

Safety Data Sheet

according to Regulation (EU) 2020/878

BUCHLER GmbH

Trade name: Didehydrocinchonine

Date of issue: 14.08.2020

Revision date: -

Version: 1

Replaces version: -

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

1.1. Product identifier

Product form : Substance
Substance name : Didehydrocinchonine
Chemical name : (S)-[(2R,4S,5S)-5-Ethynyl-1-azabicyclo[2.2.2]oct-2-yl](quinolin-4-yl)methanol
EC No : -
CAS No : 157319-37-4
Formula : C₁₉H₂₀N₂O

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

1.2.1. Relevant identified uses

Main use category : Industrial use. Professional use.
Use of the substance/mixture : Chiral resolution

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Manufacturer/Supplier

Buchler GmbH
Harxbuetteler Straße 3
38110 Braunschweig - Germany
T +49 5307 9310
www.buchler-gmbh.com
info@buchler-gmbh.com

Safety data sheet: DLAC Dienstleistungsagentur Chemie GmbH, E-Mail: sds@dlac-gmbh.de

1.4. Emergency telephone number

Country	Organisation/Company	Address	Emergency number
Germany	Giftinformationszentrum-Nord Zentrum Pharmakologie und Toxikologie der Universität Göttingen	Robert-Koch Strasse 40 D-37075 Göttingen	+49 551 19240 (German/English)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Acute toxicity (oral), Category 4 H302

Sensitisation - Skin, Category 1A H317

Full text of H statements : see section 16

Adverse physicochemical, human health and environmental effects

Harmful if swallowed. May cause an allergic skin reaction.

2.2. Label elements

Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



GHS07

Signal word (CLP) :

Warning

Hazard statements (CLP) :

H302 - Harmful if swallowed
H317 - May cause an allergic skin reaction

Precautionary statements (CLP) :

P261 - Avoid breathing dust
P270 - Do not eat, drink or smoke when using this product
P280 - Wear protective gloves, protective clothing, eye protection
P301+P312 - IF SWALLOWED: Call a POISON CENTER, doctor if you feel unwell
P302+P352 - IF ON SKIN: Wash with plenty of soap and water
P333+P313 - If skin irritation or rash occurs: Get medical advice/attention

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2.3. Other hazards

No additional information available

SECTION 3: Composition/information on ingredients

3.1. Substances

Substance name : Didehydrocinchonine

EC No : -

CAS No : 157319-37-4

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
Didehydrocinchonine	(CAS No) 157319-37-4	≤ 100	Acute Tox. 4 (Oral), H302 Skin Sens. 1A, H317

Full text of H-statements: see section 16

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

- First-aid measures general : Get medical advice/attention if you feel unwell. If possible show him this sheet. Failing this, show him the packaging or label. Never give anything by mouth to an unconscious person. Place the affected person in the recovery position.
- First-aid measures after inhalation : Remove victim to fresh air and keep at rest in a position comfortable for breathing.
- First-aid measures after skin contact : Take off immediately all contaminated clothing and wash it before reuse. Wash with plenty of soap and water. If skin irritation or rash occurs: Get medical advice/attention.
- First-aid measures after eye contact : IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
- First-aid measures after ingestion : Rinse mouth. Drink plenty of water as a precaution. Get medical advice/attention.

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

- Symptoms/injuries : Signs of cinchonism: Neurotoxic effects (e.g. headache, tinnitus, visual disturbances, confusion), gastrointestinal disorders (e.g. nausea, vomiting, diarrhoea), exanthema and haematological disorders.
- Symptoms/injuries after skin contact : May cause an allergic skin reaction.
- Symptoms/injuries after ingestion : Harmful if swallowed.

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 : Making extinguishing agents environment-friendly. Water spray. Foam. Carbon dioxide. Dry extinguishing powder.
- Unsuitable extinguishing media : Do not use a heavy water stream.

5.2. Special hazards arising from the substance or mixture

- Hazardous decomposition products in case of fire : Carbon oxides (CO, CO₂). Nitrogen oxides.

5.3. Advice for firefighters

- Firefighting instructions : Use water spray or fog for cooling exposed containers. Prevent fire-fighting water from entering environment.
- Protection during firefighting : Use a self-contained breathing apparatus and also a protective suit (EN 469).

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

- General measures : Stop leak if safe to do so. Provide adequate ventilation. Avoid contact with skin and eyes. Do not breathe dust.

