



# CHENODEOXYCHOLIC ACID (2,2,4,4-D4, 98%)

## Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

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DLM-6780

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

### 1.1. Product identifier

Product form	: Substance
Substance name	: CHENODEOXYCHOLIC ACID (2,2,4,4-D4, 98%)
EC-No.	: 207-481-8 (Unlabeled)
CAS-No.	: 99102-69-9
Product code	: DLM-6780
Formula	: C24H36D4O4
Synonyms	: Chenodiol; 3alpha,7alpha-Dihydroxy-5Beta-cholanic acid; 5Beta-Cholanic acid-3alpha,7alpha-diol

### 1.2. Relevant identified uses of the substance or mixture and uses advised against

#### 1.2.1. Relevant identified uses

Main use category	: Professional use
Industrial/Professional use spec	: For professional use only

#### 1.2.2. Uses advised against

No additional information available

### 1.3. Details of the supplier of the safety data sheet

Cambridge Isotope Laboratories, Inc.  
50 Frontage Road  
Andover, MA 01810  
USA

USA: 1-800-322-1174 Int: 1-978-749-8000

[cilsales@isotope.com](mailto:cilsales@isotope.com) [www.isotope.com](http://www.isotope.com)

### Emergency telephone number

Emergency numbers:

Chemtrec: 1-800-424-9300 (24 hours)

International: 1-703-741-5970 (24 hours)

## SECTION 2: Hazards identification

### 2.1. Classification of the substance or mixture

#### Classification according to Regulation (EC) No. 1272/2008 [CLP]

Skin Irrit. 2 H315

Eye Irrit. 2 H319

Full text of hazard classes and H-statements : see section 16

#### Classification according to Directive 67/548/EEC [DSD] or 1999/45/EC [DPD]

Xi; R36/38

Full text of R-phrases: see section 16

#### GHS-US classification

Skin Irrit. 2 H315

Eye Irrit. 2 H319

Full text of H statements : see section 16

#### Adverse physicochemical, human health and environmental effects

Liver injury may occur.

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### 2.2. Label elements

#### Labeling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



GHS07

Signal word (CLP) :

Warning

Hazard statements (CLP) :

H315 - Causes skin irritation  
H319 - Causes serious eye irritation

Precautionary statements (CLP) :

P264 - Wash hands, forearms and face thoroughly after handling.  
P280 - Wear protective gloves/protective clothing/eye protection/face protection.  
P302+P352 - IF ON SKIN: Wash with plenty of water.  
P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P332+P313 - If skin irritation occurs: Get medical advice/attention.  
P337+P313 - If eye irritation persists: Get medical advice/attention.  
P362+P364 - Take off contaminated clothing and wash it before reuse.

#### GHS-US labeling

Hazard pictograms (GHS-US) :



GHS07

Signal word (GHS-US) :

Warning

Hazard statements (GHS-US) :

H315 - Causes skin irritation  
H319 - Causes serious eye irritation

Precautionary statements (GHS-US) :

P264 - Wash hands, forearms and face thoroughly after handling.  
P280 - Wear protective gloves/protective clothing/eye protection/face protection.  
P302+P352 - If on skin: Wash with plenty of water  
P305+P351+P338 - If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P321 - Specific treatment (see supplemental first aid instruction on this label)  
P332+P313 - If skin irritation occurs: Get medical advice/attention.  
P337+P313 - If eye irritation persists: Get medical advice/attention.  
P362+P364 - Take off contaminated clothing and wash it before reuse.

### 2.3. Other hazards

No additional information available

## SECTION 3: Composition/Information on ingredients

### 3.1. Substances

Name	Product identifier	%	Classification according to Directive 67/548/EEC
CHENODEOXYCHOLIC ACID (2,2,4,4-D4, 98%)	(CAS-No.) 99102-69-9 (EC-No.) 207-481-8 (Unlabeled)	100	Xi; R36/38

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
CHENODEOXYCHOLIC ACID (2,2,4,4-D4, 98%)	(CAS-No.) 99102-69-9 (EC-No.) 207-481-8 (Unlabeled)	100	Skin Irrit. 2, H315 Eye Irrit. 2, H319

Full text of R- and H- phrases: see section 16

Name	Product identifier	%	GHS-US classification
CHENODEOXYCHOLIC ACID (2,2,4,4-D4, 98%) (Main constituent)	(CAS-No.) 99102-69-9	100	Skin Irrit. 2, H315 Eye Irrit. 2, H319

Full text of H-phrases: see section 16

### 3.2. Mixtures

Not applicable

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### SECTION 4: First aid measures

#### 4.1. Description of first aid measures

First-aid measures general	: Move out of dangerous area. Consult a physician and show this safety data sheet.
First-aid measures after inhalation	: If breathed in, move person to fresh air. If not breathing, give artificial respiration. Consult a physician.
First-aid measures after skin contact	: Wash with soap and plenty of water. Consult a physician.
First-aid measures after eye contact	: Flush eyes with water as a precaution.
First-aid measures after ingestion	: Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

Symptoms/effects after inhalation	: May be harmful if inhaled. May cause respiratory tract irritation.
Symptoms/effects after skin contact	: Causes skin irritation.
Symptoms/effects after eye contact	: Causes serious eye irritation.
Symptoms/effects after ingestion	: May be harmful if swallowed.

