

Safety Data Sheet

according to Regulation (EC) No 1907/2006

1-alpha,25-Dihydroxy-Vitamin D3-(26,26,26,27,27,27-d6)

Revision date: 28.05.2025

Product code: LS-3720

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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1. Product identifier**

1-alpha,25-Dihydroxy-Vitamin D3-(26,26,26,27,27,27-d6)

Further trade names

Calcidiol-d6

25-hydroxycholecalciferol-d6

(5Z,7E)-(3S)-9,10-seco-5,7,10(19)-cholestatriene-3,25-diol-d6

(1S,Z)-3-((E)-2-((7aR)-1-((R)-6-hydroxy-6-

(trideuteromethyl)-7,7,7-trideuteroheptan-2-yl)-7a-methyldihydro-1H-inden-4(2H,5H,6H,7H,7aH)-ylidene)ethylidene)-4-methylenecyclohexanol

Substance name: 1-alpha,25-Dihydroxy-Vitamin D3-(26,26,26,27,27,27-d6)

CAS No: 78782-99-7

EC No: 110-386-3

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

Laboratory chemical. Manufacture of the substance.

Uses advised against

Do not use for private purposes (household).

Restrictions on use: Pharmaceutical substance

1.3. Details of the supplier of the safety data sheet

Company name:	Iris Biotech GmbH	
Street:	Adalbert-Zoellner-Straße 1	
Place:	D-95615 Marktredwitz, Germany	
Telephone:	+49 9231 97121 0	Telefax: +49 9231 97121 99
E-mail:	info@iris-biotech.de	
Contact person:	Health & Safety Department	Telephone: +49 9231 97121 0
E-mail:	sds@iris-biotech.de	
Internet:	www.iris-biotech.de	
Responsible Department:	Only available during office hours.	

1.4. Emergency telephone number: +49 (0)89 19240 (POISON CENTER Munich: 24 h)**SECTION 2: Hazards identification****2.1. Classification of the substance or mixture****Regulation (EC) No 1272/2008**

Acute Tox. 2; H330

Acute Tox. 2; H310

Acute Tox. 2; H300

STOT RE 1; H372

Full text of hazard statements: see SECTION 16.

2.2. Label elements**Regulation (EC) No 1272/2008****Signal word:** Danger**Pictograms:**

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Hazard statements

H300+H310+H330 Fatal if swallowed, in contact with skin or if inhaled.
 H372 Causes damage to organs through prolonged or repeated exposure.

Precautionary statements

P260 Do not breathe dust/fume/gas/mist/vapours/spray.
 P262 Do not get in eyes, on skin, or on clothing.
 P264 Wash hands thoroughly after handling.
 P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
 P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor.
 P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
 P403+P233 Store in a well-ventilated place. Keep container tightly closed.

Additional advice on labelling

Warning - substance not yet tested completely.

2.3. Other hazards

Analogous classification: Calcitriol/ Vitamin D3 (CAS 32222-06-3)

Product is not dust explosive in its original delivery form. The addition of particulate matter, however, results in a dust explosion risk.

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.1. Substances

Chemical characterization

Calcidiol-d6

Sum formula: C₂₇H₃₈D₆O₃

Molecular weight: 422,67 g/mol g/mol

Relevant ingredients

CAS No	Chemical name	Quantity
	EC No	
	Index No	
	REACH No	
	Classification (Regulation (EC) No 1272/2008)	
78782-99-7	1-alpha,25-Dihydroxy-Vitamin D3-(26,26,26,27,27,27-d6)	100 %
	110-386-3	
	Acute Tox. 2, Acute Tox. 2, Acute Tox. 2, STOT RE 1; H330 H310 H300 H372	

Full text of H and EUH statements: see section 16.

Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
		Specific Conc. Limits, M-factors and ATE	
78782-99-7	110-386-3	1-alpha,25-Dihydroxy-Vitamin D3-(26,26,26,27,27,27-d6)	100 %
		inhalation: ATE = 0,5 mg/l (vapours); inhalation: ATE = 0,05 mg/l (dusts or mists); dermal: ATE = 50 mg/kg; oral: ATE = 5 mg/kg	

SECTION 4: First aid measures

4.1. Description of first aid measures

General information

First aider: Pay attention to self-protection! Remove affected person from the danger area and lay down. In

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case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible).

In all cases of doubt, or when symptoms persist, seek medical advice.

After inhalation

Provide fresh air. No mouth-to-mouth or mouth-to-nose resuscitation. Use Ambu bag or ventilator. Call a physician immediately. Remove casualty to fresh air and keep warm and at rest. In case of irregular breathing or respiratory arrest provide artificial respiration.

After contact with skin

After contact with skin, wash immediately with plenty of water and soap. Take off immediately all contaminated clothing and wash it before reuse. Call a physician immediately. After contact with skin, wash immediately with plenty of water and soap.

After contact with eyes

After eye contact: Rinse immediately carefully and thoroughly with eye-bath or water. Consult an ophthalmologist. If product gets into the eye, keep eyelid open and rinse immediately with large quantities of water, for at least 5 minutes. Subsequently consult an ophthalmologist.

After ingestion

Induce vomiting when the affected person is not unconscious. Call a physician immediately. Rinse mouth thoroughly with water. Never give anything by mouth to an unconscious person or a person with cramps.

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

No information available.

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

Treat symptomatically.

SECTION 5: Firefighting measures**5.1. Extinguishing media****Suitable extinguishing media**

Co-ordinate fire-fighting measures to the fire surroundings. Water spray. alcohol resistant foam. Dry extinguishing powder. Sand.

Unsuitable extinguishing media

High power water jet.

5.2. Special hazards arising from the substance or mixture

Non-flammable. Thermal decomposition can lead to the escape of irritating gases and vapours.

In case of fire may be liberated: Carbon dioxide (CO₂). Carbon monoxide (CO). Nitrogen oxides (NO_x).

5.3. Advice for firefighters

Wear a self-contained breathing apparatus and chemical protective clothing. Full protection suit.

Additional information

Suppress gases/vapours/mists with water spray jet. Collect contaminated fire extinguishing water separately.

Do not allow entering drains or surface water. Usual measures for fire prevention.

SECTION 6: Accidental release measures**6.1. Personal precautions, protective equipment and emergency procedures****General advice**

Avoid dust formation. Do not breathe dust. Avoid contact with skin, eyes and clothes. Use personal protection equipment. Provide adequate ventilation. Avoid breathing dust/fume/gas/mist/vapours/spray.

Avoid contact with skin, eyes and clothes.

Wear personal protection equipment.

In case of fire: Evacuate area.

For non-emergency personnel

Remove all sources of ignition. Provide adequate ventilation.

Use personal protection equipment.

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Evacuate the danger area, observe emergency procedures, consult an expert.

For emergency responders

Wear personal protection equipment (refer to section 8).

Take up mechanically, placing in appropriate containers for disposal. Take up dust-free and set down dust-free.

6.2. Environmental precautions

Do not allow to enter into soil/subsoil.

Do not allow to enter into surface water or drains.

6.3. Methods and material for containment and cleaning up**For containment**

Avoid dust formation.

For cleaning up

Take up mechanically. Treat the recovered material as prescribed in the section on waste disposal. Take up mechanically.

Other information

Take up mechanically, placing in appropriate containers for disposal. Avoid dust formation.

Clear contaminated areas thoroughly.

6.4. Reference to other sections

Safe handling: see section 7

Personal protection equipment: see section 8

Disposal: see section 13

Treat the recovered material as prescribed in the section on waste disposal.

