

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

# 4,5-Dichloro-2-octyl- isothiazolone



Version number: 1  
Issued: 2023-12-07

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

### 1.1. Product identifier

**Trade name**

4,5-Dichloro-2-octyl-isothiazolone

**CAS number**

64359-81-5

**EC number**

264-843-8

**Synonyms**

3(2h)-isothiazolone, 4,5-dichloro-2-octyl-

### 1.2. Relevant identified uses of the substance or mixture and uses advised against

**Relevant identified uses**

Research and development.

**Not suitable for use in**

Not suitable for human consumption or veterinary purposes.

### 1.3. Details of the supplier of the safety data sheet

**Supplier**

Molekula Group

Address

Molekula Ltd, Lingfield Way, Darlington,  
DL1 4XX Darlington  
United Kingdom

Telephone

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Email

info@molekula.com

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## 1.4. Emergency telephone number

### Poison center/Additional emergency number

0344 892 0111 - National Poisons Information Service (Newcastle Centre)

## SECTION 2: Hazards identification

### 2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

#### Classification

Serious eye damage, hazard category 1  
Hazardous to the aquatic environment — Acute hazard category 1  
Hazardous to the aquatic environment — Chronic hazard category 1  
Acute toxicity, oral, hazard category 4  
Acute toxicity, inhalation, hazard category 1  
Skin sensitisation, hazard category 1, sub-category 1A  
Skin corrosion, hazard category 1

#### Hazard statements

H302, H314, H317, H318, H330, H400, H410

### 2.2. Label elements

Labelling according to Regulation (EC) No 1272/2008

#### Hazard pictograms



#### Signal word

Danger

#### Hazard statements

H302 Harmful if swallowed.  
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.

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## **Precautionary statements**

P202 Do not handle until all safety precautions have been read and understood.  
 P260 Do not breathe dust/fumes/gas/mist/vapours/spray.  
 P262 Do not get in eyes, on skin, or on clothing.  
 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.  
 P280 Wear protective gloves/protective clothing/eye protection/face protection.  
 P284 wear respiratory protection.  
 P301 + P312 IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.  
 P301 + P330 + P331 IF SWALLOWED: rinse mouth. Do NOT induce vomiting.  
 P302 + P352 IF ON SKIN: Wash with plenty of water/.  
 P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.  
 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.  
 P310 Immediately call a POISON CENTER/doctor.  
 P320 Specific treatment is urgent (see on this label).  
 P321 Specific treatment (see on this label).  
 P330 Rinse mouth.  
 P362 + P364 Take off contaminated clothing and wash it 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 local regulations.

## **2.3. Other hazards**

No data available

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## SECTION 3: Composition/information on ingredients

### 3.2. Mixtures

Chemical name	CAS No. EC No. REACH No. Index No.	Concentration	Classification	H-phrase M factor acute M factor chronic	Note
4,5-dichloro-2-octyl- 2H-isothiazol-3-one; [DCOIT]	64359-81-5 264-843-8 - 613-335-00-8	100%	Acute Tox. 4 - oral, Skin Corr. 1, Skin Sens. 1A, Eye Dam. 1, Acute Tox. 2 - inhalation, Aquatic Acute 1, Aquatic Chronic 1	H302, H314, H317, H318, H330, H400, H410, EUH071 M-acute=100 M-chro=100	Inhalation: ATE = 0.16 mg/L (dusts/mists); Oral: ATE = 567 mg/kg; Skin Irrit. 2; H315: 0,025 % = C < 5 %; Eye Irrit. 2; H319: 0,025 % = C < 3 %; Skin Sens. 1A; H317: C = 0,0015 %

#### Molecular weight

282.22

#### Substance additional information

For the complete text of H- / EUH-statements mentioned in this section, see section 16.

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

IF exposed or concerned: Get medical advice/attention. First aiders/ medical personnel need to protect themselves. Show this Safety Data Sheet (SDS) to medical personnel.

#### Inhalation

Toxic if inhaled. IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/doctor. If breathing stops, provide artificial respiration. For breathing difficulties oxygen may be necessary.

#### Skin contact

In case of skin contact: IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower]. Immediately call a POISON CENTER/doctor. The casualty should be transferred to hospital for further treatment.

#### Eye contact

Remove contact lenses if present. Rinse eyes with water. Continue to rinse for at least 15 minutes and seek medical attention.

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## **Ingestion**

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 if the persons are fully conscious and awake).

## **Information for doctors**

No data available.

