

According to Regulation (EC) No 1907/2006

Chenodeoxycholic acid

Version number: 1
Issued: 2023-09-12



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

1.1. Product identifier

Trade name

Chenodeoxycholic acid

CAS number

474-25-9

EC number

207-481-8

Synonyms

3alpha,7alpha-Dihydroxy-5beta-cholanic acid

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

Relevant identified uses

Research and development.

Not suitable for use in

Not suitable for human consumption or veterinary purposes.

1.3. Details of the supplier of the safety data sheet

Supplier

Molekula Group

Street address

Molekula Ltd, Lingfield Way, Darlington,
DL1 4XX Darlington
United Kingdom

Telephone

+44 (0) 3302 000 333

Email

info@molekula.com

Web site

www.molekula.com

Contact person

Kevin Banks

Email address

+44 (0) 7769276927

1.4. Emergency telephone number

Poison center/Additional emergency number

0344 892 0111 - National Poisons Information Service (Newcastle Centre)

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SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

Classification

Skin irritation, hazard category 2

Eye irritation, hazard category 2

Hazard statements

H315, H319

2.2. Label elements

Labelling according to Regulation (EC) No 1272/2008

Hazard pictograms



Signal word

Warning

Hazard statements

H315 Causes skin irritation.

H319 Causes serious eye irritation.

Precautionary statements

P202 Do not handle until all safety precautions have been read and understood.

P233 Keep container tightly closed.

P260 Do not breathe dust/fumes/gas/mist/vapours/spray.

P262 Do not get in eyes, on skin, or on clothing.

P264 Wash skin thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

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

P272 Contaminated work clothing should not be allowed out of the workplace.

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

P302 + P350 IF ON SKIN: Gently wash with plenty of soap and 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.

P314 Get medical advice/attention if you feel unwell.

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

P403 Store in a well-ventilated place.

P405 Store locked up.

P501 Dispose of contents/container to local regulations.

2.3. Other hazards

No data available

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SECTION 3: Composition/information on ingredients

3.2. Mixtures

| Chemical name | CAS No. EC No. REACH No. Index No. | Concentration | Classification | H-phrase M factor acute M factor chronic | Note |
|-----------------------|---|---------------|-----------------------------|--|------|
| Chenodeoxycholic acid | 474-25-9 207-481-8 - - | 100% | Skin Irrit. 2, Eye Irrit. 2 | H315, H319 - - | - |

Molecular weight

392.57

Substance additional information

For the complete text of H- / EUH-statements mentioned in this section, see section 16.

SECTION 4: First aid measures

4.1. Description of first aid measures

Inhalation

Move to fresh air if inhaled.

Get medical attention if any discomfort continues.

Skin contact

Rinse skin with water.

If skin irritation or rash occurs: Get medical advice/attention.

Eye contact

Remove contact lenses if present. Rinse eyes with water.

If eye irritation persists: Get medical advice/attention.

Ingestion

Rinse mouth.

Get medical advice/attention if you feel unwell.

Information for doctors

No data available.

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

The severity of the symptoms described will vary dependant of the concentration and the length of exposure.

Inhalation

May cause respiratory irritation.

Skin contact

Prolonged contact may cause dryness of the skin.

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Eye contact

May be slightly irritating to the eyes.

Ingestion

May cause discomfort if swallowed.

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

Treat symptomatically. No special treatment requirement.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

In case of fire: Use foam, carbon dioxide, dry powder or water fog to extinguish.

Unsuitable extinguishing media

No specific fire fighting procedure given.

5.2. Special hazards arising from the substance or mixture

Specific hazards: None.

Thermal decomposition or combustion may liberate carbon oxides and other toxic gases or vapours.

Carbon monoxide (CO). Carbon dioxide (CO₂).

5.3. Advice for firefighters

Special protective equipment for fire-fighters

Evacuate area. Avoid breathing gas, fume, vapours or spray. Cool containers exposed to heat with water spray and remove container, if no risk is involved.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing dust/fume/gas/mist/vapours/spray. Provide adequate ventilation. For personal protection, see section 8.

6.2. Environmental precautions

Avoid discharge into drains, water courses or onto the ground.

6.3. Methods and material for containment and cleaning up

Collect spillage with shovel, broom or the like and reuse, if possible. Dispose of large amounts of spillage/waste according to agreement with local authorities.

6.4. Reference to other sections

For personal protection, see section 8. For waste disposal, see section 13.

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SECTION 7: Handling and storage

7.1. Precautions for safe handling

Preventive handling precautions

Wear protective clothing, gloves, eye and face protection. Avoid contact with skin and eyes. Do not breathe dust/fume/gas/mist/vapours/spray. Avoid ingestion and inhalation. For precautions see section 2.2.

General hygiene

Observe good chemical hygiene practices. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove contaminated clothing and launder thoroughly before re-use. Wash skin thoroughly after handling.

7.2. Conditions for safe storage, including any incompatibilities

Store at ambient temperature. Store in a dry place. Store in a closed container.