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

No additional information available

### SECTION 5: Firefighting measures

#### 5.1. Extinguishing media

Suitable extinguishing media : Use water spray, alcohol-resistant foam, dry chemical, or carbon dioxide.

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

No additional information available

#### 5.3. Advice for firefighters

Firefighting instructions	: Wear self contained breathing apparatus for fire fighting if necessary.
Protection during firefighting	: Do not enter fire area without proper protective equipment, including respiratory protection.

### SECTION 6: Accidental release measures

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

##### 6.1.1. For non-emergency personnel

Emergency procedures : Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust.

##### 6.1.2. For emergency responders

No additional information available

#### 6.2. Environmental precautions

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

#### 6.3. Methods and material for containment and cleaning up

For containment	: Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.
Methods for cleaning up	: This material and its container must be disposed of in a safe way, and as per local legislation.

#### 6.4. Reference to other sections

For further information refer to section 13.

### SECTION 7: Handling and storage

#### 7.1. Precautions for safe handling

Additional hazards when processed	: Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.
Hygiene measures	: Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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

Technical measures	: Keep container tightly closed in a cool, dry and well-ventilated place.
Storage conditions	: Store at room temperature away from light and moisture.

#### 7.3. Specific end use(s)

No additional information available

### SECTION 8: Exposure controls/personal protection

#### 8.1. Control parameters

No additional information available

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### 8.2. Exposure controls

- Appropriate engineering controls : Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.
- Personal protective equipment : Safety glasses. Gloves. Respiratory protection of the dependent type. Protective clothing.



- Materials for protective clothing : Wear suitable protective clothing and gloves.
- Hand protection : Wear suitable protective clothing and gloves.
- Eye protection : Wear safety glasses with side shields (or goggles) and a face shield.
- Skin and body protection : Choose body protection according to the amount and concentration of the dangerous substance at the work place.
- Respiratory protection : When appropriate, use NIOSH/CEN approved respirator.
- Environmental exposure controls : Avoid release to the environment.

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

- Physical state : Solid
- Appearance : Powder
- Molecular mass : 396.6 g/mol (Labeled)
- Color : White
- Odor : No data available
- Odor threshold : No data available
- pH : No data available
- Relative evaporation rate (butyl acetate=1) : No data available
- Melting point : 165 - 167 °C (329 - 333 °F )
- Freezing point : No data available
- Boiling point : No data available
- Flash point : No data available
- Auto-ignition temperature : No data available
- Decomposition temperature : No data available
- Flammability (solid, gas) : No data available
- Vapor pressure : No data available
- Relative vapor density at 20 °C : No data available
- Relative density : No data available
- Solubility : No data available
- Log Pow : No data available
- Log Kow : No data available
- Viscosity, kinematic : No data available
- Viscosity, dynamic : No data available
- Explosive properties : No data available
- Oxidizing properties : No data available
- Explosion limits : No data available

### 9.2. Other information

No additional information available

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

No additional information available

### 10.2. Chemical stability

Five years after receipt if stored as stated in "Storage" section. Re-QC after 5 years.

### 10.3. Possibility of hazardous reactions

No additional information available

### 10.4. Conditions to avoid

No additional information available

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### 10.5. Incompatible materials

Strong oxidizing agents.

### 10.6. Hazardous decomposition products

Calcium oxide

## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

Acute toxicity : Not classified

CHENODEOXYCHOLIC ACID (2,2,4,4-D4, 98%) (99102-69-9)	
LD50 oral rat	4000 mg/kg Remarks: Behavioral: Change in motor activity (specific assay). Lungs, Thorax, or Respiration: Dyspnea. diarrhea.
ATE CLP (oral)	4000.000 mg/kg body weight

Skin corrosion/irritation	: Causes skin irritation.
Serious eye damage/irritation	: Causes serious eye irritation.
Respiratory or skin sensitization	: Not classified
Germ cell mutagenicity	: Laboratory experiments have shown mutagenic effects.
Carcinogenicity	: Tumeric by RTEC criteria - kidney/liver.
Reproductive toxicity	: Overexposure may cause reproductive disorder(s) based on tests with laboratory animals. Possible risk of congenital malformation in the fetus.
Specific target organ toxicity – single exposure	: Not classified
Specific target organ toxicity – repeated exposure	: Not classified
Aspiration hazard	: Not classified
Potential Adverse human health effects and symptoms	: Liver injury may occur. Stomach - Irregularities - Based on Human Evidence. This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.
Symptoms/effects after inhalation	: May be harmful if inhaled. May cause respiratory tract irritation.
Symptoms/effects after skin contact	: Causes skin irritation.
Symptoms/effects after eye contact	: Causes serious eye irritation.
Symptoms/effects after ingestion	: May be harmful if swallowed.

