

## SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 04.07.2019

Version 5.6

**SECTION 1. Identification of the substance/mixture and of the company/undertaking****1.1 Product identifier**

Catalogue No.	818214
Product name	1,3-Dimethyltetrahydro-2(1H)-pyrimidinone for synthesis
REACH Registration Number	A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No.	7226-23-5

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

Identified uses	Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal ( <a href="http://www.merckgroup.com">www.merckgroup.com</a> ).
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**1.3 Details of the supplier of the safety data sheet**

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone: +49 6151 72-0
Responsible Department	LS-QHC * e-mail: <a href="mailto:prodsafe@merckgroup.com">prodsafe@merckgroup.com</a>

**1.4 Emergency telephone number** **Please contact the regional company representation in your country.****SECTION 2. Hazards identification****2.1 Classification of the substance or mixture****Classification (REGULATION (EC) No 1272/2008)**

Reproductive toxicity, Category 2, H361f

Acute toxicity, Category 4, Oral, H302

Serious eye damage, Category 1, H318

For the full text of the H-Statements mentioned in this Section, see Section 16.

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## 2.2 Label elements

### Labelling (REGULATION (EC) No 1272/2008)

#### Hazard pictograms



#### Signal word

Danger

#### Hazard statements

H302 Harmful if swallowed.

H318 Causes serious eye damage.

H361f Suspected of damaging fertility.

#### Precautionary statements

##### Prevention

P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

P281 Use personal protective equipment as required.

##### Response

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes.

Remove contact lenses, if present and easy to do. Continue rinsing.

P313 Get medical advice/ attention.

### Reduced labelling ( $\leq 125$ ml)

#### Hazard pictograms



#### Signal word

Danger

#### Hazard statements

H318 Causes serious eye damage.

H361f Suspected of damaging fertility.

#### Precautionary statements

P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

P281 Use personal protective equipment as required.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P313 Get medical advice/ attention.

Contains: tetrahydro-1,3-dimethyl-1H-pyrimidin-2-one

Index-No. 613-280-00-X

## 2.3 Other hazards

None known.

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## SECTION 3. Composition/information on ingredients

### 3.1 Substance

Formula	C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O (Hill)
Index-No.	613-280-00-X
EC-No.	230-625-6
Molar mass	128,17 g/mol

### Hazardous components (REGULATION (EC) No 1272/2008)

*Chemical name (Concentration)*

CAS-No.	Registration number	Classification
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tetrahydro-1,3-dimethyl-1H-pyrimidin-2-one (<= 100 % )

7226-23-5 \*)

Acute toxicity, Category 4, H302  
Serious eye damage, Category 1, H318  
Reproductive toxicity, Category 2, H361f

\*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

For the full text of the H-Statements mentioned in this Section, see Section 16.

### 3.2 Mixture

Not applicable

## SECTION 4. First aid measures

### 4.1 Description of first aid measures

After inhalation: fresh air. Call in physician.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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

Irritation and corrosion  
Risk of serious damage to eyes.

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

No information available.

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## SECTION 5. Firefighting measures

### 5.1 Extinguishing media

*Suitable extinguishing media*

Water, Foam, Carbon dioxide (CO<sub>2</sub>), Dry powder

*Unsuitable extinguishing media*

For this substance/mixture no limitations of extinguishing agents are given.

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

Combustible.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

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

Fire may cause evolution of:

nitrogen oxides

### 5.3 Advice for firefighters

*Special protective equipment 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/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## SECTION 6. Accidental release measures

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

Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

Protective equipment see section 8.

### 6.2 Environmental precautions

Do not let product enter drains.

### 6.3 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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

### 6.4 Reference to other sections

Indications about waste treatment see section 13.

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## SECTION 7. Handling and storage

### 7.1 Precautions for safe handling

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## *Advice on safe handling*

Observe label precautions.

## *Hygiene measures*

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

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

### *Storage conditions*

Tightly closed.

Recommended storage temperature see product label.

## **7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

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## **SECTION 8. Exposure controls/personal protection**

### **8.1 Control parameters**

### **8.2 Exposure controls**

#### **Engineering measures**

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

#### **Individual protection measures**

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

##### *Eye/face protection*

Tightly fitting safety goggles

##### *Hand protection*

full contact:

Glove material:	butyl-rubber
Glove thickness:	0,7 mm
Break through time:	480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,40 mm
Break through time:	30 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 898 Butoject® (full contact), KCL 730 Camatril® -Velours (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

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This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

*Other protective equipment*  
protective clothing

*Respiratory protection*  
required when vapours/aerosols are generated.  
Recommended Filter type: filter ABEK  
The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.  
These measures have to be properly documented.

## Environmental exposure controls

Do not let product enter drains.