6.1.1. For non-emergency personnel

- Emergency procedures : Only qualified personnel equipped with suitable protective equipment may intervene.

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6.1.2. For emergency responders

Protective equipment : Use personal protective equipment as required. Wear suitable respiratory equipment in case of insufficient ventilation.

6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if substance enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up : Take up mechanically (sweeping, shovelling) and collect in suitable container for disposal. Minimize generation of dust. Dispose of in accordance with relevant local regulations.

6.4. Reference to other sections

Concerning personal protective equipment to use, see section 8. Concerning disposal elimination after cleaning, see section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Provide local exhaust or general room ventilation. Avoid dust formation. Avoid contact with skin and eyes. Keep container closed when not in use.

Hygiene measures : Handle in accordance with good industrial hygiene and safety procedures. When using do not eat, drink or smoke. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Take off contaminated clothing and wash it before reuse.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Store in original container. Store tightly closed in a dry and cool place. Keep out of direct sunlight. Protect from moisture.

Storage temperature : This substance does not require any special temperature storage conditions.

Prohibitions on mixed storage : Keep away from food, drink and animal feedingstuffs.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Exposure controls

Appropriate engineering controls:

Use adequate ventilation. Avoid dust formation.

Hand protection:

Wear suitable gloves (EN 374). Latex. Nitrile rubber. Butyl rubber. 0.4 mm. The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

Eye protection:

Chemical goggles or safety glasses (EN 166).

Skin and body protection:

Wear suitable protective clothing (EN 344).

Respiratory protection:

Where exposure through inhalation may occur from use, respiratory protection is recommended. Dust production: dust mask with filter type P2.

Environmental exposure controls:

Avoid release to the environment.

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 : No data available

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Boiling point or initial boiling point and boiling range	: No data available
Flammability	: No data available
Lower and upper explosion limit	: Not applicable
Flash point	: Not applicable
Auto-ignition temperature	: Not applicable
Decomposition temperature	: No data available
pH	: No data available
Kinematic viscosity	: Not applicable
Solubility	: No data available
Partition coefficient n-octanol/water (log value)	: 2.58
Vapour pressure	: No data available
Density and/or relative density	: No data available
Relative vapour density	: Not applicable
Particle characteristics	: No data available

9.2. Other information

Explosive properties	: The substance is not explosive. Dust can form an explosive mixture with air.
Oxidising properties	: The substance has no oxidising properties.

SECTION 10: Stability and reactivity

10.1. Reactivity

No dangerous reactions known under normal conditions of use.

10.2. Chemical stability

Stable under use and storage conditions as recommended in section 7 for a minimum of 5 years.

10.3. Possibility of hazardous reactions

None under normal use.

10.4. Conditions to avoid

Direct sunlight. High temperature. The degradation product quinine is formed.

10.5. Incompatible materials

Oxidising agents.

10.6. Hazardous decomposition products

In case of fire: Carbon monoxide. Carbon dioxide. Nitrogen oxides.

SECTION 11: Toxicological information

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

Acute toxicity : Oral: Harmful if swallowed.

Didehydrocinchonine (157319-37-4)	
LD50 oral rat	350.82 mg/kg (Quinine)
Skin corrosion/irritation	: Not classified Based on available data, the classification criteria are not met
Serious eye damage/irritation	: Not classified Based on available data, the classification criteria are not met
Respiratory or skin sensitisation	: May cause an allergic skin reaction.
Germ cell mutagenicity	: Not classified Based on available data, the classification criteria are not met
Carcinogenicity	: Not classified Based on available data, the classification criteria are not met
Reproductive toxicity	: Not classified Based on available data, the classification criteria are not met
Specific target organ toxicity (single exposure)	: Not classified Based on available data, the classification criteria are not met

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Specific target organ toxicity (repeated exposure) : Not classified
Based on available data, the classification criteria are not met

Aspiration hazard : Not classified
Based on available data, the classification criteria are not met

11.2. Information on other hazards

Potential adverse human health effects and symptoms : Signs of cinchonism: Neurotoxic effects (e.g. headache, tinnitus, visual disturbances, confusion), gastrointestinal disorders (e.g. nausea, vomiting, diarrhoea), exanthema and haematological disorders.

