

Chemical Safety Data Sheet MSDS / SDS

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

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

Section 1	Section 2	Section 3	Section 4	Section 5	Section 6	Section 7	Section 8
Section 9	Section 10	Section 11	Section 12	Section 13	Section 14	Section 15	Section 16

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

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

CAS: 2682-20-4

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
Serious eye damage, Category 1
Skin sensitization, Sub-category 1A
Acute toxicity - Category 2, Inhalation
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

Hazard statement(s)

H301 Toxic if swallowed
H311 Toxic 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)

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.
P284 [In case of inadequate ventilation] wear respiratory protection.
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.
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.
P333+P317 If skin irritation or rash occurs: Get medical help.
P362+P364 Take off contaminated clothing and wash it before reuse.
P320 Specific treatment is urgent (see ... on this label).
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:	2-methyl-2H-isothiazol-3-one
Common names and synonyms:	2-methyl-2H-isothiazol-3-one
CAS number:	2682-20-4
EC number:	220-239-6

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

Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide. Special protective

equipment for firefighters: Wear self contained breathing apparatus for fire fighting if necessary.

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

Accidental Release Measures. Personal precautions: Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Environmental precautions: Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided. Methods and materials for containment and cleaning up: Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

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

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

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:	Colorless prisms
Odour:	no data available
Melting point/freezing point:	254-256 °C
Boiling point or initial boiling point and boiling range:	182.8 °C at 760 mmHg
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	64.3 °C
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	In water, 5.367X10+5 mg/L at 25 deg C (est)
Partition coefficient n-octanol/water:	log Kow = -0.83 (est)
Vapour pressure:	<0.1 mm Hg (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

Stable under recommended storage conditions.

Possibility of hazardous reactions

no data available

Conditions to avoid

no data available

Incompatible materials

Materials to avoid: Strong oxidizing agents, Amines, Mercaptans, Reducing agents.

Hazardous decomposition products

When heated to decomposition it emits toxic vapors of SO_x.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Rats(female) oral 183 mg/kg bw RH-573 Technical

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 ug/L for 96 hr (95% confidence interval: 240-320 ug/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 ug/L for 48 hr (95% confidence interval: 140-190 ug/L); Effect: intoxication, immobilization /14.17% purity

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: Utilizing a CO₂ evolution test with a freshly prepared activated sludge inoculum, methylisothiazolinone reached 54.1, 55.8 and 47.6% CO₂ evolution, at initial concentrations of 0.3, 0.03 and 0.01 ppm, respectively, over a 28 day incubation period; the results classified the compound as inherently biodegradable and demonstrated a dependence on concentration. Microcosm studies in aerobic water found degradation of methylisothiazolinone to be primarily due to biodegradation based on tests using sterile controls. The half-life of methylisothiazolinone in an aerobic microcosm using river water and sediment was 9 days(1).

Bioaccumulative potential

A BCF of 3 was reported in bluegill sunfish (*Lepomis macrochirus*) for methylisothiazolinone(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of methylisothiazolinone can be estimated to be 12(SRC). According to a classification scheme(2), this estimated Koc value suggests that methylisothiazolinone is expected to have very high mobility in soil.

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: no data available

IMDG: no data available

IATA: no data available

UN Proper Shipping Name

ADR/RID: no data available

IMDG: no data available

IATA: no data available

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

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

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

IATA: III (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/>

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