, Annex, A.3
Water solubility	soluble
Partition coefficient: n-octanol/water	log Pow: -0,34 at 30 °C - OECD Test Guideline 117 - Bioaccumulation is not expected.
Autoignition temperature	396 °C at 1.012 hPa
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
Explosive properties	No data available
Oxidizing properties	No data available

Other safety information

Surface tension 68,8 mN/m at 1g/l at 19,5 °C

OECD Test Guideline 115

Dissociation constant > 2,81 at 21 °C

OECD Test Guideline 112

SECTION 10: Stability and reactivity

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.

Chemical stability

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

Possibility of hazardous reactions

No data available

Conditions to avoid

no information available

Incompatible materials

Strong oxidizing agents

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

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

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

SECTION 12: Ecological information

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)

Toxicity to bacteria

static test EC50 - activated sludge - 41 mg/l - 3 h (OECD Test Guideline 209)

Persistence and degradability

Biodegradability Result: 55,8 % - Not readily biodegradable.

(OECD Test Guideline 301B)

Remarks: The 10 day time window criterion is not fulfilled.

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

Mobility in soil

No data available

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.

Toxics Screening Level

Due to a lack of toxicity information on this particular chemical, the screening level is being established under R232(1)(i) at 0.1 µg/m3 with annual averaging.

Other adverse effects

No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

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

UN number

ADR/RID: 3261 IMDG: 3261 IATA: 3261

UN proper shipping name

ADR/RID: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (2-Methyl-4-isothiazolin-3-one) IMDG: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (2-Methyl-4-isothiazolin-3-one)
IATA: Corrosive solid, acidic, organic, n.o.s. (2-Methyl-4-isothiazolin-3-one)

Transport hazard class(es)

ADR/RID: 8 IMDG: 8 IATA: 8

Packaging group

ADR/RID: II IMDG: II IATA: II

Environmental hazards

ADR/RID: yes IMDG Marine pollutant: yes IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

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

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: https://www.mem.gov.cn/

Measures for Environmental Management of New Chemical Substances

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: https://www.mee.gov.cn/

EC Inventory:Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: https://echa.europa.eu/

Korea Existing Chemicals List (KECL):Listed. website: http://ncis.nier.go.kr

New Zealand Inventory of Chemicals (NZIoC):Listed. website: https://www.epa.govt.nz/

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: https://emb.gov.ph/

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: https://www.epa.gov/

Vietnam National Chemical Inventory:Listed. website: https://chemicaldata.gov.vn/

SECTION 16: Other information

Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

References

【1】CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple

【2】ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

【3】ECHA - European Chemicals Agency, website: https://echa.europa.eu/

【4】eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

【5】ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg

【6】Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp

【7】HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm

【8】IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/

【9】IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home

【10】Sigma-Aldrich, website: https://www.sigmaaldrich.com/

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