

Safety Data Sheet

according to UK REACH Regulation

Valdecoxib-D3

Revision date: 19.03.2026

Product code: NS042

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

1.1. Product identifier

Valdecoxib-D3

Further trade names

4-(5-Methyl-D3-3-phenyl-isoxazol-4-yl)-benzenesulfonamide

CAS No: 1219794-90-7

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

Use of the substance/mixture

Reference standard for analysis.

1.3. Details of the supplier of the safety data sheet

Company name: WITEGA Laboratorien Berlin-Adlershof GmbH
Street: James-Franck-Strasse 4
Place: D-12489 Berlin
Telephone: +493063922001 Telefax: +493063922007
E-mail: witega@witega.de
Internet: www.witega.de

1.4. Emergency telephone number:

+493063922001

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

GB CLP Regulation

Repr. 2; H361d
Acute Tox. 4; H302
STOT RE 2; H373
Aquatic Chronic 1; H410

Full text of hazard statements: see SECTION 16.

2.2. Label elements

GB CLP Regulation

Signal word: Warning

Pictograms:



Hazard statements

H302 Harmful if swallowed.
H361d Suspected of damaging the unborn child.
H373 May cause damage to organs through prolonged or repeated exposure.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P262 Do not get in eyes, on skin, or on clothing.
P273 Avoid release to the environment.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

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2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula: C16H11D3N2O3S

Molecular weight: 317.38 g/mol

Relevant ingredients

CAS No	Chemical name	Quantity		
	EC No	Index No	REACH No	
	Classification (GB CLP Regulation)			
1219794-90-7	Valdecoxib-D3			100 %
	Repr. 2, Acute Tox. 4, STOT RE 2, Aquatic Chronic 1; H361d H302 H373 H410			

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		
1219794-90-7		Valdecoxib-D3	100 %
	oral: LD50 = 1600 mg/kg		

SECTION 4: First aid measures

4.1. Description of first aid measures

General information

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

After inhalation

Remove casualty to fresh air and keep warm and at rest. If breathing is irregular or stopped, administer artificial respiration.

After contact with skin

Remove contaminated, saturated clothing immediately. Subsequently wash off with: Water and soap

After contact with eyes

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist.

After ingestion

Rinse mouth immediately and drink plenty of water. Get immediate medical advice/attention.

Do NOT induce vomiting. 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 data available

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

No data available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

Water spray jet. Foam. Dry extinguishing powder. Carbon dioxide (CO₂).

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5.2. Special hazards arising from the substance or mixture

In case of fire may be liberated: Pyrolysis products, toxic. In case of fire and/or explosion do not breathe fumes.

5.3. Advice for firefighters

In case of fire: Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General advice

Use personal protection equipment. Do not breathe gas/fumes/vapour/spray.

6.2. Environmental precautions

Do not allow to enter into surface water or drains.

6.3. Methods and material for containment and cleaning up

Other information

Take up dust-free and set down dust-free.

6.4. Reference to other sections

Disposal: see section 13

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

If handled uncovered, arrangements with local exhaust ventilation should be used if possible.

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take precautionary measures against static discharges.

Advice on general occupational hygiene

Use personal protection equipment.

7.2. Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

Keep container tightly closed in a cool, well-ventilated place. Avoid: UV-radiation/sunlight

Further information on storage conditions

storage temperature: 2-8°C

7.3. Specific end use(s)

none

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

8.2. Exposure controls

Appropriate engineering controls

If handled uncovered, arrangements with local exhaust ventilation should be used if possible. If local exhaust ventilation is not possible or not sufficient, the entire working area should be ventilated by technical means.

Individual protection measures, such as personal protective equipment

Eye/face protection

Eye glasses with side protection

Hand protection

Wear suitable gloves. 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.

Skin protection

lab coat

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Respiratory protection

In case of inadequate ventilation wear respiratory protection.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state:	solid
Colour:	
Melting point/freezing point:	159-162 °C
Boiling point or initial boiling point and boiling range:	No data available
Flammability:	No data available
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
Water solubility:	No data available

9.2. Other information

Information with regard to physical hazard classes

Explosive properties

No data available

Self-ignition temperature

Solid:

No data available

Gas:

No data available

Oxidizing properties

No data available

Other safety characteristics

Evaporation rate:

No data available

Further Information

none

SECTION 10: Stability and reactivity

10.1. Reactivity

Reacts with : Oxidising agent, Alkali (lye), Etchant and acids

10.2. Chemical stability

The product is chemically stable under recommended conditions of storage, use and temperature.

