

# N-Methyl-3-oxodihydroisothiazole

## Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830  
Date of issue: 11/20/2019 Version: 1.0

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

#### 1.1. Product identifier

Product form	: Substance
Substance name	: N-Methyl-3-oxodihydroisothiazole
Chemical name	: 2-methylisothiazol-3(2H)-one
EC Index-No.	: 613-326-00-9
EC-No.	: 220-239-6
CAS-No.	: 2682-20-4
Product code	: 74130881
Formula	: C4H5NOS
Product group	: Raw material

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

##### 1.2.1. Relevant identified uses

Main use category	: Laboratory use, Industrial use, Professional use
Industrial/Professional use spec	: For professional use only
Use of the substance/mixture	: For analytical purposes Scientific research and development Not for human consumption or veterinary purposes.

##### 1.2.2. Uses advised against

No additional information available

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

##### Supplier

Scafell Organics  
Molekula Ltd  
Lingfield Way  
Darlington - England  
T +44 (0) 1949 823777 / +44 (0) 7590 545705  
[info@molekula.com](mailto:info@molekula.com) / [kbowen@molekula.com](mailto:kbowen@molekula.com) - [www.molekula.com](http://www.molekula.com)

#### 1.4. Emergency telephone number

Emergency number : +44 (0) 7590 545705

### SECTION 2: Hazards identification

#### 2.1. Classification of the substance or mixture

##### Classification according to Regulation (EC) No. 1272/2008 [CLP]

Acute toxicity (inhal.), Category 2	H330	
Acute toxicity (dermal), Category 3	H311	
Acute toxicity (oral), Category 3	H301	
Skin corrosion/irritation, Category 1B	H314	
Serious eye damage/eye irritation, Category 1	H318	
Skin sensitisation, category 1A	H317	
Hazardous to the aquatic environment — Acute Hazard, Category 1	H400	(M=10)
Hazardous to the aquatic environment — Chronic Hazard, Category 1	H410	
Full text of H statements : see section 16		
Specific concentration limits:		
( 0.0015 =<C <= 100)	Skin Sens. 1A, H317	

##### Adverse physicochemical, human health and environmental effects

No additional information available

#### 2.2. Label elements

##### Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP)



Signal word (CLP)

: Danger

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Hazard statements (CLP)	: H330 - Fatal if inhaled. H311 - Toxic in contact with skin. H301 - Toxic if swallowed. H314 - Causes severe skin burns and eye damage. H317 - May cause an allergic skin reaction. H410 - Very toxic to aquatic life with long lasting effects.
Precautionary statements (CLP)	: P260 - Do not breathe dust/fume/gas/mist/vapours/spray. P273 - Avoid release to the environment. P280 - Wear protective gloves/protective clothing/eye protection/face protection. P284 - Wear respiratory protection. P301+P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor. P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
EUH-statements	: EUH071 - Corrosive to the respiratory tract.

### 2.3. Other hazards

This substance/mixture does not meet the PBT criteria of REACH regulation, annex XIII

This substance/mixture does not meet the vPvB criteria of REACH regulation, annex XIII

## SECTION 3: Composition/information on ingredients

### 3.1. Substances

Name	Product identifier	%
N-Methyl-3-oxodihydroisothiazole	(CAS-No.) 2682-20-4 (EC-No.) 220-239-6 (EC Index-No.) 613-326-00-9	100

Full text of H-statements: see section 16

### 3.2. Mixtures

Not applicable

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

First-aid measures general	: If possible show this sheet, if not available show packaging or label. Never give anything by mouth to an unconscious person. Do not leave affected person unattended.
First-aid measures after inhalation	: If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing. Give oxygen or artificial respiration if necessary. If breathing difficulties persist : Get medical advice/attention.
First-aid measures after skin contact	: After contact with skin, take off immediately all contaminated clothing, and wash immediately with plenty of water. Do not remove clothing if it sticks to the skin. If irritation persists, consult a doctor.
First-aid measures after eye contact	: Rinse immediately with plenty of water. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.
First-aid measures after ingestion	: Rinse mouth out with water. Do not induce vomiting. Get medical advice/attention.

