

Calcitriol (1,25-Dihydroxyvitamin D3) SDS/MSDS (Safety Data Sheet)

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

* Product Name: Calcitriol (1,25-Dihydroxyvitamin D3)

* Catalog Number: S1466

* CAS Number: 32222-06-3

* IUPAC Name: (1R,3S,Z)-5-((E)-2-((1R,3aS,7aR)-1-((R)-6-hydroxy-6-methylheptan-2-yl)-7a-methyl-octahydroinden-4-ylidene)ethylidene)-4-methylenecyclohexane-1,3-diol

Relevant identified uses and uses advised against

* Identified uses: For research and development use only; laboratory chemicals; manufacture of substances.

* Uses advised against: Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

* Company: Selleck Chemicals

* TollFree: +1 877 796-6397

* Tel: +1 832 582-8158

* Fax: +1 832 582-8590

Emergency telephone number

* Emergency phone #: +1 832 582-8158

2. HAZARDS IDENTIFICATION

2.1 GHS classification in accordance with 29 CFR 1910 (OSHA HCS):

Acute toxicity (oral): Category 1. H300

Acute toxicity (dermal): Category 1. H310

Acute toxicity (inhalation): Category 1. H330

Reproductive toxicity: Category 2. H361

2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Danger

Hazard statement(s)

H300: Fatal if swallowed

H310: Fatal in contact with skin

H330: Fatal if inhaled

H361: Suspected of damaging fertility or the unborn child

Precautionary statement(s)

None.

Prevention	P203: Obtain, read and follow all safety instructions before use. P260: Do not breathe dust/fume/gas/mist/vapors/spray. P262: Do not get in eyes, on skin, or on clothing. P264: Wash hands thoroughly after handling. P270: Do not eat, drink or smoke when using this product. P271: Use only outdoors or in a well-ventilated area. P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection. P284: [In case of inadequate ventilation] Wear respiratory protection.
Response	P301+P316: IF SWALLOWED: Get emergency medical help immediately. P302+P352: IF ON SKIN: wash with plenty of water. P304+P340: IF INHALED: Remove person to fresh air and keep comfortable for breathing. P316: Get emergency medical help immediately. P318: if exposed or concerned, get medical advice. P320: Specific treatment is urgent. P321: Specific treatment (see information on this label and safety datasheet)). P330: Rinse mouth. P361+P364: Take off immediately all contaminated clothing and wash it before reuse.
Storage	P403+P233: Store in a well-ventilated place. Keep container tightly closed. P405: Store locked up.
Disposal	P501: P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Other hazards

None.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Product name: Calcitriol (1,25-Dihydroxyvitamin D3)

CAS Number: 32222-06-3

PubChem CID: 5280453

Molecular formula: C₂₇H₄₄O₃

Molecular weight: 416.6 g/mol

IUPAC name: trans-(1R,3S,5Z)-5-[(2E)-2-[(1R,3aS,7aR)-1-[(2R)-6-hydroxy-6-methylheptan-2-yl]-7a-methyl-2,3,3a,5,6,7-hexahydro-1H-inden-4-ylidene]ethylidene]-4-methylidenecyclohexane-1,3-diol

3.2 Mixtures

Not applicable (pure substance).

4. FIRST-AID MEASURES

4.1 Description of first aid measures

Inhalation: Move to fresh air. Keep at rest in a position comfortable for breathing. Seek medical attention if symptoms persist.

Skin contact: Wash with plenty of soap and water. Remove contaminated clothing. Seek medical attention if irritation develops.

Eye contact: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing. Seek medical attention.

Ingestion: Rinse mouth. Do NOT induce vomiting unless directed by medical personnel. Seek medical attention.

4.2 Most important symptoms and effects, both acute and delayed

See Section 11 (Toxicological Information).

4.3 Indication of any immediate medical attention and special treatment needed

Treat symptomatically. Contact a poison control center or physician for severe exposure.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media

Suitable: Water spray, dry chemical, carbon dioxide (CO₂), alcohol-resistant foam.

Unsuitable: None known.