SECTION 7: Handling and storage**7.1. Precautions for safe handling****Advice on safe handling**

If handled uncovered, arrangements with local exhaust ventilation have to be used. Avoid dust formation. Do not breathe dust. Provide adequate ventilation.

Avoid breathing dust/fume/gas/mist/vapours/spray.

Avoid contact with skin, eyes and clothes.

Advice on protection against fire and explosion

Usual measures for fire prevention.

Advice on general occupational hygiene

Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme.

Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat, drink, smoke, sniff. Take off contaminated clothing. Wash hands before breaks and after work. When using do not eat, drink, smoke, sniff. Avoid contact with skin, eyes and clothes. Provide adequate ventilation.

7.2. Conditions for safe storage, including any incompatibilities**Requirements for storage rooms and vessels**

Keep container tightly closed. Keep locked up. Store in a place accessible by authorized persons only. Provide adequate ventilation as well as local exhaust at critical locations. Keep container tightly closed in a cool, well-ventilated place.

Handle and store contents under inert gas. Protect from moisture.

storage temperature: -20 °C

Hints on joint storage

No special measures are necessary.

Further information on storage conditions

Protect from light!

Keep under argon.

7.3. Specific end use(s)

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Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

SECTION 8: Exposure controls/personal protection**8.1. Control parameters****Additional advice on limit values**

To date, no national critical limit values exist.

8.2. Exposure controls**Appropriate engineering controls**

If handled uncovered, arrangements with local exhaust ventilation have to be used. Do not breathe dust. The receiver of our product is singularly responsible for adhering to existing laws and regulations.

Individual protection measures, such as personal protective equipment**Eye/face protection**

Wear eye protection/face protection.

Tightly fitting safety goggles. Face shield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Hand protection

When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. Wear suitable gloves.

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands. The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Skin protection

Use of protective clothing.

Respiratory protection

In case of inadequate ventilation wear respiratory protection. If technical exhaust or ventilation measures are not possible or insufficient, respiratory protection must be worn.

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

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.

Thermal hazards

No data available

Environmental exposure controls

Discharge into the environment must be avoided.

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SECTION 9: Physical and chemical properties**9.1. Information on basic physical and chemical properties**

Physical state:	solid	
Colour:	white/ whitish	
Odour:	No data available	
Odour threshold:	No data available	
Melting point/freezing point:		No data available
Boiling point or initial boiling point and boiling range:		No data available
Flammability:		not determined
Lower explosion limits:		No data available
Upper explosion limits:		No data available
Flash point:		No data available
Auto-ignition temperature:		No data available
Decomposition temperature:		No data available
pH-Value:		No data available
Viscosity / kinematic:		not applicable
Water solubility:		No data available
Solubility in other solvents		
not determined		
Dissolution rate:		No data available
Partition coefficient n-octanol/water:		No data available
Dispersion stability:		No data available
Vapour pressure:		No data available
Density:		No data available
Relative density:		No data available
Bulk density:		No data available
Relative vapour density:		No data available
Particle characteristics:		No data available

9.2. Other information**Information with regard to physical hazard classes**

Explosive properties

The product is not: Explosive. Product is not dust explosive in its original delivery form. The addition of particulate matter, however, results in a dust explosion risk.

Sustained combustibility: No data available

Self-ignition temperature

Solid: No data available

Gas: not applicable

Oxidizing properties

No data available

Other safety characteristics

Solvent content: No data available

Viscosity / dynamic: not applicable

Flow time: not applicable

SECTION 10: Stability and reactivity**10.1. Reactivity**

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

10.2. Chemical stability

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Stable under recommended storage conditions.

10.3. Possibility of hazardous reactions

No data available

10.4. Conditions to avoid

 Protect from moisture.
 Keep away from heat.
 Protect from light!

10.5. Incompatible materials

Oxidizing agents, strong.

10.6. Hazardous decomposition products

 Thermal decomposition can lead to the escape of irritating gases and vapours.
 In case of fire may be liberated: Carbon dioxide (CO₂). Carbon monoxide (CO). Nitrogen oxides (NO_x).

