

## Chemical Safety Data Sheet MSDS / SDS

## 9(S)-HPOT

Revision Date:2026-05-31 Revision Number:1

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

## Product identifier

Product name : 9(S)-HPOT  
CBnumber : CB4194123  
CAS : 111004-08-1  
Synonyms : 9(S)-HpOTrE,9-hydroperoxy-10,12,15-octadecatrienoic acid

## 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

## SECTION 2: Hazards identification

## GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

## Precautionary statements

No data available

## Hazard statements

No data available

## SECTION 3: Composition/information on ingredients

## Substance

Product name : 9(S)-HPOT  
Synonyms : 9(S)-HpOTrE,9-hydroperoxy-10,12,15-octadecatrienoic acid  
CAS : 111004-08-1

MF : C18H30O4  
MW : 310.43

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## SECTION 4: First aid measures

### Description of first aid measures

#### General information

Immediately remove any clothing soiled by the product.

#### After inhalation

Supply fresh air; consult doctor in case of complaints.

#### After skin contact

Immediately rinse with water.

#### After eye contact

Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.

#### After swallowing

If symptoms persist consult doctor.

#### Information for 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

CO<sub>2</sub>, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

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

Can release vapors that form explosive mixtures at temperatures at or above the flashpoint.

Container explosion may occur under fire conditions.

Emits toxic fumes under fire conditions.

Sensitive to static discharge.

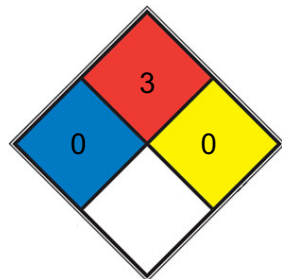
Vapors can travel to a source of ignition and flash back.

## Advice for firefighters

## Protective equipment

No special measures required.

## NFPA 704



|          |   |                                                                                                                                                                                                                                                                                                                                                             |
|----------|---|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| ■ HEALTH | 0 | Poses no health hazard, no precautions necessary and would offer no hazard beyond that of ordinary combustible materials                                                                                                                                                                                                                                    |
| ■ FIRE   | 3 | Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature conditions . Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, <a href="#">acetone</a> ) |
| ■ REACT  | 0 | Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, <a href="#">N2</a> )                                                                                                                                                                                                                                     |
| □ SPEC.  |   |                                                                                                                                                                                                                                                                                                                                                             |
| □ HAZ.   |   |                                                                                                                                                                                                                                                                                                                                                             |

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Wear protective equipment. Keep unprotected persons away.

### Environmental precautions

Dilute with plenty of water.

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

### Methods and material for containment and cleaning up

Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).

Dispose contaminated material as waste according to section 13.

Ensure adequate ventilation.

### 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.

### Protective Action Criteria for Chemicals

### **PAC-1**

64-17-5 ethanol 1,800 ppm

### **PAC-2**

64-17-5 ethanol 3300\* ppm

### **PAC-3**

64-17-5 ethanol 15000\* ppm

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## **SECTION 7: Handling and storage**

### **Handling**

#### **Precautions for safe handling**

No special precautions are necessary if used correctly.

Avoid breathing dust/fume/gas/mist/vapours/spray.

Avoid prolonged or repeated exposure.

Keep away from sources of ignition.

Take precautionary measures against static discharge.re.

#### **Information about protection against explosions and fires**

Keep ignition sources away - Do not smoke.

Protect against electrostatic charges.

#### **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**

Store in a cool location.

#### **Information about storage in one common storage facility**

Not required.

#### **Further information about storage conditions**

Keep receptacle tightly sealed.

Store in cool, dry conditions in well sealed receptacles.

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

No further relevant information available.

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

## Additional information about design of technical systems

No further data; see section 7.