5.2 Specific hazards arising from the substance or mixture

Combustible. Heating may produce toxic fumes.

5.3 Advice for firefighters

Wear self-contained breathing apparatus (SCBA) and full protective clothing.

Fight fire from upwind. Cool containers with water spray until fire is extinguished.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear appropriate personal protective equipment (see Section 8).

Avoid breathing dust/vapor. Ensure adequate ventilation.

Evacuate personnel to safe areas. Keep people away from and upwind of spill.

WARNING: Highly toxic — only trained personnel should handle spills.

6.2 Environmental precautions

Prevent product from entering drains, waterways, or soil.

Contain spill with inert absorbent material.

6.3 Methods and materials for containment and cleaning up

SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational exposure or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or water; effects on animal, aquatic, and plant life; and conformance with environmental and public health regulations.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Calcitriol capsules should be protected from moisture, heat, and light and stored in tight, light-resistant containers at 15-30 °C. Calcitriol oral solution should be protected from light and stored at 15-30 °C. Calcitriol injection should be

stored at room temperature (25 °C); freezing should be avoided. Although brief exposure to temperatures up to 40 °C does not adversely affect the injection, exposure to excessive heat should be avoided.

7.2 Conditions for safe storage, including any incompatibilities

Calcitriol capsules should be protected from moisture, heat, and light and stored in tight, light-resistant containers at 15-30 °C. Calcitriol oral solution should be protected from light and stored at 15-30 °C. Calcitriol injection should be stored at room temperature (25 °C); freezing should be avoided. Although brief exposure to temperatures up to 40 °C does not adversely affect the injection, exposure to excessive heat should be avoided.

Store away from incompatible materials (see Section 10).

[Note: Specific storage temperature not available in public databases. Refer to supplier Certificate of Analysis (COA) for exact storage conditions.]

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Exposure controls

8.1.1 Occupational exposure limits (OEL)

OSHA PEL: Not established.

ACGIH TLV: Not established.

NIOSH REL: Not established.

No occupational exposure limit values are established for this substance.

Use the lowest feasible exposure level (ALARA principle).

8.1.2 Appropriate engineering controls

Use only in a chemical fume hood or with local exhaust ventilation.

Ensure adequate ventilation to keep airborne concentrations below exposure limits.

8.2 Individual protection measures

8.2.1 Eye/face protection

Wear safety glasses with side shields.

8.2.2 Skin protection

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

8.2.3 Respiratory protection

Wear NIOSH-approved respirator with appropriate cartridges. SCBA for high concentrations.

8.2.4 Thermal hazards

Not applicable.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance: White solid; [Merck Index]

b) Odor: No data available

c) Odor threshold: No data available

d) pH: No data available

e) Melting point/freezing point: 113-114

f) Initial boiling point and boiling range: No data available

- g) Flash point: No data available
- h) Evaporation rate: No data available
- i) Flammability (solid, gas): No data available
- j) Upper/lower flammability or explosive limits: No data available
- k) Vapor pressure: No data available
- l) Vapor density: No data available
- m) Relative density: No data available
- n) Water solubility: Insoluble
- o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 5.1
- p) Auto-ignition temperature: No data available
- q) Decomposition temperature: No data available
- r) Viscosity: No data available
- s) Explosive properties: No data available
- t) Oxidizing properties: No data available

9.2 Other information

Topological Polar Surface Area (TPSA): 60.7 Å²

Complexity: 688

10. STABILITY AND REACTIVITY

10.1 Reactivity

No specific reactivity hazards identified under normal handling conditions.

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No hazardous reactions under normal conditions.

10.4 Conditions to avoid

Avoid heat, sparks, open flames, direct sunlight, and moisture.

10.5 Incompatible materials

Strong oxidizing agents, strong acids, strong bases.

10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO₂).

See also Section 5 (Fire-fighting measures) for combustion products.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity:

No acute toxicity data available.

Skin corrosion/irritation:

No data available.

Serious eye damage/eye irritation:

No data available.

Respiratory or skin sensitization:

No data available.

Germ cell mutagenicity:

No data available.

Carcinogenicity:

No data available.