Further information

In case of fire: See chapter 5.

SECTION 11: Toxicological information
11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008
Toxicokinetics, metabolism and distribution

No data available

Acute toxicity

 Fatal if inhaled.
 Fatal in contact with skin.
 Fatal if swallowed.
 Analogous classification: Calcitriol/ Vitamin D3 (CAS 32222-06-3)

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
78782-99-7	1-alpha,25-Dihydroxy-Vitamin D3-(26,26,26,27,27,27-d6)				
	oral	ATE 5 mg/kg			
	dermal	ATE 50 mg/kg			
	inhalation vapour	ATE 0,5 mg/l			
	inhalation dust/mist	ATE 0,05 mg/l			

Irritation and corrosivity

 Skin corrosion/irritation: Based on available data, the classification criteria are not met.
 Serious eye damage/eye irritation: Based on available data, the classification criteria are not met.

Sensitising effects

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

Carcinogenic/mutagenic/toxic effects for reproduction

 Germ cell mutagenicity: Based on available data, the classification criteria are not met.
 Carcinogenicity: Based on available data, the classification criteria are not met.
 Reproductive toxicity: Based on available data, the classification criteria are not met.
 IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

STOT-single exposure

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

STOT-repeated exposure

 Causes damage to organs through prolonged or repeated exposure. (1-alpha,25-Dihydroxy- Vitamin D3-(26,26,26,27,27,27-d6))
 Analogous classification: Calcitriol/ Vitamin D3 (CAS 32222-06-3)

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Aspiration hazard

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

Information on likely routes of exposure

No data available

Specific effects in experiment on an animal

No data available

Practical experience

No data available

11.2. Information on other hazards**Endocrine disrupting properties**

No data available

Other information

Analogous classification: Calcitriol/ Vitamin D3 (CAS 32222-06-3)

Further information

RTECS: No data available

To our knowledge, the chemical, physical and toxicological properties have not been extensively studied. Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information**12.1. Toxicity**

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

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

This substance does not meet the PBT/vPvB criteria of REACH, annex XIII.

The product has not been tested.

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

12.7. Other adverse effects

Warning - substance not yet tested completely.

Further information

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil.

Avoid release to the environment.

SECTION 13: Disposal considerations**13.1. Waste treatment methods****Disposal recommendations**

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil. Dispose of waste according to applicable legislation.

Consult the appropriate local waste disposal expert about waste disposal.

Handle contaminated packages in the same way as the substance itself.

Contaminated packaging

Hazardous waste according to Directive 2008/98/EC (waste framework directive). Handle contaminated packages in the same way as the substance itself.

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SECTION 14: Transport information**Land transport (ADR/RID)**

14.1. UN number or ID number: UN 2811
14.2. UN proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (Calcitriol-d6)
14.3. Transport hazard class(es): 6.1
14.4. Packing group: II
Hazard label: 6.1



Classification code: T2
Special Provisions: 274 614
Limited quantity: 500 g
Excepted quantity: E4
Transport category: 2
Hazard No: 60
Tunnel restriction code: D/E

Inland waterways transport (ADN)

14.1. UN number or ID number: UN 2811
14.2. UN proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (Calcitriol-d6)
14.3. Transport hazard class(es): 6.1
14.4. Packing group: II
Hazard label: 6.1



Classification code: T2
Special Provisions: 274 614 802
Limited quantity: 500 g
Excepted quantity: E4

Marine transport (IMDG)

14.1. UN number or ID number: UN 2811
14.2. UN proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (Calcitriol-d6)
14.3. Transport hazard class(es): 6.1
14.4. Packing group: II
Hazard label: 6.1



Special Provisions: 274
Limited quantity: 500 g
Excepted quantity: E4
EmS: F-A, S-A

