

## Chemical Safety Data Sheet MSDS / SDS

**ethyl 1-benzyl-3-hydroxy-2(5H)-oxopyrrole-4-carboxylate**Revision Date:2026-06-06 Revision Number:1

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

Product name : ethyl 1-benzyl-3-hydroxy-2(5H)-oxopyrrole-4-carboxylate  
CBnumber : CB51373216  
CAS : 4450-98-0  
Synonyms : 1h-pyrrole-3-carboxylic acid, 2,5-dihydro-4-hydroxy-5-oxo-1-(phenylmethyl)-, ethyl ester

**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  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 010-86108875

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**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Danger

**Precautionary statements**

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

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

Continuerinsing.

**Hazard statements**

H302 Harmful if swallowed

H318 Causes serious eye damage

**SECTION 3: Composition/information on ingredients****Substance**

Product name	: ethyl 1-benzyl-3-hydroxy-2(5H)-oxopyrrole-4-carboxylate
Synonyms	: 1h-pyrrole-3-carboxylic acid, 2,5-dihydro-4-hydroxy-5-oxo-1-(phenylmethyl)-, ethyl ester
CAS	: 4450-98-0
MF	: C14H15NO4
MW	: 261.27

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## SECTION 4: First aid measures

### Description of first aid measures

#### General information

Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.

#### After inhalation

Supply fresh air; consult doctor in case of complaints.

#### After skin contact

Generally the product does not irritate the skin.

#### After eye contact

Rinse opened eye for several minutes under running water. Then consult a doctor.

#### After swallowing

Immediately call a doctor.

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

No further relevant information available.

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

No further relevant information available.

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## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing agents

Use fire fighting measures that suit the environment.

A solid water stream may be inefficient.

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

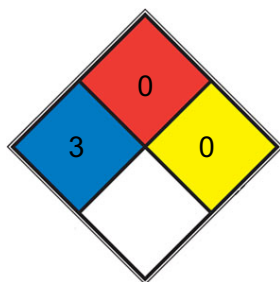
No further relevant information available.

#### Advice for firefighters

## Protective equipment

No special measures required.

## NFPA 704



HEALTH 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

FIRE 0 Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand. Materials that will not burn in air when exposed to a temperature of 820 °C (1,500 °F) for a period of 5 minutes.(e.g. Carbon tetrachloride)

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium,[N2](#))

SPEC.  
 HAZ.

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## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Wear protective equipment. Keep unprotected persons away.

### Environmental precautions

Do not allow to enter sewers/ surface or ground water.

### Methods and material for containment and cleaning up

Use neutralizing agent.

Dispose contaminated material as waste according to section 13.

### Protective Action Criteria for Chemicals

#### PAC-1

Substance is not listed.

#### PAC-2

Substance is not listed.

#### PAC-3

Substance is not listed.

## Reference to other sections

See Section 7 for information on safe handling.

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

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## SECTION 7: Handling and storage

### Precautions for safe handling

Thorough dedusting.

### Information about protection against explosions and fires

No special measures required.

### Conditions for safe storage, including any incompatibilities

#### Storage

Store in accordance with information listed on the product insert.

### Requirements to be met by storerooms and receptacles

No special requirements.

### Information about storage in one common storage facility

Not required.

Further information about storage conditions: Keep receptacle tightly sealed.
Specific end use(s) No further relevant information available.

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## SECTION 8: Exposure controls/personal protection

### Control parameters

### Components with limit values that require monitoring at the workplace

Not required.

### Additional information

The lists that were valid during the creation were used as basis.

### Exposure controls

#### Appropriate engineering controls

No further data; see section 7.

#### Personal protective equipment

#### General protective and hygienic measures

Keep away from foodstuffs, beverages and feed.

Immediately remove all soiled and contaminated clothing.

Wash hands before breaks and at the end of work.

Avoid contact with the eyes.

Avoid contact with the eyes and skin.

### **Breathing equipment**

Not required.

### **Protection of hands**

Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.

Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

### **Material of gloves**

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

### **Penetration time of glove material**

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

### **Eye protection**

Tightly sealed goggles

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## SECTION 9: Physical and chemical properties

### **Information on basic physicochemical properties**

#### **Physical State**

Solid

#### **Color**

white

#### **Odor**

Characteristic

#### **Structural Formula**

C<sub>14</sub>H<sub>15</sub>NO<sub>4</sub>

#### **Molecular Weight**

261.3 g/mol

#### **Storage Buffer**

**Odor Threshold**

Not determined.

**Formulation****Melting point/Melting range**

Undetermined.

**Boiling point/Boiling range**

479.8±45.0 °C(Predicted)

**Flammability**

Product is not flammable.

**Explosion limits**

Lower: Not determined.

Upper: Not determined.

**Flash point**

Not applicable.

**Decomposition temperature**

Not determined.

**pH**

Not applicable.

**Viscosity****Kinematic**

Not applicable.

**SOLUBILITY**

DMF: 20 mg/ml; DMSO: 14 mg/ml; Ethanol: 14 mg/ ml; PBS (pH 7.2): 0.2 mg/ml

**Dynamic**

Not applicable.