## **4.2. Most important symptoms and effects, both acute and delayed**

The severity of the symptoms described will vary dependant of the concentration and the length of exposure. See section 11 for more detailed information on health effects and symptoms.

## **Inhalation**

Single exposure may cause the following adverse effects: Difficulty in breathing. Unconsciousness, possibly death.

## **Skin contact**

Single exposure may cause the following adverse effects: Unconsciousness, possibly death.

## **Eye contact**

Single exposure may cause the following adverse effects: Severe irritation. Unconsciousness, possibly death.

## **Ingestion**

Single exposure may cause the following adverse effects: Severe abdominal pain. May cause severe internal injury. Unconsciousness, possibly death.

## **4.3. Indication of any immediate medical attention and special treatment needed**

Treat symptomatically. No special treatment requirement.

## **SECTION 5: Firefighting measures**

### **5.1. Extinguishing media**

#### **Suitable extinguishing media**

In case of fire: Use foam, carbon dioxide, dry powder or water fog to extinguish.

#### **Unsuitable extinguishing media**

No specific fire fighting procedure given.

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## 5.2. Special hazards arising from the substance or mixture

Specific hazards: Toxic. Corrosive.

Thermal decomposition or combustion may liberate carbon oxides and other toxic gases or vapours.

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

Nitrous gases (NO<sub>x</sub>).

Sulfur oxides

Hydrogen Chloride gas

Combustible.

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

## 5.3. Advice for firefighters

### **Special protective equipment for fire-fighters**

Evacuate area. Avoid breathing gas, fume, vapours or spray. Cool containers exposed to heat with water spray and remove container, if no risk is involved.

## SECTION 6: Accidental release measures

### 6.1. Personal precautions, protective equipment and emergency procedures

Avoid breathing dust/fume/gas/mist/vapours/spray. Provide adequate ventilation. Avoid contact with skin and eyes. Avoid dust formation. For personal protection, see section 8.

### 6.2. Environmental precautions

Avoid discharge into drains, water courses or onto the ground.

### 6.3. Methods and material for containment and cleaning up

Collect spillage with shovel, broom or the like and reuse, if possible. Dispose of large amounts of spillage/waste according to agreement with local authorities.

### 6.4. Reference to other sections

For personal protection, see section 8. For waste disposal, see section 13.

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

#### **Preventive handling precautions**

For precautions see section 2.2. Do not handle until all safety precautions have been read and understood. Do not handle broken packages without protective equipment. This product is toxic. Keep containers tightly closed. Immediate first aid is necessary. Wear protective clothing, gloves, eye and face protection. Avoid contact with skin and eyes. Do not breathe dust/fume/gas/mist/vapours/spray. Avoid ingestion and inhalation. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Do not reuse empty containers. Work under hood

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## General hygiene

Observe good chemical hygiene practices. Remove contaminated clothing immediately and wash skin with soap and water. Remove contaminated clothing and launder thoroughly before re-use. Wash skin thoroughly after handling.

## 7.2. Conditions for safe storage, including any incompatibilities

Store at room temperature. Store in a dry place. Store in a closed container.

Storage class : Toxic storage.

## 7.3. Specific end use(s)

No specific usage precautions noted.

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

No data available

### 8.2. Exposure controls

#### Personal Protective Equipment Symbols



#### Eye / face protection

Wear eye protection.

#### Hand protection

Wear protective gloves.

Always inspect gloves before use. If signs of wear and tear are noticed then the gloves should be replaced.

No specific hygiene procedures noted, but good personal hygiene practices are always advisable, especially when working with chemicals.

Wash contaminated skin thoroughly after handling.

#### Other skin protection

Wash skin thoroughly after handling.

#### Respiratory protection

Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided.

#### Environmental exposure controls

Avoid discharge into drains.

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## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

#### Physical state

Solid

#### Colour

White.

#### Odour

No data available

#### Melting point / freezing point

44 - 46 °C

#### Boiling point or initial boiling point and boiling range

No data available

#### Flammability

No data available

#### Lower and upper explosion limit

No data available

#### Flash point

No data available

#### Auto-ignition temperature

No data available

#### Decomposition temperature

No data available

#### pH

No data available

#### Kinematic viscosity

No data available

#### Solubility

No data available

#### Partition coefficient n-octanol/water

No data available

#### Vapour pressure

No data available



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## Density and/or relative density

No data available

## Relative vapour density

No data available

## Particle characteristics

No data available

## 9.2. Other information

No data available

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

There are no known reactivity hazards associated with this product.

