

## Chemical Safety Data Sheet MSDS / SDS

**3alpha,7alpha-dihydroxy-12-oxo-5beta-cholan-24-oic 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 : 3alpha,7alpha-dihydroxy-12-oxo-5beta-cholan-24-oic acid  
CBnumber : CB6890359  
CAS : 2458-08-4  
EINECS Number : 219-542-6  
Synonyms : 12-Ketochenodeoxycholic acid,3,7-Dihydroxy-12-oxocholanoic 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

Warning

**Precautionary statements**

P362 Take off contaminated clothing and wash before reuse.  
P332+P313 IF SKIN irritation occurs: Get medical advice/attention.  
P321 Specific treatment (see ... on this label).  
P302+P352 IF ON SKIN: wash with plenty of soap and water.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P264 Wash skin thoroughly after handling.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.  
Continuerinsing.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P264 Wash skin thoroughly after handling.

## Hazard statements

H315 Causes skin irritation

H319 Causes serious eye irritation

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## SECTION 3: Composition/information on ingredients

### Substance

Product name	: 3alpha,7alpha-dihydroxy-12-oxo-5beta-cholan-24-oic acid
Synonyms	: 12-Ketochenodeoxycholic acid,3,7-Dihydroxy-12-oxocholanoic acid
CAS	: 2458-08-4
EC number	: 219-542-6
MF	: C24H38O5
MW	: 406.56

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## SECTION 4: First aid measures

### General advice

Show this material safety data sheet to the doctor in attendance.

### If inhaled

After inhalation: fresh air.

### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

### In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

### If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

### Protection of first-aiders

For personal protection see section 8.

### Notes to physician

No data available

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## SECTION 5: Firefighting measures

### **Suitable extinguishing media**

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

### **Unsuitable extinguishing media**

For this substance/mixture no limitations of extinguishing agents are given.

### **Specific hazards during fire fighting**

Combustible. Development of hazardous combustion gases or vapours possible in the event of fire.

### **Hazardous combustion products**

Carbon oxides

### **Specific extinguishing methods**

Prevent fire extinguishing water from contaminating surface water or the ground water system.

### **Special protective equipment for fire-fighters**

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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## SECTION 6: Accidental release measures

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

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.

### **Environmental precautions**

Do not let product enter drains.

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

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

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## SECTION 7: Handling and storage

### **Handling**

#### **Avoidance of contact**

Strong oxidizing agents

#### **Storage**

#### **Further information on storage conditions**

Tightly closed. Dry.

#### **Storage class**

13, Non Combustible Solids

**Recommended storage temperature**

-20 °C

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**SECTION 8: Exposure controls/personal protection****Ingredients with workplace control parameters**

Contains no substances with occupational exposure limit values.

**Engineering measures**

No data available

**Personal protective equipment****Respiratory protection**

required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

**Recommended Filter type**

Filter type P2

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

**Eye/face protection**

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Safety glasses

**Skin and body protection**

protective clothing

**Hand protection****Material**

Nitrile rubber

**Break through time**

480 min

**Glove thickness**

0.11 mm

**Protective index**

Full contact

**Manufacturer**

KCL 741 L

**Material**

Nitrile rubber

**Break through time**

480 min

**Glove thickness**

0.11 mm

**Protective index**

Splash contact

**Manufacturer**

KCL 741 L

**Remarks**

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D- 36124 Eichenzell, Internet: www.kcl.de).

**Hygiene measures**

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

solid

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**Color**

White to off-white

**Odor**

No data available

**Odor Threshold**

No data available

**pH**

No data available

**Melting point/ range**

214 - 216 °C

**Boiling point/boiling range**

583°C[at 101 325 Pa]

**Flash point**

No data available

**Evaporation rate**

No data available

**Flammability (solid, gas)**

The product is not flammable.

