

## Chemical Safety Data Sheet MSDS / SDS

**16alpha,17,21-trihydroxypregna-1,4,9(11)-triene-3,20-dione 21-acetate**

Revision Date:2024-03-16 Revision Number:1

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

Product name : 16alpha,17,21-trihydroxypregna-1,4,9(11)-triene-3,20-dione 21-acetate  
CBnumber : CB1894903  
CAS : 77017-20-0  
EINECS Number : 278-593-2  
Synonyms : 2-((8S,10S,13S,14S,16R,17S)-16,17-dihydroxy-10,13-dimethyl-3-oxo-6,7,8,10,12,13,14,15,16,17-decahydro-3H-cyclopenta[a]phenanthren-17-yl)-2-oxoethyl acetate, 16alpha,17,21-trihydroxypregna-1,4,9(11)-triene-3,20-dione 21-acetate

**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 : 400-158-6606

**SECTION 2: Hazards identification****Classification of the substance or mixture**

Skin irritation, Category 2  
Eye irritation, Category 2  
Specific target organ toxicity – single exposure, Category 3  
Reproductive toxicity, Category 2  
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 2

**Label elements****Pictogram(s)**

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Signal word : Warning

**Hazard statement(s)**

H315 Causes skin irritation  
H319 Causes serious eye irritation

H335 May cause respiratory irritation

H361 Suspected of damaging fertility or the unborn child

H411 Toxic to aquatic life with long lasting effects

#### **Precautionary statement(s)**

##### **Prevention**

P264 Wash ... thoroughly after handling.

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

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P271 Use only outdoors or in a well-ventilated area.

P203 Obtain, read and follow all safety instructions before use.

P273 Avoid release to the environment.

##### **Response**

P302+P352 IF ON SKIN: Wash with plenty of water/...

P321 Specific treatment (see ... on this label).

P332+P317 If skin irritation occurs: Get medical help.

P362+P364 Take off contaminated clothing and wash it before reuse.

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

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P319 Get medical help if you feel unwell.

P318 IF exposed or concerned, get medical advice.

P391 Collect spillage.

##### **Storage**

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

P405 Store locked up.

##### **Disposal**

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

##### **Other hazards**

no data available

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## SECTION 3: Composition/information on ingredients

### **Substance**

Product name : 16alpha,17,21-trihydroxypregna-1,4,9(11)-triene-3,20-dione 21-acetate

Synonyms : 2-((8S,10S,13S,14S,16R,17S)-16,17-dihydroxy-10,13-dimethyl-3-oxo-6,7,8,10,12,13,14,15,16,17-decahydro-3H-cyclopenta[a]phenanthren-17-yl)-2-oxoethyl acetate, 16alpha,17,21-trihydroxypregna-1,4,9(11)-triene-3,20-dione 21-acetate

CAS : 77017-20-0

EC number : 278-593-2

MF : C23H28O6

## SECTION 4: First aid measures

### Description of first aid measures

#### If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately.

Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

#### Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

#### Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

#### Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

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

no data available

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

no data available

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## SECTION 5: Firefighting measures

### Extinguishing media

Use dry chemical, carbon dioxide or alcohol-resistant foam.

### Specific Hazards Arising from the Chemical

no data available

### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

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## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

### Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

## Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

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## SECTION 7: Handling and storage

### Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

### Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

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## SECTION 8: Exposure controls/personal protection