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

Symptoms/effects	: Corrosive to the respiratory tract. May cause an allergic skin reaction. May cause allergy or asthma symptoms or breathing difficulties if inhaled.
Symptoms/effects after inhalation	: Fatal if inhaled. Material is destructive to tissue of the mucuous membranes and upper respiratory tract. Cough, shortness of breath, headache, nausea. Depression of the central nervous system, headaches, dizziness, drowsiness, loss of coordination. May cause circulatory shock, respiratory depression and convulsions.
Symptoms/effects after skin contact	: Toxic in contact with skin. Causes severe burns. May produce skin irritation, blistering, ulcers, and deep scarring.
Symptoms/effects after eye contact	: Causes serious eye damage. May cause severe chemical burns to skin and cornea.
Symptoms/effects after ingestion	: Swallowing a small quantity of this material will result in serious health hazard. Symptoms of ingestion include drowsiness, weakness, headache, dizziness, nausea, vomiting. burns of the upper digestive and respiratory tracts, abdominal pain, bloody vomiting, severe damage to the delicate tissue and danger of perforation.

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

Immediately call a POISON CENTER/doctor.

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

Suitable extinguishing media	: Foam. Dry powder. Carbon dioxide. Water spray. Sand.
Unsuitable extinguishing media	: Do not use a heavy water stream.

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

Hazardous decomposition products in case of fire	: Carbon oxides (CO, CO <sub>2</sub> ). Sulphur oxides. Nitrogen oxides.
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### 5.3. Advice for firefighters

Precautionary measures fire	: Keep container tightly closed and away from heat, sparks and flame. Keep away from combustible materials.
Firefighting instructions	: Use water spray or fog for cooling exposed containers. Exercise caution when fighting any chemical fire. Prevent fire fighting water from entering the environment.
Protection during firefighting	: Do not enter fire area without proper protective equipment, including respiratory protection.
Other information	: Warn all persons of toxic hazard.

## SECTION 6: Accidental release measures

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

General measures	: Isolate from fire, if possible, without unnecessary risk. Avoid dust formation. No flames, no sparks. Eliminate all sources of ignition.
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#### 6.1.1. For non-emergency personnel

Protective equipment	: Wear recommended personal protective equipment.
Emergency procedures	: Evacuate unnecessary personnel. Mark out the contaminated area with signs and prevent access to unauthorized personnel. Do not touch or walk on the spilled product. Avoid contact with skin, eyes and clothing.
Measures in case of dust release	: Keep upwind. Avoid creating or spreading dust. Ventilate the area thoroughly, especially low lying areas (basements, workpits etc).

#### 6.1.2. For emergency responders

Protective equipment	: Equip cleanup crew with proper protection. Use self-contained breathing apparatus and chemically protective clothing.
Emergency procedures	: Ventilate area.

### 6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if product enters sewers or public waters.

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

Methods for cleaning up	: On land, sweep or shovel into suitable containers. Shovel or sweep up and put in a closed container for disposal.
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### 6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

Precautions for safe handling	: Avoid creating or spreading dust. Provide local exhaust or general room ventilation.
Hygiene measures	: Take off immediately all contaminated clothing and wash it before reuse. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Do not eat, drink or smoke when using this product.

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

Technical measures	: Ensure adequate ventilation, especially in confined areas.
Storage conditions	: Keep only in the original container in a cool, well ventilated place away from : Heat sources, Direct sunlight. Keep container closed when not in use. Air sensitive. Store contents under inert gas.
Incompatible products	: Strong oxidizing agents. Air contact.
Incompatible materials	: Sources of ignition. Direct sunlight. Heat sources.
Heat and ignition sources	: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
Storage area	: Store below 20 °C. Keep container tightly closed and dry. Keep in a cool, well-ventilated place away from acids.