### 10.2. Chemical stability

Stable under normal temperature conditions. Stable under the prescribed storage conditions.

### 10.3. Possibility of hazardous reactions

There are no known conditions that are likely to result in a hazardous situation.

### 10.4. Conditions to avoid

strong heating Moisture.

### 10.5. Incompatible materials

Strong oxidising agents. Acids. Bases.

### 10.6. Hazardous decomposition products

See section 5.

## SECTION 11: Toxicological information

### 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

#### Acute toxicity

Product / Substance name CAS / EC no.	Dose descriptor	Value / Dose	Exposure route
4,5-dichloro-2-octyl- 2H-iso-thiazol-3-one; [DCOIT] 64359-81-5 / 264-843-8	Acute toxicity estimate Oral	567 mg/kg	-
4,5-dichloro-2-octyl- 2H-iso-thiazol-3-one; [DCOIT] 64359-81-5 / 264-843-8	ATE = Acute Toxicity Estimate.	0.16 mg/l	Inhalation.

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## Aspiration hazard

Based on available data, the classification criteria are not met.

## 11.2. Information on other hazards

No data available

## SECTION 12: Ecological information

### 12.1. Toxicity

No data available

### 12.2. Persistence and degradability

No data available

### 12.3. Bioaccumulative potential

No data available

### 12.4. Mobility in soil

No data available

### 12.5. Results of PBT and vPvB assessment

No data available

### 12.6. Endocrine disrupting properties

This product does not contain any known or suspected endocrine disruptors.

### 12.7. Other adverse effects

No data available

## SECTION 13: Disposal considerations

### 13.1. Waste treatment methods

#### Disposal considerations

Dispose of contents/container in accordance with local/regional/national/international regulations.

## SECTION 14: Transport information

### 14.1. UN number

2923

### 14.2. UN proper shipping name

#### ADR / RID / ADN proper shipping name

CORROSIVE SOLID, TOXIC, N.O.S. (4,5-Dichloro-2-octyl-isothiazolone)

#### IMDG proper shipping name

CORROSIVE SOLID, TOXIC, N.O.S. (4,5-Dichloro-2-octyl-isothiazolone)

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## IATA proper shipping name

Corrosive solid, toxic, n.o.s. (4,5-Dichloro-2-octyl-isothiazolone)

### 14.3. Transport hazard class(es)

#### Label

ADR/RID/ADN



8



6.1

IMDG



8



6.1

IATA



8



6.1

#### ADR / RID Class

8

#### ADR / RID Classification code

CT2

#### ADR / RID hazard identification number

86

#### IMDG Class

8 (6.1)

#### IATA Class

8 (6.1)

#### ADN Class

8

#### ADN Class Code

CT2

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## 14.4. Packing group

ADR / RID / ADN: III  
IMDG: III  
IATA: III

## 14.5. Environmental hazards

**IMDG EmS**  
F-A, S-B

## 14.6. Special precautions for user

Tunnel restriction code: E  
Transport category: 3

## 14.7. Maritime transport in bulk according to IMO instruments

IBC Instruction: IBC08

## SECTION 15: Regulatory information

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

#### **EU regulations**

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.  
This material safety data sheet complies with the requirements of Regulation (EU) 2020/878.

#### **National regulations**

Directive: 2012/18/EU:  
ACUTE TOXIC  
ENVIRONMENTAL HAZARDS

### 15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

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## SECTION 16: Other information

### Phrase meaning

Eye Dam. 1 - Serious eye damage, hazard category 1

Aquatic Acute 1 - Hazardous to the aquatic environment — Acute hazard category 1

Aquatic Chronic 1 - Hazardous to the aquatic environment — Chronic hazard category 1

Acute Tox. 4 - oral - Acute toxicity, oral, hazard category 4

Acute Tox. 1 - inhalation - Acute toxicity, inhalation, hazard category 1

Skin Sens. 1A - Skin sensitisation, hazard category 1, sub-category 1A

Skin Corr. 1 - Skin corrosion, hazard category 1

Acute Tox. 2 - inhalation - Acute toxicity, inhalation, hazard category 2

H302 Harmful if swallowed.

H314 Causes severe skin burns and eye damage.

H317 May cause an allergic skin reaction.

H318 Causes serious eye damage.

H330 Fatal if inhaled.

H400 Very toxic to aquatic life.

H410 Very toxic to aquatic life with long lasting effects.

EUH071 Corrosive to the respiratory tract.