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity : Not classified

Chronic aquatic toxicity : Not classified

Didehydrocinchonine (157319-37-4)

EC50 daphnia	79.96 mg/l 24 h, Daphnia magna (Cinchonine)
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EC50 daphnia	14.25 mg/l 48 h, Daphnia magna (Cinchonine)
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ErC50 algae	11.13 mg/l 72 h, Dunaliella salina (Quinine)
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12.2. Persistence and degradability

Didehydrocinchonine (157319-37-4)

Persistence and degradability	Readily biodegradable.
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Biodegradation	72 – 96.9 % 28 d (OECD 301 B) (Cinchonin)
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12.3. Bioaccumulative potential

Didehydrocinchonine (157319-37-4)

Bioconcentration factor (BCF REACH)	13 l/kg
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Log Pow	2.58
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12.4. Mobility in soil

Didehydrocinchonine (157319-37-4)

Log Koc	1.8 – 4.2
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12.5. Results of PBT and vPvB assessment

This substance does not meet the PBT- or vPvB criteria of REACH regulation, annex XIII.

12.6. Endocrine disrupting properties

No additional information available

12.7. Other adverse effects

No additional information available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Regional legislation (waste) : Dispose in a safe manner in accordance with local/national regulations.

Waste treatment methods : This material and its container must be disposed of as hazardous waste. Do not dispose of with domestic waste. Do not empty into drains.

Waste disposal recommendations : Empty the packaging completely prior to disposal. When totally empty, containers are recyclable like any other packing.

European List of Waste (LoW) code : 07 00 00 - WASTES FROM ORGANIC CHEMICAL PROCESSES
07 01 00 - wastes from the manufacture, formulation, supply and use (MFSU) of basic organic chemicals

Waste code : The waste code number according to the Ordinance on the European Waste Catalogue (AVV) depends on the waste producer and can therefore vary for any given product. The waste code number is therefore to be gleaned separately from each waste producer.

SECTION 14: Transport information

In accordance with ADR / IMDG / IATA

14.1. UN number or ID number

UN-No. (ADR) : Not applicable

UN-No. (IMDG) : Not applicable

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UN-No. (IATA) : Not applicable

14.2. UN proper shipping name

Proper Shipping Name (ADR) : Not applicable

Proper Shipping Name (IMDG) : Not applicable

Proper Shipping Name (IATA) : Not applicable

14.3. Transport hazard class(es)

ADR

Transport hazard class(es) (ADR) : Not applicable

IMDG

Transport hazard class(es) (IMDG) : Not applicable

IATA

Transport hazard class(es) (IATA) : Not applicable

14.4. Packing group

Packing group (ADR) : Not applicable

Packing group (IMDG) : Not applicable

Packing group (IATA) : Not applicable

14.5. Environmental hazards

Dangerous for the environment : No

Marine pollutant : No

Other information : No supplementary information available

14.6. Special precautions for user

- Overland transport

Not applicable

- Transport by sea

Not applicable

- Air transport

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

15.1.1. EU-Regulations

Didehydrocinchonine is not on the REACH Candidate List

Didehydrocinchonine is not on the REACH Annex XIV List

15.1.2. National regulations

No additional information available

15.2. Chemical safety assessment

For this substance a chemical safety assessment was not carried out.

SECTION 16: Other information

Data source : REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006

Changes compared to earlier Versions : -

Abbreviations and acronyms:

ADN	European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways
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ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road
BCF	Bioconcentration factor
DNEL	Derived-No Effect Level
EC50	Median effective concentration
IATA	International Air Transport Association
IMDG	International Maritime Dangerous Goods
LC50	Median lethal concentration
LD50	Median lethal dose
NOEC	No-Observed Effect Concentration
NOAEL	No-Observed Adverse Effect Level
NOAEC	No-Observed Adverse Effect Concentration
LOAEL	Lowest Observed Adverse Effect Level
PBT	Persistent Bioaccumulative Toxic
PNEC	Predicted No-Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals Regulation (EC) No 1907/2006
STP	Sewage treatment plant
vPvB	Very Persistent and Very Bioaccumulative

Full text of H- and EUH-statements:

Acute Tox. 4 (Oral)	Acute toxicity (oral), Category 4
Skin Sens. 1A	Sensitisation - Skin, Category 1A
H302	Harmful if swallowed
H317	May cause an allergic skin reaction

SDS EU (REACH Annex II)

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.