Reproductive toxicity:

Suspected of damaging fertility or the unborn child (H361).

Specific target organ toxicity (single exposure):

No data available.

Specific target organ toxicity (repeated exposure):

No data available.

Aspiration hazard:

No data available.

11.2 Additional information

Carcinogen classification:

No indication of carcinogenicity to humans (not listed by IARC).

Exposure routes:

Intravenous, Oral.

Rapidly absorbed from the intestine.

Signs and symptoms of exposure:

Overdose evident in elevated blood calcium levels causing symptoms of anorexia, nausea and vomiting, polyuria, polydipsia, weakness, pruritus, and nervousness, potentially with irreversible calcification of soft tissue in the kidney and liver.

Data source: Hazardous Substances Data Bank (HSDB) via PubChem.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

1,25-Dihydroxycholecalciferol's production and use for the management of hypocalcemia in patients undergoing chronic renal dialysis may result in its release to the environment through various waste streams. If released to air, an estimated vapor pressure of 1.2×10^{-12} mm Hg at 25 °C indicates 1,25-dihydroxycholecalciferol will exist solely in the particulate phase in the atmosphere. Particulate-phase 1,25-dihydroxycholecalciferol will be removed from the atmosphere by wet or dry deposition. 1,25-Dihydroxycholecalciferol does absorb at wavelengths >290 nm and therefore may be susceptible to direct photolysis by sunlight. If released to soil, 1,25-dihydroxycholecalciferol is expected to have no mobility based upon an estimated Koc of 1.1×10^5 . Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 3.1×10^{-7} atm-cu m/mole. 1,25-Dihydroxycholecalciferol is not expected to volatilize from dry soil surfaces based upon its vapor pressure. Biodegradation data for 1,25-dihydroxycholecalciferol were not available. If released into water, 1,25-dihydroxycholecalciferol is expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from water surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. An estimated BCF of 9600 suggests the potential for bioconcentration in aquatic

organisms is very high. Hydrolysis is n

12.2 Persistence and degradability

No data available.

12.3 Bioaccumulative potential

Log P (n-octanol/water): 5.1

Potential for bioaccumulation exists (Log P > 3).

12.4 Mobility in soil

No data available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available.

12.6 Other adverse effects

No other adverse ecological effects identified.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers and do not mix with other waste. Handle uncleaned containers in the same manner as the product itself.

14. TRANSPORT INFORMATION

14.1 UN number

Not regulated as dangerous goods (research quantities typically exempt).

14.2 UN proper shipping name

Not subject to transport regulations (small quantities for research use).

14.3 Transport hazard class(es)

Not classified as dangerous goods for transport (research quantities).

14.4 Packing group

Not applicable (not regulated as dangerous goods in typical research quantities).

14.5 Environmental hazards

Marine pollutant: No (not classified as environmentally hazardous per GHS).

14.6 Special precautions for user

Transport in original packaging. Ensure containers are tightly sealed.

For bulk or commercial quantities, consult applicable transport regulations (DOT, IATA, IMDG).

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

Not applicable.

15. REGULATORY INFORMATION

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

US EPA / TSCA: Subject to EPA TSCA regulations

EU ECHA / REACH: Not available in public databases.

SARA 302 Components:

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components:

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards:

Acute (short-term) health hazard

Chronic (long-term) health hazard

Massachusetts Right To Know Components:

This material contains components subject to the Massachusetts Right to Know Act. See Section 2 for hazard classification.

Pennsylvania Right To Know Components:

This material contains components subject to the Pennsylvania Right to Know Act. See Section 2 for hazard classification.

New Jersey Right To Know Components:

This material contains components subject to the New Jersey Right to Know Act. See Section 2 for hazard classification.

California Prop. 65 Components:

This product does not contain any chemicals known to the State of California to cause cancer, birth defects, or any other reproductive harm.

15.2 Chemical safety assessment

A chemical safety assessment has not been carried out for this substance.

For research-use-only compounds, no CSA is required under REACH Annex I.

16. OTHER INFORMATION

Revision Date: 2026/09/08

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product.

Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or contact with the product.