### Control parameters

#### Occupational Exposure limit values

no data available

#### Biological limit values

no data available

### Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

### Individual protection measures

#### Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

#### Skin protection

Wear fire/flare resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

#### Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

#### Thermal hazards

no data available

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

|  |   |
|--|---|
| Physical state   | Solid. Crystalline.   |
| Colour   | Brown.  |
| Odour  | no data available   |
| Melting point/freezing point                             | 203.4 °C. Atm. press.:101.3 kPa.  |
| Boiling point or initial boiling point and boiling range | 515.48 °C. Atm. press.:760 mm Hg. Remarks:Calculated by Adapted Stein and Brown Method.               |
| Flammability   | no data available   |
| Lower and upper explosion limit/flammability limit       | no data available   |
| Flash point  | 280.46 °C. Atm. press.:760 mm Hg.   |
| Auto-ignition temperature                                | 357 °C. Atm. press.:760 mm Hg. Remarks:Stimated by OECD Toolbox.                                      |
| Decomposition temperature                                | no data available   |
| pH   | no data available   |
| Kinematic viscosity                                      | no data available   |
| Solubility   | In water: 38.72 mg/L. Temperature:25 °C. Remarks:Calculated from ALogPs value of 2.26.                |
| Partition coefficient n-octanol/water                    | log Pow = 2.26. Remarks:Calculated by OECD Toolbox.   |
| Vapour pressure  | See below. Temperature:25 °C. Remarks:2.47 E-013 mm Hg - Calculated by MPBVP (Modified Grain Method). |
| Density and/or relative density                          | 0.457 g/cm <sup>3</sup> . Temperature:25 °C.;0.685 g/cm <sup>3</sup> . Temperature:25 °C.             |
| Relative vapour density                                  | no data available   |
| Particle characteristics                                 | no data available   |

## SECTION 10: Stability and reactivity

### Reactivity

no data available

### Chemical stability

no data available

### Possibility of hazardous reactions

no data available

### Conditions to avoid

no data available

### Incompatible materials

no data available

### Hazardous decomposition products

no data available

## SECTION 11: Toxicological information

### Acute toxicity

- Oral: no data available
- Inhalation: no data available
- Dermal: LD50 - mouse and rat - 2 540 mg/kg bw.

### Skin corrosion/irritation

no data available

### Serious eye damage/irritation

no data available

### Respiratory or skin sensitization

no data available

### Germ cell mutagenicity

no data available

### Carcinogenicity

no data available

### Reproductive toxicity

no data available

### STOT-single exposure

no data available

### STOT-repeated exposure

no data available

### Aspiration hazard

no data available

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## SECTION 12: Ecological information

### Toxicity

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: LC50 - Daphnia magna - 4.43 mg/L - 48 h.

Toxicity to algae: EC50 - Pseudokirchneriella subcapitata (previous names: Raphidocelis subcapitata, Selenastrum capricornutum) - 27.1 mg/L.

Toxicity to microorganisms: no data available

### Persistence and degradability

no data available

### **Bioaccumulative potential**

no data available

### **Mobility in soil**

no data available

### **Other adverse effects**

no data available

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## SECTION 13: Disposal considerations

### **Disposal methods**

#### **Product**

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

#### **Contaminated packaging**

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

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## SECTION 14: Transport information

### **UN Number**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **UN Proper Shipping Name**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

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

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **Packing group, if applicable**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

## **Environmental hazards**

ADR/RID: Yes

IMDG: Yes

IATA: Yes

## **Special precautions for user**

no data available

## **Transport in bulk according to IMO instruments**

no data available

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# SECTION 15: Regulatory information

## **Safety, health and environmental regulations specific for the product in question**

### **European Inventory of Existing Commercial Chemical Substances (EINECS)**

Listed.

### **EC Inventory**

Listed.

### **United States Toxic Substances Control Act (TSCA) Inventory**

Not Listed.

### **China Catalog of Hazardous chemicals 2015**

Not Listed.

### **New Zealand Inventory of Chemicals (NZIoC)**

Not Listed.

### **PICCS**

Not Listed.

### **Vietnam National Chemical Inventory**

Not Listed.

### **IECSC**

Not Listed.

### **Korea Existing Chemicals List (KECL)**

Not Listed.

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# SECTION 16: Other information

## **Abbreviations and acronyms**

CAS: Chemical Abstracts Service

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

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association



TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

## References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: [http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

### 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.