## SECTION 12: Ecological information

### 12.1. Toxicity

Ecology - general : The product is not considered harmful to aquatic organisms or to cause long-term adverse effects in the environment.

CHENODEOXYCHOLIC ACID (2,2,4,4-D4, 98%) (99102-69-9)	
LC50 fish 1	> 100 mg/l Semi static test - Danio rerio (zebra fish) - 96 h - (OECD Test Guideline 203) - Remarks: (in analogy to similar products)
ErC50 (algae)	> 100 mg/l static test - Pseudokirchneriella subcapitata - 72 h(OECD Test Guideline 201) - Remarks: (in analogy to similar products) - (Chenodeoxycholic acid)
ErC50 (other aquatic plants)	Bacteria - Remarks: (in analogy to similar products) - (Chenodeoxycholic acid)

### 12.2. Persistence and degradability

CHENODEOXYCHOLIC ACID (2,2,4,4-D4, 98%) (99102-69-9)	
Persistence and degradability	Biodegradability aerobic - Exposure time: 28 d - Result: 82 % -Readily biodegradable - (OECD Test Guideline 301F) - Remarks: The 10 day time window criterion is not fulfilled.

### 12.3. Bioaccumulative potential

No additional information available

### 12.4. Mobility in soil

No additional information available

### 12.5. Results of PBT and vPvB assessment

No additional information available

### 12.6. Other adverse effects

No additional information available

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### SECTION 13: Disposal considerations

#### 13.1. Waste treatment methods

- Regional legislation (waste) : Waste materials should be disposed of under conditions which meet Federal, State, and local environmental control regulations.
- Product/Packaging disposal recommendations : Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.
- Ecology - waste materials : Dispose of as unused product.

### SECTION 14: Transport information

In accordance with ADR / RID / IMDG / IATA / ADN

#### 14.1. UN number

Not applicable

#### 14.2. UN proper shipping name

Not applicable

#### 14.3. Additional information

- Other information : No supplementary information available.
- Special transport precautions : Not dangerous goods.

#### Overland transport

No additional information available

#### Transport by sea

No additional information available

#### Air transport

No additional information available

#### 14.4. Environmental hazards

- Other information : No supplementary information available.

#### 14.5. Special precautions for user

- Special transport precautions : Not dangerous goods.

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

Not applicable

### SECTION 15: Regulatory information

#### 15.1. US Federal regulations

CHENODEOXYCHOLIC ACID (2,2,4,4-D4, 98%) (99102-69-9)	
SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302
SARA Section 311/312 Hazard Classes	Delayed (chronic) health hazard
SARA Section 313 - Emission Reporting	Not subject to reporting requirements of the United States SARA Section 313

#### 15.2. International regulations

##### CANADA

CHENODEOXYCHOLIC ACID (2,2,4,4-D4, 98%) (99102-69-9)
Listed on the Canadian DSL (Domestic Substances List)

#### 15.2.1. National regulations

No additional information available

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### 15.3. US State regulations

CHENOEXOXYCHOLIC ACID (2,2,4,4-D4, 98%)(99102-69-9)	
U.S. - California - Proposition 65 - Carcinogens List	No
U.S. - California - Proposition 65 - Developmental Toxicity	Yes
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	Yes
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	Yes
State or local regulations	RTK - U.S. - Pennsylvania - RTK (Right to Know) List RTK - U.S. - New Jersey - Right to Know Hazardous Substance List

### SECTION 16: Other information

Other information : This product is not radioactive. The data given for this product are those of the corresponding unlabeled compound, unless specifically indicated otherwise. Health and safety data for labeled compounds are generally not available, but are assumed to be similar or identical to the corresponding unlabeled compound.

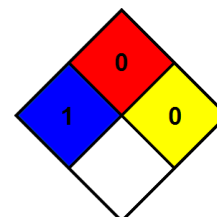
Full text of R-, H- and EUH-phrases:

Eye Irrit. 2	Serious eye damage/eye irritation Category 2
Skin Irrit. 2	Skin corrosion/irritation Category 2
H315	Causes skin irritation
H319	Causes serious eye irritation
R36/38	Irritating to eyes and skin
Xi	Irritant

NFPA health hazard : 1 - Materials that, under emergency conditions, can cause significant irritation.

NFPA fire hazard : 0 - Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand.

NFPA reactivity : 0 - Material that in themselves are normally stable, even under fire conditions.



### Hazard Rating

Health : 1 Slight Hazard - Irritation or minor reversible injury possible

Flammability : 0 Minimal Hazard

Physical : 0 Minimal Hazard

CIL Substance SDS

*This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product*