### 7.3. Specific end use(s)

For analytical purposes. Scientific research and development. Not for human consumption or veterinary purposes.

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

No additional information available

### 8.2. Exposure controls

#### Appropriate engineering controls:

Handle in accordance with good industrial hygiene and safety procedures.

#### Personal protective equipment:

Avoid all unnecessary exposure.

#### Materials for protective clothing:

Wear suitable protective clothing, gloves and eye/face protection

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<b>Hand protection:</b>					
The protective gloves to be used must comply with the specifications of the regulation 2016/425 and the resultant standard EN 374					
<b>Type</b>	<b>Material</b>	<b>Permeation</b>	<b>Thickness (mm)</b>	<b>Penetration</b>	<b>Standard</b>
Disposable gloves	Nitrile rubber (NBR)	6 (> 480 minutes)	0.11		EN 374
<b>Eye protection:</b>					
Emergency eye wash fountains should be available in the immediate vicinity of any potential exposure. Use eye protection according to EN 166, designed to protect against powders and dusts.					
<b>Type</b>	<b>Use</b>		<b>Characteristics</b>	<b>Standard</b>	
Safety goggles, Face shield	Fine dust, Dust		tightly fitting safety goggles, With side shields	EN 166	
<b>Skin and body protection:</b>					
Emergency safety showers should be available in the immediate vicinity of any potential exposure. Keep suitable chemically resistant protective clothing readily available for emergency use					
<b>Type</b>			<b>Standard</b>		
Total impervious protective suits, gloves, and boots must be worn to prevent any contact with the product			EN ISO 13982		
<b>Respiratory protection:</b>					
Keep self contained breathing apparatus readily available for emergency use. Where exposure through inhalation may occur from use, respiratory protection equipment is recommended					
<b>Device</b>	<b>Filter type</b>		<b>Condition</b>	<b>Standard</b>	
Respiratory protective device with a particle filter	Type P3		Dust protection	EN 143	

### Other information:

Do not eat, drink or smoke during use.

## SECTION 9: Physical and chemical properties

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

Physical state	: Solid
Appearance	: lumps. Powder. Paste.
Molecular mass	: 115.15 g/mol
Colour	: White to off-white.
Odour	: No data available.
Odour threshold	: No data available
pH	: No data available
Relative evaporation rate (butylacetate=1)	: No data available
Melting point	: 48 - 50 °C
Freezing point	: No data available
Boiling point	: 93 °C
Flash point	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Flammability (solid, gas)	: Non flammable.
Vapour pressure	: No data available
Relative vapour density at 20 °C	: No data available
Relative density	: No data available
Solubility	: No data available
Log Pow	: 0.119
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidising properties	: No data available
Explosive limits	: No data available

### 9.2. Other information

No additional information available

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### SECTION 10: Stability and reactivity

#### 10.1. Reactivity

The product is non-reactive under normal conditions of use, storage and transport.

#### 10.2. Chemical stability

Stable under recommended handling and storage conditions (see section 7).

#### 10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

#### 10.4. Conditions to avoid

Protect from sunlight. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

#### 10.5. Incompatible materials

Strong oxidizers. Air contact.

#### 10.6. Hazardous decomposition products

No hazardous decomposition products known at room temperature. Thermal decomposition generates : Carbon oxides (CO, CO<sub>2</sub>). Nitrogen oxides. Sulphur oxides.

