

## Chemical Safety Data Sheet MSDS / SDS

**2-[[[(4R)-4-[(3R,5R,8R,9S,10S,13R,14S,17R)-3-hydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]pentanoyl]amino]ethanesulfonic acid**

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

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

Product name : 2-[[[(4R)-4-[(3R,5R,8R,9S,10S,13R,14S,17R)-3-hydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]pentanoyl]amino]ethanesulfonic acid

CBnumber : CB21236073

CAS : 516-90-5

Synonyms : Lithocholyltaurine,5B-Cholanic Acid-3A-OI N-(2-Sulphoethyl)-Amide

**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 | : 2-[[[(4R)-4-[(3R,5R,8R,9S,10S,13R,14S,17R)-3-hydroxy-10,13-dimethyl-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-17-yl]pentanoyl]amino]ethanesulfonic acid |
| Synonyms     | : Lithocholytaurine,5B-Cholanic Acid-3A-OI N-(2-Sulphoethyl)-Amide                                                                                                                           |
| CAS          | : 516-90-5                                                                                                                                                                                   |
| MF           | : C26H45NO5S                                                                                                                                                                                 |
| MW           | : 483.7                                                                                                                                                                                      |

## SECTION 4: First aid measures

### 4.1 Description of first aid measures

#### Eye contact

Remove any contact lenses, locate eye-wash station, and flush eyes immediately with large amounts of water. Separate eyelids with fingers to ensure adequate flushing. Promptly call a physician.

#### Skin contact

Rinse skin thoroughly with large amounts of water. Remove contaminated clothing and shoes and call a physician.

#### Inhalation

Immediately relocate self or casualty to fresh air. If breathing is difficult, give cardiopulmonary resuscitation (CPR). Avoid mouth- to-mouth resuscitation.

#### Ingestion

Wash out mouth with water; Do NOT induce vomiting; call a physician.

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

The most important known symptoms and effects are described in the labelling (see section 2).

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

Treat symptomatically.

## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Use water spray, dry chemical, foam, and carbon dioxide fire extinguisher.

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

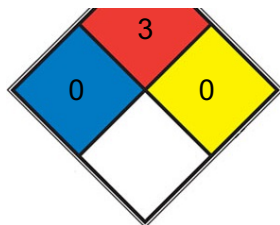
During combustion, may emit irritant fumes.

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus and protective clothing.

### 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, [acetone](#))

■ REACT 0

Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N<sub>2</sub>](#))

□

SPEC.

HAZ.

## SECTION 6: Accidental release measures

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

Use full personal protective equipment. Avoid breathing vapors, mist, dust or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

Refer to protective measures listed in sections 8.

### 6.2 Environmental precautions

Try to prevent further leakage or spillage. Keep the product away from drains or water courses.

### 6.3 Methods and materials for containment and cleaning up

Absorb solutions with finely-powdered liquid-binding material (diatomite, universal binders); Decontaminate surfaces and equipment by scrubbing with alcohol; Dispose of contaminated material according to Section 13.

### 6.4 Reference to other sections

For disposal see section 13.

## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Avoid inhalation, contact with eyes and skin. Avoid dust and aerosol formation. Use only in areas with appropriate exhaust ventilation.

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

Keep container tightly sealed in cool, well-ventilated area. Keep away from direct sunlight and sources of ignition.

#### Recommended storage temperature

Powder -20°C 3 years

In solvent -80°C 6 months -20°C 1 month

Shipping at room temperature if less than 2 weeks.

### 7.3 Specific end use(s)

No data available.

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Components with workplace control parameters

This product contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Engineering controls

Ensure adequate ventilation. Provide accessible safety shower and eye wash station.

#### Personal protective equipment

##### Eye protection

Safety goggles with side-shields.

##### Hand protection

Protective gloves.

##### Skin and body protection

Impervious clothing.

##### Respiratory protection

Suitable respirator.