**Solubility in / Miscibility with**

DMSO: ≥10mg/mL

**Water**

Not determined.

**Partition coefficient (n-octanol/water)**

Not determined.

### **Vapor Pressure**

Not applicable.

### **Density**

1.340±0.06 g/cm<sup>3</sup>(Predicted)

### **Relative Density**

1.340±0.06 g/cm<sup>3</sup>(Predicted)

### **Vapor Density**

Not applicable.

### **Particle characteristics**

Not determined.

### **Other information**

### **Appearance**

### **Form**

Solid

### **Important information on protection of health and environment, and on safety.**

### **Ignition temperature**

Not determined.

### **Danger of explosion**

Product does not present an explosion hazard.

### **Change in condition**

### **Evaporation Rate**

Not applicable.

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## **SECTION 10: Stability and reactivity**

### **Reactivity**

No further relevant information available.

### **Chemical stability**

### **Thermal decomposition / conditions to be avoided**

No decomposition if used according to specifications.

### **Possibility of hazardous reactions**

No dangerous reactions known.

### **Conditions to avoid**

No further relevant information available.

### **Incompatible materials**

No further relevant information available.

### **Hazardous decomposition products**

carbon oxides, nitrogen oxides

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## **SECTION 11: Toxicological information**

### **Information on toxicological effects**

#### **Acute toxicity**

#### **Primary irritant effect**

##### **on the skin**

No irritant effect.

##### **on the eye**

Strong irritant with the danger of severe eye injury.

#### **Sensitization**

No sensitizing effects known.

### **Additional toxicological information**

#### **Interactive effects**

No interactive effects between components are known.

### **Carcinogenic categories**

#### **IARC (International Agency for Research on Cancer)**

Substance is not listed.

#### **NTP (National Toxicology Program)**

Substance is not listed.

#### **OSHA-Ca (Occupational Safety & Health Administration)**

Substance is not listed.

## **Alternative sources for toxicological information**

No non-standard sources for toxicological information were used.

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## **SECTION 12: Ecological information**

### **Toxicity**

#### **Aquatic toxicity**

No further relevant information available.

#### **Persistence and degradability**

No further relevant information available.

#### **Bioaccumulative potential**

No further relevant information available.

#### **Mobility in soil**

No further relevant information available.

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

#### **PBT**

Not applicable.

#### **vPvB**

Not applicable.

#### **PBT:**

Not applicable.

#### **vPvB:**

Not applicable.

### **Other adverse effects**

### **Additional ecological information**

#### **General notes**

Water hazard class 1 (Self-assessment) slightly hazardous for water

Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

Must not reach bodies of water or drainage ditch undiluted or unneutralized.

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## **SECTION 13: Disposal considerations**

## **Waste treatment methods**

### **Recommendation**

Must not be disposed of together with household garbage. Do not allow product to reach sewage system.

### **Uncleaned packagings**

### **Recommendation**

Disposal must be made according to official regulations.

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## **SECTION 14: Transport information**

### **UN-Number**

DOT, IMDG, IATA not regulated

### **UN proper shipping name**

DOT, IMDG, IATA not regulated

### **Transport hazard class(es)**

DOT, ADN, IMDG, IATA

Class not regulated

### **Packing group**

DOT, IMDG, IATA not regulated

### **Environmental hazards**

Not applicable.

### **Special precautions for user**

Not applicable.

### **Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code**

MARPOL73/78 and the IBC Code Not applicable.

### **UN "Model Regulation"**

not regulated

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## **SECTION 15: Regulatory information**

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

No further relevant information available.

### **Sara**

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Section 355 (extremely hazardous substances):	Substance is not listed.
Section 313 (Specific toxic chemical listings):	Substance is not listed.
TSCA (Toxic Substances Control Act):	Substance is not listed.
Hazardous Air Pollutants:	Substance is not listed.
Chemicals known to cause cancer:	Substance is not listed.
Chemicals known to cause reproductive toxicity for females:	Substance is not listed.
Chemicals known to cause reproductive toxicity for males:	Substance is not listed.
Chemicals known to cause developmental toxicity:	Substance is not listed.

### **Carcinogenic categories**

EPA (Environmental Protection Agency):	Substance is not listed.
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### **TLV (Threshold Limit Value)**

Substance is not listed.

### **NIOSH-Ca (National Institute for Occupational Safety and Health)**

Substance is not listed.

### **Chemical safety assessment**

A Chemical Safety Assessment has not been carried out.

## **SECTION 16: Other information**

### **Abbreviations and acronyms**

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

CAS: Chemical Abstracts Service (division of the American Chemical Society)

NFPA: National Fire Protection Association (USA)

HMS: Hazardous Materials Identification System (USA)

PBT: Persistent, Bioaccumulative and Toxic vPvB: very Persistent and very Bioaccumulative

NIOSH: National Institute for Occupational Safety

OSHA: Occupational Safety & Health

TLV: Threshold Limit Value

PEL: Permissible Exposure Limit

REL: Recommended Exposure Limit

Acute toxicity - oral 4: Acute toxicity – Category 4

Eye damage 1: Serious eye damage/eye irritation – Category 1

#### **Disclaimer:**

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.