Method: Flammability (solids)

**Burning rate**

No data available

**Self-ignition**

> 400 °C

Method: Relative self-ignition temperature for solids does not ignite

**Upper explosion limit / Upper flammability limit**

No data available

**Lower explosion limit / Lower flammability limit**

No data available

**Vapor pressure**

< 0.1 hPa (20 °C)

Method: OECD Test Guideline 104

**Relative vapor density**

No data available

**Relative density**

1.18[at 20°C]

**Density**

1.18[at 20°C]

**Water solubility**

4.698mg/L at 25°C

**Partition coefficient: n-octanol/water**

log Pow: 2.97 (20 °C)

Method: OECD Test Guideline 107 Bioaccumulation is not expected.

**Autoignition temperature**

No data available

**Decomposition temperature**

No data available

**Viscosity, dynamic**

No data available

**Viscosity, kinematic**

No data available

**Flow time**

No data available

Explosive properties : Method: Explosive properties

Oxidizing properties : Method: Regulation (EC) No. 440/2008, Annex, A.17 none

### **Molecular weight**

406.57 g/mol

### **Particle characteristics Particle size**

No data available

### **Solubility**

Chloroform: Slightly Soluble

Methanol: Slightly Soluble

### **Physical state**

Solid

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

### **Reactivity**

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### **Chemical stability**

The product is chemically stable under standard ambient conditions (room temperature) .

### **Possibility of hazardous reactions**

No data available

### **Conditions to avoid**

no information available

### **Incompatible materials**

Strong oxidizing agents

### **Hazardous decomposition products**

In the event of fire: see section 5

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## **SECTION 11: Toxicological information**

### **11.1 Information on toxicological effects**

#### **Acute toxicity**

Oral: No data available

Inhalation: Irritating to respiratory system.

Dermal: No data available

#### **Skin corrosion/irritation**

Remarks: Causes skin irritation.

(ECHA)

#### **Serious eye damage/eye irritation**

Remarks: Causes serious eye irritation.

(ECHA)

#### **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**

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

#### **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

### **11.2 Additional Information**

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## **SECTION 12: Ecological information**

### **Ecotoxicity**

#### **Components:**

#### **(3 $\alpha$ ,5 $\beta$ ,7 $\alpha$ )-3,7-Dihydroxy-12-oxocholan-24-oic acid:**

##### **Toxicity to fish**

LC50 (Danio rerio (zebra fish)): > 70.29 mg/l End point: mortality Exposure time: 96 h Test Type: semi-static test Analytical monitoring: yes  
Method: OECD Test Guideline 203 GLP: yes Remarks: (in analogy to similar products) The value is given in analogy to the following  
substances: Ursodeoxycholic acid

##### **Toxicity to algae/aquatic plants**

ErC50 (Pseudokirchneriella subcapitata (green algae)): > 97.9 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes  
Method: OECD Test Guideline 201 GLP: yes Remarks: (in analogy to similar products) The value is given in analogy to the following  
substances: Ursodeoxycholic acid

##### **Toxicity to microorganisms**

EC50 (activated sludge): > 1,000 mg/l Exposure time: 3 h Test Type: static test Method: OECD Test Guideline 209 GLP: yes Remarks: (in  
analogy to similar products) The value is given in analogy to the following substances: Ursodeoxycholic acid

### **Ecotoxicology Assessment**

### Acute aquatic toxicity

This product has no known ecotoxicological effects.

### Persistence and degradability

#### Components:

#### (3 $\alpha$ ,5 $\beta$ ,7 $\alpha$ )-3,7-Dihydroxy-12-oxocholan-24-oic acid:

#### Biodegradability

aerobic Inoculum: activated sludge Concentration: 100 mg/l Result: Readily biodegradable. Biodegradation: 82 % Exposure time: 28 d Method: OECD Test Guideline 301F GLP: yes Remarks: The 10 day time window criterion is not fulfilled.

### Bioaccumulative potential

#### Components:

#### (3 $\alpha$ ,5 $\beta$ ,7 $\alpha$ )-3,7-Dihydroxy-12-oxocholan-24-oic acid:

#### Partition coefficient: noctanol/water

log Pow: 2.97 (20 °C) pH: 6 Method: OECD Test Guideline 107 Remarks: Bioaccumulation is not expected.