### SECTION 11: Toxicological information

#### 11.1. Information on toxicological effects

Acute toxicity (oral)	: Oral: Toxic if swallowed.
Acute toxicity (dermal)	: Dermal: Toxic in contact with skin.
Acute toxicity (inhalation)	: Inhalation: Fatal if inhaled.
Skin corrosion/irritation	: Causes severe skin burns and eye damage.
Additional information	: Based on available data, the classification criteria are not met
Serious eye damage/irritation	: Causes serious eye damage.
Additional information	: Based on available data, the classification criteria are not met
Respiratory or skin sensitisation	: May cause an allergic skin reaction.
Additional information	: Based on available data, the classification criteria are not met
Germ cell mutagenicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Carcinogenicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Reproductive toxicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
STOT-single exposure	: Not classified
Additional information	: Based on available data, the classification criteria are not met
STOT-repeated exposure	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Aspiration hazard	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Potential adverse human health effects and symptoms	: Based on available data, the classification criteria are not met.

### SECTION 12: Ecological information

#### 12.1. Toxicity

Hazardous to the aquatic environment, short-term (acute)	: Very toxic to aquatic life.
Hazardous to the aquatic environment, long-term (chronic)	: Very toxic to aquatic life with long lasting effects.

#### N-Methyl-3-oxodihydroisothiazole (2682-20-4)

EC50 Daphnia 1	0.18 mg/l Daphnia magna (Water flea) 48hr
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#### 12.2. Persistence and degradability

#### N-Methyl-3-oxodihydroisothiazole (2682-20-4)

Persistence and degradability	No data available.
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#### 12.3. Bioaccumulative potential

#### N-Methyl-3-oxodihydroisothiazole (2682-20-4)

Log Pow	0.119
Bioaccumulative potential	No data available.

#### 12.4. Mobility in soil

No additional information available

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### 12.5. Results of PBT and vPvB assessment

#### N-Methyl-3-oxodihydroisothiazole (2682-20-4)

This substance/mixture does not meet the PBT criteria of REACH regulation, annex XIII

This substance/mixture does not meet the vPvB criteria of REACH regulation, annex XIII

### 12.6. Other adverse effects

Additional information : Avoid release to the environment.

## SECTION 13: Disposal considerations






### 13.1. Waste treatment methods

Product/Packaging disposal recommendations : Dispose in a safe manner in accordance with local/national regulations.

Ecology - waste materials : Avoid release to the environment. Hazardous waste due to toxicity.

## SECTION 14: Transport information

In accordance with ADR / RID / IMDG / IATA / ADN

ADR	IMDG	IATA	ADN	RID
<b>14.1. UN number</b>				
3261	3261	3261	3261	3261
<b>14.2. UN proper shipping name</b>				
CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S.	CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S.	Corrosive solid, acidic, organic, n.o.s.	CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S.	CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S.
<b>Transport document description</b>				
UN 3261 CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (N-Methyl-3-oxodihydroisothiazole), 8, II, (E), ENVIRONMENTALLY HAZARDOUS	UN 3261 CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (N-Methyl-3-oxodihydroisothiazole), 8, II, MARINE POLLUTANT/ENVIRONMENTALLY HAZARDOUS	UN 3261 Corrosive solid, acidic, organic, n.o.s. (N-Methyl-3-oxodihydroisothiazole), 8, II, ENVIRONMENTALLY HAZARDOUS	UN 3261 CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (N-Methyl-3-oxodihydroisothiazole), 8, II, ENVIRONMENTALLY HAZARDOUS	UN 3261 CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (N-Methyl-3-oxodihydroisothiazole), 8, II, ENVIRONMENTALLY HAZARDOUS
<b>14.3. Transport hazard class(es)</b>				
8	8	8	8	8
				
<b>14.4. Packing group</b>				
II	II	II	II	II
<b>14.5. Environmental hazards</b>				
Dangerous for the environment : Yes	Dangerous for the environment : Yes Marine pollutant : Yes	Dangerous for the environment : Yes	Dangerous for the environment : Yes	Dangerous for the environment : Yes