10.3. Possibility of hazardous reactions

No known hazardous reactions.

10.4. Conditions to avoid

Do not expose to temperatures exceeding 50 °C/122 °F.

10.5. Incompatible materials

Oxidising agent, Alkali (lye), Etchant and acids

10.6. Hazardous decomposition products

In case of fire may be liberated: Pyrolysis products, toxic.

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in GB CLP Regulation

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Acute toxicity

Harmful if swallowed.

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
1219794-90-7	Valdecoxib-D3				
	oral	LD50 1600 mg/kg	Rat		

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

Suspected of damaging the unborn child. (Valdecoxib-D3)

Germ cell mutagenicity: Based on available data, the classification criteria are not met.

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

STOT-single exposure

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

STOT-repeated exposure

May cause damage to organs through prolonged or repeated exposure. (Valdecoxib-D3)

Aspiration hazard

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

Specific effects in experiment on an animal

No data available

SECTION 12: Ecological information

12.1. Toxicity

Very toxic to aquatic life with long lasting effects.

No data available

12.2. Persistence and degradability

No data available

12.3. Bioaccumulative potential

No indication of bioaccumulation potential.

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 UK REACH.

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

12.6. Endocrine disrupting properties

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

12.7. Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

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Disposal recommendations

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

Contaminated packaging

This material and its container must be disposed of as hazardous waste.

SECTION 14: Transport information

Land transport (ADR/RID)

14.1. UN number or ID number: UN 3077
14.2. UN proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
14.3. Transport hazard class(es): 9
14.4. Packing group: III
 Hazard label: 9



Classification code: M7
 Special Provisions: 274 335 375 601
 Limited quantity: 5 kg
 Excepted quantity: E1
 Transport category: 3
 Hazard No: 90
 Tunnel restriction code: -

Inland waterways transport (ADN)

14.1. UN number or ID number: UN 3077
14.2. UN proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
14.3. Transport hazard class(es): 9
14.4. Packing group: III
 Hazard label: 9



Classification code: M7
 Special Provisions: 274 335 375 601
 Limited quantity: 5 kg
 Excepted quantity: E1

Marine transport (IMDG)

14.1. UN number or ID number: UN 3077
14.2. UN proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
14.3. Transport hazard class(es): 9
14.4. Packing group: III
 Hazard label: 9



Special Provisions: 274 335 966 967 969
 Limited quantity: 5 kg
 Excepted quantity: E1
 EmS: F-A, S-F

Air transport (ICAO-TI/IATA-DGR)

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14.1. UN number or ID number: UN 3077
14.2. UN proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
14.3. Transport hazard class(es): 9
14.4. Packing group: III
 Hazard label: 9



Special Provisions: A97 A158 A179 A197 A215
 Limited quantity Passenger: 30 kg G
 Passenger LQ: Y956
 Excepted quantity: E1
 IATA-packing instructions - Passenger: 956
 IATA-max. quantity - Passenger: 400 kg
 IATA-packing instructions - Cargo: 956
 IATA-max. quantity - Cargo: 400 kg

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: Yes



14.6. Special precautions for user

No transport as bulk according to IBC Code.

14.7. Maritime transport in bulk according to IMO instruments

No transport as bulk according to IBC Code.

SECTION 15: Regulatory information

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

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

15.2. Chemical safety assessment

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

SECTION 16: Other information

Abbreviations and acronyms

Acute Tox: Acute toxicity
 Repr: Reproductive toxicity
 STOT RE: Specific target organ toxicity - repeated exposure
 Aquatic Chronic: Chronic aquatic hazard

Relevant H and EUH statements (number and full text)

H302 Harmful if swallowed.
 H361d Suspected of damaging the unborn child.
 H373 May cause damage to organs through prolonged or repeated exposure.
 H410 Very toxic to aquatic life with long lasting effects.

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Further Information

This information is based on our present state of knowledge. However, it should not constitute a guarantee for any specific product properties and shall not establish a legally valid relationship. The substances are only for R&D. Do not use as a drug, in household or other applications.