

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

# Calcitriol

Version number: 2  
 Issued: 2024-03-26  
 Replaces SDS: 2019-09-30



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

### 1.1. Product identifier

**Trade name**

Calcitriol

**CAS number**

32222-06-3

**EC number**

250-963-8

**Synonyms**

(1R,3S,Z)-5-((E)-2-((1R,3aS,7aR)-1-((R)-6-hydroxy-6-methylheptan-2-yl)-7a-methylhexahydro-1H-inden-4(2H)-ylidene)ethylidene)-4-methylenecyclohexane-1,3-diol

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

**Relevant identified uses**

Research and development. Laboratory Chemicals. Manufacture of substances.

**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

**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

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+44 (0) 7769276927

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## 1.4. Emergency telephone number

### Poison center/Additional emergency number

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

## SECTION 2: Hazards identification

### 2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

#### Classification

Reproductive toxicity, hazard category 1A

Specific Target Organ Toxicity — Repeated exposure, hazard category 1

Acute toxicity, oral, hazard category 1

Acute toxicity, dermal, hazard category 1

Acute toxicity, inhalation, hazard category 1

#### Hazard statements

H300, H310, H330, H361d, H372

### 2.2. Label elements

Labelling according to Regulation (EC) No 1272/2008

#### Hazard pictograms



#### Signal word

Danger

#### Hazard statements

H300 Fatal if swallowed.

H310 Fatal in contact with skin.

H330 Fatal if inhaled.

H361d Suspected of damaging the unborn child.

H372 Causes damage to organs through prolonged or repeated exposure .

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## **Precautionary statements**

P201 Obtain special instructions before use.  
 P202 Do not handle until all safety precautions have been read and understood.  
 P260 Do not breathe dust/fumes/gas/mist/vapours/spray.  
 P262 Do not get in eyes, on skin, or on clothing.  
 P263 Avoid contact during pregnancy and while nursing.  
 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.  
 P284 wear respiratory protection.  
 P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor.  
 P302 + P352 IF ON SKIN: Wash with plenty of water/.  
 P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
 P308 + P313 IF exposed or concerned: Get medical advice/attention.  
 P314 Get medical advice/attention if you feel unwell.  
 P330 Rinse mouth.  
 P403 + P233 Store in a well-ventilated place. Keep container tightly closed.  
 P405 Store locked up.  
 P501 Dispose of contents/container to local regulations.

## **2.3. Other hazards**

No data available

## **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
Calcitriol	32222-06-3 250-963-8 - -	100%	Acute Tox. 1 - oral, Acute Tox. 1 - dermal, Acute Tox. 1 - inhala- tion, STOT RE 1, Repr. 1A	H300, H310, H330, H361d, H372 - -	-

## **Molecular weight**

416.64

## **Substance additional information**

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

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## SECTION 4: First aid measures

### 4.1. Description of first aid measures

IF exposed or concerned: Get medical advice/attention. First aiders/ medical personnel need to protect themselves. Show this Safety Data Sheet (SDS) to medical personnel.

#### Inhalation

Toxic if inhaled. IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/doctor. If breathing stops, provide artificial respiration. For breathing difficulties oxygen may be necessary.

#### Skin contact

In case of skin contact: IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower]. Immediately call a POISON CENTER/doctor. The casualty should be transferred to hospital for further treatment.

#### Eye contact

Remove contact lenses if present. Rinse eyes with water. Continue to rinse for at least 15 minutes and seek medical attention.

#### Ingestion

IF SWALLOWED: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only if the persons are fully conscious and awake). Administer activated charcoal (20 - 40g in a 10% slurry) and consult a doctor as quickly as possible. Do not attempt to neutralise.

#### 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. See section 11 for more detailed information on health effects and symptoms.

#### Inhalation

Single exposure may cause the following adverse effects: Difficulty in breathing. Unconsciousness, possibly death.

#### Skin contact

Single exposure may cause the following adverse effects: Unconsciousness, possibly death.

#### Eye contact

Single exposure may cause the following adverse effects: Severe irritation. Unconsciousness, possibly death.

#### Ingestion

Single exposure may cause the following adverse effects: Severe abdominal pain. May cause severe internal injury. Unconsciousness, possibly death.

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## 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: Toxic. Combustible.

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

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

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

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

### 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 breathing dust/fume/gas/mist/vapours/spray. Provide adequate ventilation. Avoid contact with skin and eyes. Avoid dust formation. 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

For precautions see section 2.2. Do not handle until all safety precautions have been read and understood. Do not handle broken packages without protective equipment. This product is toxic. Work under hood. Keep containers tightly closed. Immediate first aid is necessary. 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. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Do not reuse empty containers.