No supplementary information available

### 14.6. Special precautions for user

#### Overland transport

Classification code (ADR) : C4  
Special provisions (ADR) : 274  
Limited quantities (ADR) : 1kg  
Excepted quantities (ADR) : E2  
Packing instructions (ADR) : P002, IBC08  
Special packing provisions (ADR) : B4  
Mixed packing provisions (ADR) : MP10  
Portable tank and bulk container instructions (ADR) : T3  
Portable tank and bulk container special provisions (ADR) : TP33

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Tank code (ADR) : SGAN, L4BN

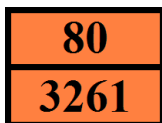
Vehicle for tank carriage : AT

Transport category (ADR) : 2

Special provisions for carriage - Packages (ADR) : V11

Hazard identification number (Kemler No.) : 80

Orange plates :



Tunnel restriction code (ADR) : E

EAC code : 2X

### Transport by sea

Special provisions (IMDG) : 274

Packing instructions (IMDG) : P002

IBC packing instructions (IMDG) : IBC08

IBC special provisions (IMDG) : B21, B4

Tank instructions (IMDG) : T3

Tank special provisions (IMDG) : TP33

EmS-No. (Fire) : F-A

EmS-No. (Spillage) : S-B

Stowage category (IMDG) : B

Properties and observations (IMDG) : Causes burns to skin, eyes and mucous membranes.

### Air transport

PCA Excepted quantities (IATA) : E2

PCA Limited quantities (IATA) : Y844

PCA limited quantity max net quantity (IATA) : 5kg

PCA packing instructions (IATA) : 859

PCA max net quantity (IATA) : 15kg

CAO packing instructions (IATA) : 863

CAO max net quantity (IATA) : 50kg

Special provisions (IATA) : A3, A803

ERG code (IATA) : 8L

### Inland waterway transport

Classification code (ADN) : C4

Special provisions (ADN) : 274

Limited quantities (ADN) : 1 kg

Excepted quantities (ADN) : E2

Equipment required (ADN) : PP, EP

Number of blue cones/lights (ADN) : 0

### Rail transport

Classification code (RID) : C4

Special provisions (RID) : 274

Excepted quantities (RID) : E2

Packing instructions (RID) : P002, IBC08

Special packing provisions (RID) : B4

Mixed packing provisions (RID) : MP10

Portable tank and bulk container instructions (RID) : T3

Portable tank and bulk container special provisions (RID) : TP33

Tank codes for RID tanks (RID) : SGAN, L4BN

Transport category (RID) : 2

Special provisions for carriage – Packages (RID) : W11

Colis express (express parcels) (RID) : CE10

Hazard identification number (RID) : 80

### 14.7. Transport in bulk according to Annex II of Marpol and the IBC Code

Not applicable

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### SECTION 15: Regulatory information

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

##### 15.1.1. EU-Regulations

No REACH Annex XVII restrictions

N-Methyl-3-oxodihydroisothiazole is not on the REACH Candidate List

Directive 2012/18/EU (SEVESO III)

##### 15.1.2. National regulations

No additional information available

#### 15.2. Chemical safety assessment

No chemical safety assessment has been carried out for the substance or the mixture by the supplier

### SECTION 16: Other information

Data sources : REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.

Other information : None.

Full text of H- and EUH-statements:	
Acute Tox. 2 (Inhalation)	Acute toxicity (inhal.), Category 2
Acute Tox. 3 (Dermal)	Acute toxicity (dermal), Category 3
Acute Tox. 3 (Oral)	Acute toxicity (oral), Category 3
Aquatic Acute 1	Hazardous to the aquatic environment — Acute Hazard, Category 1
Aquatic Chronic 1	Hazardous to the aquatic environment — Chronic Hazard, Category 1
Eye Dam. 1	Serious eye damage/eye irritation, Category 1
Skin Corr. 1B	Skin corrosion/irritation, Category 1B
Skin Sens. 1A	Skin sensitisation, category 1A
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.
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.

SDS EU (REACH Annex II)

*This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.*