7.3. Specific end use(s)

No specific usage precautions noted.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Exposure limits

No occupational exposure limit assigned.

8.2. Exposure controls

Personal Protective Equipment Symbols



Eye / face protection

Wear eye protection.

Hand protection

Wear protective gloves. No specific hygiene procedures noted, but good personal hygiene practices are always advisable, especially when working with chemicals.

Wash contaminated skin thoroughly after handling.

Other skin protection

Wash skin thoroughly after handling.

Respiratory protection

Provide adequate ventilation.

Environmental exposure controls

Avoid discharge into drains.

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SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state

Solid

Colour

White.

Odour

Odourless.

Melting point / freezing point

165 - 167 °C

Boiling point or initial boiling point and boiling range

No data available

Flammability

No data available

Lower and upper explosion limit

No data available

Flash point

No data available

Auto-ignition temperature

No data available

Decomposition temperature

No data available

pH

No data available

Kinematic viscosity

No data available

Solubility

No data available

Partition coefficient n-octanol/water

No data available

Vapour pressure

No data available

Density and/or relative density

No data available

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Relative vapour density

No data available

Particle characteristics

No data available

9.2. Other information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

There are no known reactivity hazards associated with this product.

10.2. Chemical stability

Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions

No data available

10.4. Conditions to avoid

Heating.

10.5. Incompatible materials

Strong oxidising agents.

10.6. Hazardous decomposition products

See section 5.

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Acute toxicity

| Product / Substance name CAS / EC no. | Dose descriptor | Value / Dose | Exposure route | Test animals |
|---|-----------------|--------------|------------------|--------------|
| Chenodeoxycholic acid 474-25-9 / 207-481-8 | LD50 | 4000 mg/kg | Oral | Rat |
| Chenodeoxycholic acid 474-25-9 / 207-481-8 | LD50 | 105 mg/kg | Intraperitoneal. | Rat |
| Chenodeoxycholic acid 474-25-9 / 207-481-8 | LD50 | 106 mg/kg | Intravenous. | Rat |

Skin corrosion/irritation

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| Product / Substance name CAS / EC no. | Result |
|---|-------------------------|
| Chenodeoxycholic acid 474-25-9 / 207-481-8 | Causes skin irritation. |

Serious eye damage/irritation

| Product / Substance name CAS / EC no. | Result |
|---|--------------------------------|
| Chenodeoxycholic acid 474-25-9 / 207-481-8 | Causes serious eye irritation. |

Germ cell mutagenicity

| Product / Substance name CAS / EC no. | Result |
|---|-----------------------------------|
| Chenodeoxycholic acid 474-25-9 / 207-481-8 | Lab tests show mutagenic effects. |

Aspiration hazard

Based on available data, the classification criteria are not met.

11.2. Information on other hazards

No data available

SECTION 12: Ecological information

12.1. Toxicity

Acute fish toxicity

| Product / Substance name CAS / EC no. | Measurement type | Value / Result | Duration of exposure | Species |
|---|------------------|----------------|----------------------|-----------------------------------|
| Chenodeoxycholic acid 474-25-9 / 207-481-8 | LC50 | >100 mg/l | 96 hours | Brachydanio rerio (Zebra Fish) |

Acute algae toxicity

| Product / Substance name CAS / EC no. | Measurement type | Value / Result | Duration of exposure | Species |
|--|------------------|----------------|----------------------|--------------------------|
| Chenodeoxycholic acid | ErC50 | >100 mg/l | 72 hours | Pseudokirchneriella sub- |

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| Product / Substance name CAS / EC no. | Measurement type | Value / Result | Duration of exposure | Species |
|--|------------------|----------------|----------------------|----------|
| 474-25-9 / 207-481-8 | | | | capitata |

12.2. Persistence and degradability

Persistence and degradability

| Product / Substance name CAS / EC no. | Type of test | Duration | Result | Degradation | Remark |
|---|--------------|----------|--------|---------------------------------------|--|
| Chenodeoxycholic acid 474-25-9 / 207-481-8 | aerobic | 28 days | 82% | The product is readily biodegradable. | Readily biodegradable but failing the 10 day window. |

12.3. Bioaccumulative potential

No data available

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

No data available

12.6. Endocrine disrupting properties

No data available

12.7. Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal considerations

Dispose of contents/container in accordance with local/regional/national/international regulations.

SECTION 14: Transport information

14.1. UN number

Not applicable

14.2. UN proper shipping name

Not applicable

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14.3. Transport hazard class(es)

Not applicable

14.4. Packing group

Not applicable

14.5. Environmental hazards

Not applicable

14.6. Special precautions for user

Not applicable

14.7. Maritime transport in bulk according to IMO instruments

Not applicable

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

EU regulations

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

National regulations

No data available

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

SECTION 16: Other information

Phrase meaning

Skin Irrit. 2 - Skin irritation, hazard category 2

Eye Irrit. 2 - Eye irritation, hazard category 2

H315 Causes skin irritation.

H319 Causes serious eye irritation.