

## Chemical Safety Data Sheet MSDS / SDS

## 5-hydroxyeicosatetraenoic acid lactone

Revision Date:2026-03-20 Revision Number:1

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

## Product identifier

Product name : 5-hydroxyeicosatetraenoic acid lactone  
CBnumber : CB01399103  
CAS : 81517-87-5  
Synonyms : 6-[(1E,3Z,6Z,9Z)-pentadeca-1,3,6,9-tetraenyl]oxan-2-one;2H-Pyran-2-one, tetrahydro-6-(1E,3Z,6Z,9Z)-1,3,6,9-pentadecatetraen-1-yl-

## 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) : No data available  
Signal word : No data available

## Precautionary statements

No data available

## Hazard statements

No data available

## SECTION 3: Composition/information on ingredients

## Substance

Product name : 5-hydroxyeicosatetraenoic acid lactone  
Synonyms : 6-[(1E,3Z,6Z,9Z)-pentadeca-1,3,6,9-tetraenyl]oxan-2-one;2H-Pyran-2-one, tetrahydro-6-(1E,3Z,6Z,9Z)-1,3,6,9-pentadecatetraen-1-yl-

|     |              |
|-----|--------------|
| CAS | : 81517-87-5 |
| MF  | : C20H30O2   |
| MW  | : 302.45     |

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## SECTION 4: First aid measures

### Description of first aid measures

#### General information

Immediately remove any clothing soiled by the product.

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. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.

In case of unconsciousness place patient stably in side position for transportation.

#### 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

Immediately call a 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

No further relevant information available.

#### Advice for firefighters

## **Protective equipment**

Mouth respiratory protective device.

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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**

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**

75-05-8 Acetonitrile 13 ppm

#### **PAC-2**

75-05-8 Acetonitrile 50 ppm

#### **PAC-3**

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

### **Handling**

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

Ensure good ventilation/exhaustion at the workplace.

Prevent formation of aerosols.

#### **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:

| 75-05-8 Acetonitrile |                                                |
|----------------------|------------------------------------------------|
| PEL                  | Long-term value: 70 mg/m <sup>3</sup> , 40 ppm |
| REL                  | Long-term value: 34 mg/m <sup>3</sup> , 20 ppm |
| TLV                  | Long-term value: 20 ppm<br>Skin, A4            |

### 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**

In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.

### **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

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## **SECTION 9: Physical and chemical properties**

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

#### **Appearance**

#### **Physical State**

Liquid

#### **Color**

According to product specification

#### **Odor**

Aromatic

#### **Structural Formula**

C<sub>20</sub>H<sub>30</sub>O<sub>2</sub>

#### **Molecular Weight**

302.5 g/mol

#### **Odor Threshold**

Not determined.

### **Formulation**

A solution in acetonitrile

### **pH**

Not determined.

### **Change in condition**

### **Melting point/Melting range**

-46 °C (-50.8 °F)

### **Boiling point/Boiling range**

81 °C (177.8 °F)

### **Flash point**

5 °C (41 °F)

### **Flammability (solid,gas)**

Highly flammable.

### **Auto igniting**

525 °C (977 °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: 4.4 Vol %

Upper: 16 Vol %

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

97 hPa (72.8 mm Hg)

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

330 hPa (247.5 mm Hg)

### **Density at 20 °C (68 °F)**

0.7822 g/cm<sup>3</sup> (6.52746 lbs/gal)

**Relative Density**

0.979±0.06 g/cm<sup>3</sup>(Predicted)

**Vapor Density**

Not determined.

**Evaporation Rate**

Not determined.

**Solubility in / Miscibility with**

DMF: 50 mg/ml

DMSO: 50 mg/ml

Ethanol: 50 mg/ml PBS pH 7.2: 1 mg/ml

**Water**

Fully miscible.

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

Not determined.

**Viscosity****Dynamic**

at 20 °C (68 °F): 0.39 mPas

**Kinematic**

Not determined.

**SOLUBILITY**

DMF: 50 mg/ml; DMSO: 50 mg/ml; Ethanol: 50 mg/ml; PBS pH 7.2: 1 mg/ml

**VOC content**

0.00 % 0.0 g/l / 0.00 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

oxidizing agents, reducing agents

### Hazardous decomposition products

carbon dioxide, carbon monoxide, nitrogen oxides

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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                                                                                                                                                                                  |
|-------------------------------|------------|----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| ATE (Acute Toxicity Estimate) | Oral       | LD50     | 500 mg/kg                                                                                                                                                                              |
| ATE (Acute Toxicity Estimate) | Dermal     | LD50     | 1,100 mg/kg                                                                                                                                                                            |
| ATE (Acute Toxicity Estimate) | Inhalative | LC50/4 h | 11 mg/l                                                                                                                                                                                |
| 75-05-8 Acetonitrile          | Oral       | TDLO     | 64 ml/kg (man)                                                                                                                                                                         |
| 75-05-8 Acetonitrile          | Oral       | LD50     | 2,460 mg/kg (rat)                                                                                                                                                                      |
| 75-05-8 Acetonitrile          | Dermal     | LD50     | 980 mg/kg (rabbit)                                                                                                                                                                     |
| 75-05-8 Acetonitrile          | Inhalative | LC50/4 h | 7,551 mg/m <sup>3</sup> (rat)                                                                                                                                                          |
| 75-05-8 Acetonitrile          | Inhalative | LC50     | 7,551 mg/m <sup>3</sup> /8h (rat)<br>TCLO 160 mg/m <sup>3</sup> /4h (hmn)<br>Irritation of eyes Irritation 100 µl/24 hr (rabbit) moderate<br>Irritation 100 il/24 hr (rabbit) moderate |

#### 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

Harmful

Irritant

## **Carcinogenic categories**

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

None of the ingredients is listed.

### **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 2 (Self-assessment) hazardous for water

Do not allow product to reach ground water, water course or sewage system.

Danger to drinking water if even small quantities leak into the ground.

#### **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 UN1648

**UN proper shipping name**

DOT, IATA Acetonitrile solution

IMDG ACETONITRILE 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**

B

**Stowage Code**

SW2 Clear of living quarters.

**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 1648 ACETONITRILE 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): | 75-05-8 Acetonitrile               |
| TSCA (Toxic Substances Control Act):            | 75-05-8 Acetonitrile ACTIVE        |
| Hazardous Air Pollutants 75-05-8 Acetonitrile   |                                    |

### 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:            | None of the ingredients is listed. |

### Carcinogenic categories

|                                        |
|----------------------------------------|
| EPA (Environmental Protection Agency): |
|----------------------------------------|

### 75-05-8

Acetonitrile CBD, D

### TLV (Threshold Limit Value)

### 75-05-8

Acetonitrile A4

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

None of the ingredients is listed.

### Chemical safety assessment

## 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)

HMS: 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

Acute Toxicity - Oral 4: Acute toxicity – Category 4

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.