## Control parameters

Components with limit values that require monitoring at the workplace:

| 64-17-5 ethanol |                                                    |
|-----------------|----------------------------------------------------|
| PEL             | Long-term value: 1900 mg/m <sup>3</sup> , 1000 ppm |
| REL             | Long-term value: 1900 mg/m <sup>3</sup> , 1000 ppm |
| TLV             | Short-term value: 1000 ppm<br>A3                   |

## Additional information

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

## Exposure controls

### 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. As the product is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.

### 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

## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

#### Appearance

#### Physical State

Liquid

#### Color

According to product specification

#### Odor

Characteristic

#### Structural Formula

C<sub>18</sub>H<sub>30</sub>O<sub>4</sub>

#### Molecular Weight

310.4 g/mol

#### Odor Threshold

Not determined.

#### Formulation

A solution in ethanol

#### pH

Not determined.

#### Change in condition

#### Melting point/Melting range

-114 °C (-173.2 °F)

#### Boiling point/Boiling range

78 °C (172.4 °F)

#### Flash point

13 °C (55.4 °F)

#### Flammability (solid,gas)

Highly flammable.

#### Auto igniting

425 °C (797 °F)

### **Decomposition temperature**

Not determined.

### **Ignition temperature**

Product is not selfigniting.

### **Danger of explosion**

Product is not explosive. However, formation of explosive air/ vapor mixtures are possible.

### **Explosion limits**

Lower: 3.3 Vol %

Upper: 19 Vol %

### **Vapor Pressure at 20 °C (68 °F)**

59 hPa (44.3 mm Hg)

### **Vapor Pressure at 50 °C (122 °F)**

280 hPa (210 mm Hg)

### **Density at 20 °C (68 °F)**

0.79 g/cm<sup>3</sup> (6.59255 lbs/gal)

### **Relative Density**

1.016±0.06 g/cm<sup>3</sup>(Predicted)

### **Vapor Density**

Not determined.

### **Evaporation Rate**

Not determined.

### **Solubility in / Miscibility with**

DMF: >50 mg/ml (from 13(S)-HODE); DMSO: >50 mg/ml (from 13(S)-HODE); Ethanol: >50 mg/ml (from 13(S)-HODE); PBS pH 7.2: >1 mg/ml (from 13(S)-HODE)

### **Water at 20 °C (68 °F)**

1,000 g/l

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

Not determined.

### **Viscosity**

### **Dynamic**

at 20 °C (68 °F): 1.2 mPas

**Kinematic**

Not determined.

**SOLUBILITY**

DMF: >50 mg/ml; DMSO: >50 mg/ml; Ethanol: >50 mg/ml;

PBS pH 7.2: >1 mg/ml

**Organic solvents**

99.9 %

**VOC content**

99.90 % 999.0 g/l / 8.34 lb/gal

**Solids content**

0.0 %

**Other information**

No information available

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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**

No dangerous decomposition products known.

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**SECTION 11: Toxicological information**

## Information on toxicological effects

### Acute toxicity

LD/LC50 values that are relevant for classification:

| Substance / Estimate | Route      | Endpoint | Value                                         |
|----------------------|------------|----------|-----------------------------------------------|
| 64-17-5 ethanol      | Oral       | LD50     | 10,470 mg/kg (rat)<br>OECD Test Guideline 401 |
| 64-17-5 ethanol      | Inhalative | LC50/4 h | 117–125 mg/l (rat)<br>OECD 403 (rat)          |

### Primary irritant effect

#### on the skin

No irritant effect.

#### on the eye

Irritating effect.

### Sensitization

No sensitizing effects known.

### Additional toxicological information

The product shows the following dangers according to internally approved calculation methods for preparations  
Irritant

### Carcinogenic categories

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

64-17-5 ethanol 1

#### NTP (National Toxicology Program)

None of the ingredients is listed.

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

None of the ingredients is listed.

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## SECTION 12: Ecological information

### Toxicity

#### Aquatic toxicity

No further relevant information available.

#### Persistence and degradability

No further relevant information available.