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID number: UN 2811
14.2. UN proper shipping name: TOXIC SOLID, ORGANIC, N.O.S. (Calcitriol-d6)
14.3. Transport hazard class(es): 6.1
14.4. Packing group: II
Hazard label: 6.1

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Special Provisions:	A3 A5	
Limited quantity Passenger:	1 kg	
Passenger LQ:	Y644	
Excepted quantity:	E4	
IATA-packing instructions - Passenger:		669
IATA-max. quantity - Passenger:		25 kg
IATA-packing instructions - Cargo:		676
IATA-max. quantity - Cargo:		100 kg

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

14.6. Special precautions for user

Warning: Acute Toxicity.

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 regulatory information**

Information according to Directive 2012/18/EU (SEVESO III): H2 ACUTE TOXIC

Additional information

Safety Data Sheet according to Regulation (EC) No. 1907/2006 (REACH)

National regulatory information

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC). Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

Water hazard class (D): 3 - highly hazardous to water

Skin resorption/Sensitization: Permeates easily through outer skin and causes poisoning.

15.2. Chemical safety assessment

For this substance a chemical safety assessment has not been carried out.

SECTION 16: Other information**Changes**

This data sheet contains changes from the previous version in section(s): 1,2,4,5,6,7,8,9,10,11,12,13,14,15,16.

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Abbreviations and acronyms

Acute Tox: Acute toxicity
STOT RE: Specific target organ toxicity - repeated exposure
ADR: Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road).
IMDG: International Maritime Code for Dangerous Goods
IATA: International Air Transport Association
GHS: Globally Harmonized System of Classification and Labelling of Chemicals
EINECS: European Inventory of Existing Commercial Chemical Substances
ELINCS: European List of Notified Chemical Substances
CAS: Chemical Abstracts Service
LC50: Lethal concentration, 50%
LD50: Lethal dose, 50%
CLP: Classification, labelling and Packaging
REACH: Registration, Evaluation and Authorization of Chemicals
GHS: Globally Harmonised System of Classification, Labelling and Packaging of Chemicals
UN: United Nations
CAS: Chemical Abstracts Service
DNEL: Derived No Effect Level
DMEL: Derived Minimal Effect Level
PNEC: Predicted No Effect Concentration
ATE: Acute toxicity estimate
LL50: Lethal loading, 50%
EL50: Effect loading, 50%
EC50: Effective Concentration 50%
ErC50: Effective Concentration 50%, growth rate
NOEC: No Observed Effect Concentration
BCF: Bio-concentration factor
PBT: persistent, bioaccumulative, toxic
vPvB: very persistent, very bioaccumulative
RID: Regulations concerning the international carriage of dangerous goods by rail
ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways (Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures)
EmS: Emergency Schedules
MFAG: Medical First Aid Guide
IATA: International Air Transport Association
ICAO: International Civil Aviation Organization
MARPOL: International Convention for the Prevention of Marine Pollution from Ships
IBC: Intermediate Bulk Container
SVHC: Substance of Very High Concern
For abbreviations and acronyms, see table at <http://abbrev.esdscom.eu>
EC/EEC: European Community/European Economic Community
EU: European Union
M-factor: Multiplying factor
ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
IATA: International Air Transport Association
DGR: Dangerous Goods Regulations
ICAO: International Civil Aviation Organization
TI: Technical Instructions
For abbreviations and acronyms, see: ECHA Guidance on information requirements and chemical safety assessment, chapter R.20 (Table of terms and abbreviations).

Relevant H and EUH statements (number and full text)

H300 Fatal if swallowed.

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H300+H310+H330	Fatal if swallowed, in contact with skin or if inhaled.
H310	Fatal in contact with skin.
H330	Fatal if inhaled.
H372	Causes damage to organs through prolonged or repeated exposure.

Further Information

The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights. The receiver of our product is singularly responsible for adhering to existing laws and regulations.

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.