#### General hygiene

Observe good chemical hygiene practices. Remove contaminated clothing immediately and wash skin with soap and water. Remove contaminated clothing and launder thoroughly before re-use. Wash skin thoroughly after handling.

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

Store in a dry place. Store in a closed container.

Storage class : Toxic storage.

Recommended storage temperature: -20 to -15°C (-4 to 5°F)

### 7.3. Specific end use(s)

No specific usage precautions noted.

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

No data available

### 8.2. Exposure controls

#### Personal Protective Equipment Symbols



#### Eye / face protection

Wear eye protection.

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## Hand protection

Wear protective gloves. Recommended gloves: Nitrile.

Glove Thickness: 0.11mm

Breakthrough time: 8 hours

Always inspect gloves before use. If signs of wear and tear are noticed then the gloves should be replaced.

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. If ventilation is insufficient, suitable respiratory protection must be provided.

## Environmental exposure controls

Avoid discharge into drains.

## SECTION 9: Physical and chemical properties

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

#### Physical state

Solid

#### Colour

White / off-white.

#### Odour

No data available

#### Melting point / freezing point

99 °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

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## 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

## 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

Violent reactions possible with:  
 Strong oxidising agents.

### 10.4. Conditions to avoid

Air sensitive. Light sensitive. Moisture Sensitive.



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## 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
Calcitriol 32222-06-3 / 250-963-8	LD50	0.62 mg/kg	Oral	Rat
Calcitriol 32222-06-3 / 250-963-8	ATE = Acute Toxicity Estimate.	0.051 mg/l	Inhalation.	-
Calcitriol 32222-06-3 / 250-963-8	ATE = Acute Toxicity Estimate.	50.1 mg/kg	Dermal	-

#### Reproductive toxicity

Product / Substance name CAS / EC no.	Result
Calcitriol 32222-06-3 / 250-963-8	May damage fertility. Suspected of damaging the unborn child.

#### STOT-repeated exposure

Product / Substance name CAS / EC no.	Result
Calcitriol 32222-06-3 / 250-963-8	Causes damage to organs through prolonged or repeated exposure.

#### Aspiration hazard

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

### 11.2. Information on other hazards

No data available

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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

No data available

### 12.6. Endocrine disrupting properties

This product does not contain any known or suspected endocrine disruptors.

### 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

2811

### 14.2. UN proper shipping name

#### ADR / RID / ADN proper shipping name

TOXIC SOLID, ORGANIC, N.O.S. (Calcitriol)

#### IMDG proper shipping name

TOXIC SOLID, ORGANIC, N.O.S. (Calcitriol)

#### IATA proper shipping name

Toxic solid, organic, n.o.s. (Calcitriol)

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## 14.3. Transport hazard class(es)

### Label

ADR/RID/ADN



6.1

IMDG



6.1

IATA



6.1

### ADR / RID Class

6.1

### ADR / RID Classification code

T2

### ADR / RID hazard identification number

66

### IMDG Class

6.1

### IATA Class

6.1

### ADN Class

6.1

### ADN Class Code

T2

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## 14.4. Packing group

ADR / RID / ADN: I  
 IMDG: I  
 IATA: I

## 14.5. Environmental hazards

Not applicable

## 14.6. Special precautions for user

### Special precautions for user

Tunnel restriction code: C/E  
 Transport category: 1

### IMDG EmS

F-A, S-A

## 14.7. Maritime transport in bulk according to IMO instruments

IBC Instruction: IBC99

## 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.  
 This material safety data sheet complies with the requirements of Regulation (EU) 2020/878.

#### National regulations

Directive: H1 ACUTE TOXIC

### 15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

## SECTION 16: Other information

### Phrase meaning

Repr. 1A - Reproductive toxicity, hazard category 1A  
 STOT RE 1 - Specific Target Organ Toxicity — Repeated exposure, hazard category 1  
 Acute Tox. 1 - oral - Acute toxicity, oral, hazard category 1  
 Acute Tox. 1 - dermal - Acute toxicity, dermal, hazard category 1  
 Acute Tox. 1 - inhalation - Acute toxicity, inhalation, hazard category 1  
 H300 Fatal if swallowed.  
 H310 Fatal in contact with skin.  
 H330 Fatal if inhaled.  
 H361d Suspected of damaging the unborn child.  
 H372 Causes damage to organs through prolonged or repeated exposure .  
 H372 Causes damage to organs through prolonged or repeated exposure .?.