### **Behavior in environmental systems**

#### **Bioaccumulative potential**

No further relevant information available.

#### **Mobility in soil**

No further relevant information available.

### **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.

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

#### **PBT**

Not applicable.

#### **vPvB**

Not applicable.

#### **PBT:**

Not applicable.

#### **vPvB:**

Not applicable.

### **Other adverse effects**

No further relevant information available.

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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.

### **Recommended cleansing agent**

Water, if necessary with cleansing agents.

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## SECTION 14: Transport information

### UN-Number

DOT, IMDG, IATA UN1170

### UN proper shipping name

DOT Ethanol solutions

IMDG ETHANOL SOLUTION (ETHYL ALCOHOL  
SOLUTION)

IATA Ethanol solution

### Transport hazard class(es)

#### DOT

Class: 3 Flammable liquids

Label: 3

#### IMDG, IATA

Class: 3 Flammable liquids

Label: 3

### Packing group

DOT, IMDG, IATA II

### Environmental hazards

Not applicable.

### Special precautions for user

Warning: Flammable liquids

### Hazard identification number (Kemler code)

33

### EMS Number

F-E,S-D

### Stowage Category

A

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

Not applicable.

### Transport/Additional information

DOT:

## Quantity limitations

On passenger aircraft/rail: 5 L

On cargo aircraft only: 60 L

## IMDG:

## Limited quantities (LQ)

1L

## Excepted quantities (EQ)

Code: E2

Maximum net quantity per inner packaging: 30 ml

Maximum net quantity per outer packaging: 500 ml

## IATA:

## Remarks

When sold in quantities of less than or equal to 1 mL, or 1 g, with an Excepted Quantity Code of

E1, E2, E4, or E5, this item meets the De Minimis

Quantities exemption, per IATA 2.6.10.

Therefore packaging does not have to be labeled as

Dangerous Goods/Excepted Quantity.

## UN "Model Regulation"

UN 1170 ETHANOL SOLUTION (ETHYL ALCOHOL

SOLUTION), 3, II

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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

|                                                 |                                    |
|-------------------------------------------------|------------------------------------|
| Section 355 (extremely hazardous substances):   | None of the ingredients is listed. |
| Section 313 (Specific toxic chemical listings): | None of the ingredients is listed. |
| TSCA (Toxic Substances Control Act):            | 64-17-5 ethanol ACTIVE             |
| Hazardous Air Pollutants:                       | None of the ingredients is listed. |

## Proposition 65

|                                                             |                                    |
|-------------------------------------------------------------|------------------------------------|
| Chemicals known to cause cancer:                            | None of the ingredients is listed. |
| Chemicals known to cause reproductive toxicity for females: | None of the ingredients is listed. |
| Chemicals known to cause reproductive toxicity for males:   | None of the ingredients is listed. |
| Chemicals known to cause developmental toxicity:            | 64-17-5 ethanol<br>Chemical Book   |

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### Carcinogenic categories

|                                                                   |                                    |
|-------------------------------------------------------------------|------------------------------------|
| EPA (Environmental Protection Agency):                            | None of the ingredients is listed. |
| TLV (Threshold Limit Value):                                      | 64-17-5 ethanol A3                 |
| NIOSH-Ca (National Institute for Occupational Safety and Health): | None of the ingredients is listed. |

### Chemical safety assessment

A Chemical Safety Assessment has not been carried out.

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## SECTION 16: Other information

### Abbreviations and acronyms

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

EINECS: European Inventory of Existing Commercial Chemical Substances

ELINCS: European List of Notified Chemical Substances

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

NFPA: National Fire Protection Association (USA)

HMIS: Hazardous Materials Identification System (USA)

VOC: Volatile Organic Compounds (USA, EU)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

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

Flammable Liquids 2: Flammable liquids – Category 2

Eye Irritation 2A: Serious eye damage/eye irritation – Category 2A

#### 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.