### Mobility in soil

No data available

### Other adverse effects

No data available

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## SECTION 13: Disposal considerations

### Disposal methods

#### Waste from residues

Offer surplus and non-recyclable solutions to a licensed disposal company.

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## SECTION 14: Transport information

### International Regulations

#### IATA-DGR

UNID No. : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

Packing instruction (cargo aircraft) : Not applicable

Packing instruction (passenger aircraft) : Not applicable

### **IMDG-Code**

UN number : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

EmS Code : Not applicable

Marine pollutant : no

### **Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code**

Not applicable for product as supplied.

National regulation GB 6944/12268

UN number : Not applicable

Proper shipping name : Not applicable

Class : Not applicable

Subsidiary risk : Not applicable

Packing group : Not applicable

Labels : Not applicable

### **Special precautions for user**

Remarks : Not classified as dangerous in the meaning of transport regulations.

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## **SECTION 15: Regulatory information**

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

### **National regulatory information**

#### **Regulations on Safety Management of Hazardous Chemicals**

#### **Catalogue of Hazardous Chemicals**

Not applicable

#### **Hazardous Chemicals for Priority Management**

Not applicable under SAWS

#### **Regulation of Environmental Management on the First Import of Chemicals and the Import and Export of Toxic Chemicals**

#### **China Severely Restricted Toxic Chemicals for Import and Export**

Not applicable

## Measures on the Environmental Administration of New Chemical Substances Registration

### Registration/Notification number

B1A222216660

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## SECTION 16: Other information

### Full text of other abbreviations

AiIC - Australian Inventory of Industrial Chemicals

ANTT - National Agency for Transport by Land of Brazil

ASTM - American Society for the Testing of Materials

bw - Body weight

CMR - Carcinogen, Mutagen or Reproductive Toxicant

DIN - Standard of the German Institute for Standardisation

DSL - Domestic Substances List (Canada)

EC<sub>x</sub> - Concentration associated with x% response

EL<sub>x</sub> - Loading rate associated with x% response

EmS - Emergency Schedule

ENCs - Existing and New Chemical Substances (Japan)

ErC<sub>x</sub> - Concentration associated with x% growth rate response

ERG - Emergency Response Guide

GHS - Globally Harmonized System

GLP - Good Laboratory Practice

IARC - International Agency for Research on Cancer

IATA - International Air Transport Association

IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk

IC<sub>50</sub> - Half maximal inhibitory concentration

ICAO - International Civil Aviation Organization

IECSC - Inventory of Existing Chemical Substances in China

IMDG - International Maritime Dangerous Goods

IMO - International Maritime Organization

ISHL - Industrial Safety and Health Law (Japan)

ISO - International Organisation for Standardization

KECI - Korea Existing Chemicals Inventory

LC<sub>50</sub> - Lethal Concentration to 50 % of a test population

LD<sub>50</sub> - Lethal Dose to 50% of a test population (Median Lethal Dose)

MARPOL - International Convention for the Prevention of Pollution from Ships

n.o.s. - Not Otherwise Specified

Nch - Chilean Norm

NO(A)EC - No Observed (Adverse) Effect Concentration

NO(A)EL - No Observed (Adverse) Effect Level

NOELR - No Observable Effect Loading Rate

NOM - Official Mexican Norm  
NTP - National Toxicology Program  
NZIoC - New Zealand Inventory of Chemicals  
OECD - Organization for Economic Co-operation and Development  
OPPTS - Office of Chemical Safety and Pollution Prevention  
PBT - Persistent, Bioaccumulative and Toxic substance  
PICCS - Philippines Inventory of Chemicals and Chemical Substances  
(Q)SAR - (Quantitative) Structure Activity Relationship  
REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals  
SADT - Self-Accelerating Decomposition Temperature  
SDS - Safety Data Sheet  
TCSI - Taiwan Chemical Substance Inventory  
TDG - Transportation of Dangerous Goods  
TECI - Thailand Existing Chemicals Inventory  
TSCA - Toxic Substances Control Act (United States)  
UN - United Nations  
UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods  
vPvB - Very Persistent and Very Bioaccumulative  
WHMIS - Workplace Hazardous Materials Information System

**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.