## SECTION 9. Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	odourless
Odour Threshold	Not applicable
pH	11 at 100 g/l 20 °C
Melting point	-24 °C
Boiling point/boiling range	247 °C at 1.013 hPa
Flash point	121 °C Method: DIN 51758
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1,6 %(V)
Upper explosion limit	9,3 %(V)

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Vapour pressure	0,5 hPa at 57 °C
Relative vapour density	No information available.
Density	1,064 g/cm <sup>3</sup> at 20 °C
Relative density	No information available.
Water solubility	at 20 °C soluble
Partition coefficient: n-octanol/water	log Pow: 0,05 (25 °C) (experimental) (External MSDS) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	3,41 mPa.s at 20 °C
Explosive properties	Not classified as explosive.
Oxidizing properties	none

## 9.2 Other data

Ignition temperature	255 °C Method: DIN 51794
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## SECTION 10. Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.  
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

### 10.2 Chemical stability

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

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

Risk of explosion with:

chromium(VI) oxide

### 10.4 Conditions to avoid

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Strong heating.

## 10.5 Incompatible materials

no information available

## 10.6 Hazardous decomposition products

in the event of fire: See section 5.

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## SECTION 11. Toxicological information

### 11.1 Information on toxicological effects

#### *Acute oral toxicity*

LD50 Rat: 1.770 mg/kg

OECD Test Guideline 401

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

#### *Acute inhalation toxicity*

Symptoms: Possible damages:, mucosal irritations

#### *Acute dermal toxicity*

This information is not available.

#### *Skin irritation*

Rabbit

Result: No irritation

OECD Test Guideline 404

#### *Eye irritation*

Causes serious eye damage.

#### *Sensitisation*

This information is not available.

#### *Germ cell mutagenicity*

#### *Genotoxicity in vitro*

Mutagenicity (mammal cell test):

Result: negative

(External MSDS)

Ames test

Result: negative

(Lit.)

#### *Carcinogenicity*

This information is not available.

#### *Reproductive toxicity*

This information is not available.

#### *Teratogenicity*

This information is not available.



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## *CMR effects*

Reproductive toxicity:  
Suspected of damaging fertility.

## *Specific target organ toxicity - single exposure*

This information is not available.

## *Specific target organ toxicity - repeated exposure*

This information is not available.

## *Aspiration hazard*

This information is not available.

### **11.2 Further information**

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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## **SECTION 12. Ecological information**

### **12.1 Toxicity**

#### *Toxicity to fish*

LC50 *Leuciscus idus* (Golden orfe): 1.000 - 2.200 mg/l; 96 h  
(External MSDS)

#### *Toxicity to bacteria*

EC50 activated sludge: > 1.000 mg/l; 3 h  
OECD Test Guideline 209

### **12.2 Persistence and degradability**

#### *Biodegradability*

< 10 %; 28 d  
OECD Test Guideline 301E  
Not readily biodegradable.

#### *Biochemical Oxygen Demand (BOD)*

< 2 mg/g (5 d)

(External MSDS)

### **12.3 Bioaccumulative potential**

#### *Partition coefficient: n-octanol/water*

log Pow: 0,05 (25 °C)  
(experimental)

(External MSDS) Bioaccumulation is not expected.

### **12.4 Mobility in soil**

No information available.

### **12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

### **12.6 Other adverse effects**

#### *Additional ecological information*

Discharge into the environment must be avoided.

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## SECTION 13. Disposal considerations

### *Waste treatment methods*

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14. Transport information

### Land transport (ADR/RID)

**14.1 - 14.6** Not classified as dangerous in the meaning of transport regulations.

### Inland waterway transport (ADN)

Not relevant

### Air transport (IATA)

**14.1 - 14.6** Not classified as dangerous in the meaning of transport regulations.

### Sea transport (IMDG)

**14.1 - 14.6** Not classified as dangerous in the meaning of transport regulations.

### 14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

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## SECTION 15. Regulatory information

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

#### *EU regulations*

Major Accident Hazard Legislation	SEVESO III Not applicable
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Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.
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Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC not regulated

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Substances of very high concern (SVHC)

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of  $\geq 0.1\%$  (w/w).

*National legislation*

Storage class 10 - 13

## 15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out.

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## SECTION 16. Other information

### Full text of H-Statements referred to under sections 2 and 3.

H302 Harmful if swallowed.  
H318 Causes serious eye damage.  
H361f Suspected of damaging fertility.

### Training advice

Provide adequate information, instruction and training for operators.

### Labelling

*Hazard pictograms*



*Signal word*

Danger

*Hazard statements*

H302 Harmful if swallowed.  
H318 Causes serious eye damage.  
H361 Suspected of damaging fertility or the unborn child.

*Precautionary statements*

Prevention

P280 Wear eye protection.

Response

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes.

Remove contact lenses, if present and easy to do. Continue rinsing.

P313 Get medical advice/ attention.

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Contains: tetrahydro-1,3-dimethyl-1H-pyrimidin-2-one

## **Key or legend to abbreviations and acronyms used in the safety data sheet**

Used abbreviations and acronyms can be looked up at [www.wikipedia.org](http://www.wikipedia.org).

## **Regional representation**

This information is given on the authorised Safety Data Sheet for your country.

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*The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.*

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