##### Environmental exposure controls

Keep the product away from drains, water courses or the soil. Clean spillages in a safe way as soon as possible.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

|                                              |                   |
|----------------------------------------------|-------------------|
| Appearance                                   | Solid             |
| Odor                                         | No data available |
| Odor threshold                               | No data available |
| pH                                           | No data available |
| Melting/freezing point                       | No data available |
| Boiling point/range                          | No data available |
| Flash point                                  | No data available |
| Evaporation rate                             | No data available |
| Flammability (solid, gas)                    | No data available |
| Upper/lower flammability or explosive limits | No data available |
| Vapor pressure                               | No data available |

|                           |                           |
|---------------------------|---------------------------|
| Vapor density             | No data available         |
| Relative density          | 1.0476 (rough estimate)   |
| Water Solubility          | No data available         |
| Partition coefficient     | No data available         |
| Auto-ignition temperature | No data available         |
| Decomposition temperature | No data available         |
| Viscosity                 | No data available         |
| Explosive properties      | No data available         |
| Oxidizing properties      | No data available         |
| Physical state            | powder                    |
| Colour                    | Colorless to light yellow |

## 9.2 Other safety information

No data available.

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available.

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available.

### 10.4 Conditions to avoid

No data available.

### 10.5 Incompatible materials

Strong acids/alkalis, strong oxidising/reducing agents.

### 10.6 Hazardous decomposition products

Under fire conditions, may decompose and emit toxic fumes.

Other decomposition products - no data available.

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

Classified based on available data. For more details, see section 2

#### Skin corrosion/irritation

Classified based on available data. For more details, see section 2

**Serious eye damage/irritation**

Classified based on available data. For more details, see section 2

**Respiratory or skin sensitization**

Classified based on available data. For more details, see section 2

**Germ cell mutagenicity**

Classified based on available data. For more details, see section 2

**Carcinogenicity****IARC**

No component of this product present at a level equal to or greater than 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

**ACGIH**

No component of this product present at a level equal to or greater than 0.1% is identified as a potential or confirmed carcinogen by ACGIH.

**NTP**

No component of this product present at a level equal to or greater than 0.1% is identified as a anticipated or confirmed carcinogen by NTP.

**OSHA**

No component of this product present at a level equal to or greater than 0.1% is identified as a potential or confirmed carcinogen by OSHA.

**Reproductive toxicity**

Classified based on available data. For more details, see section 2

**Specific target organ toxicity - single exposure**

Classified based on available data. For more details, see section 2

**Specific target organ toxicity - repeated exposure**

Classified based on available data. For more details, see section 2

**Aspiration hazard**

Classified based on available data. For more details, see section 2

**Additional information**

This information is based on our current knowledge. However the chemical, physical, and toxicological properties have not been completely investigated.

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## SECTION 12: Ecological information

**12.1 Toxicity**

No data available.

**12.2 Persistence and degradability**

No data available.

**12.3 Bioaccumulative potential**

No data available.

**12.4 Mobility in soil**

No data available.

**12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment unavailable as chemical safety assessment not required or not conducted.

## 12.6 Other adverse effects

No data available.

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# SECTION 13: Disposal considerations

## 13.1 Waste treatment methods

### Product

Dispose substance in accordance with prevailing country, federal, state and local regulations.

### Contaminated packaging

Conduct recycling or disposal in accordance with prevailing country, federal, state and local regulations.

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# SECTION 14: Transport information

## DOT (US)

### Proper shipping name

Not dangerous goods

### UN number

-

### Class

-

### Packing group

-

## IMDG

### Proper shipping name

Not dangerous goods

### UN number

-

### Class

-

### Packing group

-

## IATA

### Proper shipping name

Not dangerous goods

### UN number

-

### Class

-

**Packing group**

- Packing group: -

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## SECTION 15: Regulatory information

**SARA 302 Components**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**SARA 313 Components**

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards**

No SARA Hazards.

**Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know Components**

No components are subject to the Pennsylvania Right to Know Act.

**New Jersey Right To Know Components**

No components are subject to the New Jersey Right to Know Act.

**California Prop. 65 Components**

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or anyother reproductive harm.

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## SECTION 16: Other information

**Abbreviations and acronyms**

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

DOT: US Department of Transportation

NFPA: National Fire Protection Association



NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

**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.