

Chemical Safety Data Sheet MSDS / SDS

5-chloro-2-methyl-2H-isothiazol-3-one SDS

Revision Date:2024-04-25 Revision Number:1

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

Product name: 5-chloro-2-methyl-2H-isothiazol-3-one

CAS: 26172-55-4

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.in

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SECTION 2: Hazards identification**Classification of the substance or mixture**

Acute toxicity - Category 3, Oral

Acute toxicity - Category 3, Dermal

Skin corrosion, Sub-category 1B
Skin sensitization, Category 1
Serious eye damage, Category 1
Specific target organ toxicity - single exposure, Category 3
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1

GHS label elements, including precautionary statements

Pictogram(s)



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
H318 Causes serious eye damage
H335 May cause respiratory irritation
H400 Very toxic to aquatic life

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P272 Contaminated work clothing should not be allowed out of the workplace.
P271 Use only outdoors or in a well-ventilated area.
P273 Avoid release to the environment.

Response

P301+P316 IF SWALLOWED: Get emergency medical help immediately.
P321 Specific treatment (see ... on this label).
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P316 Get emergency medical help immediately.

P361+P364 Take off immediately all contaminated clothing and wash it before reuse.
P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P363 Wash contaminated clothing before reuse.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P333+P317 If skin irritation or rash occurs: Get medical help.
P362+P364 Take off contaminated clothing and wash it before reuse.
P305+P354+P338 IF IN EYES: Immediately rinse with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P317 Get medical help.
P319 Get medical help if you feel unwell.
P391 Collect spillage.

Storage

P405 Store locked up.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	5-chloro-2-methyl-2H-isothiazol-3-one
Common names and synonyms:	5-chloro-2-methyl-2H-isothiazol-3-one
CAS number:	26172-55-4
EC number:	247-500-7
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms/effects, acute and delayed

no data available

Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Poisons A and B

SECTION 5: Firefighting measures

Suitable extinguishing media

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

Specific hazards arising from the chemical

no data available

Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Liquid
Colour:	Crystals from ligroin (60-90 deg C)
Odour:	no data available

Melting point/freezing point:	54-55 deg C
Boiling point or initial boiling point and boiling range:	200.2°C at 760 mmHg
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	74.9°C
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	Solubility in g/100 mL solvent: water, infinite
Partition coefficient n-octanol/water:	log Kow = 0.401 at 24 deg C
Vapour pressure:	0.328mmHg at 25°C
Density and/or relative density:	1.25 (14% aq.)
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

no data available

Possibility of hazardous reactions

no data available

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits toxic vapors of NO_x, SO_x, and Cl-

SECTION 11: Toxicological information**Acute toxicity**

Oral: no data available

Inhalation: no data available

Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information**Toxicity**

Toxicity to fish: LC50; Species: *Lepomis macrochirus* (Bluegill) weight 0.58 g; Conditions: freshwater, flow through; Concentration: 300 µg/L for 96 hr (95% confidence interval: 260-340 µg/L) /14.17% purity

Toxicity to daphnia and other aquatic invertebrates: EC50; Species: *Daphnia magna* (Water Flea) age <24 hr; Conditions: freshwater, flow through; Concentration: 180 µg/L for 48 hr (95% confidence interval: 120-300 µg/L); Effect: intoxication, immobilization /14.17% purity

Toxicity to algae: EC50; Species: *Anabaena flosaquae* (Blue-Green Algae); Conditions: freshwater, static; Concentration: 290 ug/L for 5 days (95% confidence interval: 190-450 ug/L); Effect: population, abundance /13.9% purity

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: Utilizing a CO₂ evolution test with a freshly prepared activated sludge inoculum, 5-chloro-2-methyl-4-isothiazolin-3-one reached 38.8% and 62.0% CO₂ evolution, at initial concentrations of 0.3 and 0.03 ppm, respectively, over a 28 day incubation period(1); the results classified the compound as inherently biodegradable and demonstrated a dependence on concentration(1). Microcosm studies found degradation of 5-chloro-2-methyl-4-isothiazolin-3-one to be primarily due to biodegradation based on tests using sterile controls(1). The half-life of 5-chloro-2-methyl-4-isothiazolin-3-one in an aerobic microcosm using river water and sediment was 17 days(1). At 1 ppm, [¹⁴C][5-chloro-2-methyl-4-isothiazolin-3-one], ring-labeled at the 4 and 5 carbons, degraded with a half-life of 5.4 hours in sandy loam soil that was incubated in the dark at 24-26 deg C for 64 days, and 75% of field moisture capacity(2). 5-Chloro-2-methyl-4-isothiazolin-3-one, present at 100 mg/L, reached 0% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test(3); 5-chloro-2-methyl-4-isothiazolin-3-one is a biocide(1), and the high concentration (100 ppm) may have been toxic to the microorganisms(SRC).

Bioaccumulative potential

A BCF of 5 was determined in bioaccumulation studies performed with bluegill sunfish(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

Ring-labeled [4,5-¹⁴C][5-chloro-2-methyl-4-isothiazolin-3-one] was very mobile in sandy loam, silt loam, clay loam, and sand soils under aerobic conditions; with Freundlich K_d values of 0.1-1.5, and in sandy loam sediment with a Freundlich K_d value of 4.9 being measured(1). K_{oc} values were 30-144 for the soils and 310 for the sediment(1). According to a classification scheme(2), these K_{oc} values suggest that 5-chloro-2-methyl-4-isothiazolin-3-one is expected to have very high to high mobility in soil and moderate mobility in sediment.

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN1760 (For reference only, please check.)

IMDG: UN1760 (For reference only, please check.)

IATA: UN1760 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: CORROSIVE LIQUID, N.O.S. (For reference only, please check.)

IMDG: CORROSIVE LIQUID, N.O.S. (For reference only, please check.)

IATA: CORROSIVE LIQUID, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 8 (For reference only, please check.)

IMDG: 8 (For reference only, please check.)

IATA: 8 (For reference only, please check.)

Packing group, if applicable

ADR/RID: I (For reference only, please check.)

IMDG: I (For reference only, please check.)

IATA: I (For reference only, please check.)

Environmental hazards

ADR/RID: Yes

IMDG: Yes

IATA: Yes

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

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

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

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

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

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

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

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

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

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

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Disclaimer: 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. We as supplier shall not be held liable for any