according to Regulation (EU) 2020/878



Trade name: (8α,9R)-1-(9-anthracenylmethyl)-9-hydroxy-6'-

methoxy-cinchonanium chloride

Date of issue: 06.07.2023

Revision date: 15.02.2024

Version: 2 Replaces version: 1

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

1.1. Product identifier

Product form : Substance

Substance name : (8a,9R)-1-(9-anthracenylmethyl)-9-hydroxy-6'-methoxy-cinchonanium chloride

EC no : -

CAS No : 199588-84-6 Formula : C35H35CIN2O2

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 : Research and development of synthesis, Phase transfer catalyst

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

info@buchler-gmbh.com - www.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	Robert-Koch Strasse 40	+49 551 19240
	Zentrum Pharmakologie und Toxikologie der Universität Göttingen	D-37075 Göttingen	(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 1 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

Contains no substance(s) included in the list established in accordance with Article 59(1) of REACH for having endocrine disrupting properties, or is not identified as having endocrine disrupting properties in accordance with the criteria set out in Commission Delegated Regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605.

SECTION 3: Composition/information on ingredients

3.1. **Substances**

: (8α,9R)-1-(9-anthracenylmethyl)-9-hydroxy-6'-methoxy-cinchonanium chloride Substance name

EC No

CAS No : 199588-84-6

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
(8α,9R)-1-(9-anthracenylmethyl)-9- hydroxy-6'-methoxy-cinchonanium chloride	(CAS No) 199588-84-6	≤ 100	Acute Tox. 4 (Oral), H302 Skin Sens. 1, H317

Full text of H-statements: see section 16

Mixtures

Not applicable

SECTION 4: First aid measures

Description of first aid measures

: Get medical advice/attention if you feel unwell. If possible, show him this sheet. Failing this, First-aid measures general 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.

Rinse mouth. Drink water as a precaution. Call a POISON CENTER or doctor/physician if you First-aid measures after ingestion

feel unwell.

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.

: May cause an allergic skin reaction. Symptoms/injuries after skin contact

Symptoms/injuries after ingestion Harmful if swallowed.

Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

SECTION 5: Firefighting measures

Extinguishing media 5.1.

Suitable extinguishing media : Adapt extinguishing agent to suit the environment. Water spray. Foam. Carbon dioxide. Dry

extinguishing powder.

Unsuitable extinguishing media : Do not use a heavy water stream.

Special hazards arising from the substance or mixture

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

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

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

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6.1.1. For non-emergency personnel

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

For emergency responders 6.1.2

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

insufficient ventilation.

Environmental precautions 6.2.

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

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.

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

Precautions for safe handling

Precautions for safe handling : Provide local exhaust or general room ventilation. Wear personal protective equipment. Avoid

dust formation. Do not breathe dust. 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

7.2. Conditions for safe storage, including any incompatibilities

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

sunlight. Protect from moisture.

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

Control parameters

(8α,9R)-1-(9-anthracenylmethyl)-9-hydroxy-6'-methoxy-cinchonanium chloride (199588-84-6)				
Ireland	Local name	Dusts non-specific		
Ireland	OEL (8 hours ref) (mg/m³)	10 mg/m³ (total inhalable) 4 mg/m³ (respirable)		
United Kingdom	Local name	Dust		
United Kingdom	WEL TWA (mg/m³)	10 mg/m³ (total inhalable) 4 mg/m³ (respirable)		

Exposure controls

Appropriate engineering controls:

Provide local exhaust or general room ventilation to minimize dust concentrations.

Hand protection:

Wear suitable gloves (EN 374). 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:

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Avoid release to the environment.

SECTION 9: Physical and chemical properties

Information on basic physical and chemical properties

Physical state : Solid, powder Colour : White - Yellow Odour : Odourless : No data available Melting point/freezing point Boiling point or initial boiling point and boiling : No data available

range

: No data available Flammability Lower and upper explosion limit : Not applicable Flash point : Not applicable Auto-ignition temperature : Not applicable Decomposition temperature : No data available рΗ : No data available Kinematic viscosity : Not applicable Solubility No data available Partition coefficient n-octanol/water (log value) : No data available 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

: The substance is not explosive. Explosive properties

Oxidising properties : The substance has no oxidising properties.

Molecular mass : 551.13 g/mol

SECTION 10: Stability and reactivity

10.1. Reactivity

No dangerous reactions known under normal conditions of use.

Chemical stability

Stable under use and storage conditions as recommended in section 7.

Possibility of hazardous reactions

None under normal use.

Conditions to avoid

Direct sunlight. High temperature.

10.5. Incompatible materials

Oxidizing agents.

Hazardous decomposition products

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

SECTION 11: Toxicological information

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

: Oral: Harmful if swallowed. Acute toxicity

(8α,9R)-1-(9-anthracenylmethyl)-9-hydroxy-6'-methoxy-cinchonanium chloride (199588-84-6)

LD50 oral 350.18 mg/kg (QSAR via T.E.S.T.)

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

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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

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

11.2.1. Endocrine disrupting properties

Endocrine disruption for human health

: The substance/mixture has no endocrine disrupting properties.

11.2.2. Other information

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

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

No additional information available

12.4. Mobility in soil

No additional information available

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

Endocrine disruption for the environment : The substance/mixture has no endocrine disrupting properties.

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 (EWC)

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.

number to distribute to be greated departately from each waste produced.

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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
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

REACH Annex XIV (Authorisation List)

Contains no substance(s) listed on REACH Annex XIV (Authorisation List).

REACH Candidate List (SVHC)

Contains no substance(s) listed on the REACH Candidate List.

PIC Regulation (Prior Informed Consent)

Contains no substance(s) listed on the PIC list (Regulation EU 649/2012 concerning the export and import of hazardous chemicals).

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POP Regulation (Persistent Organic Pollutants)

Contains no substance(s) listed on the POP list (Regulation EU 2019/1021 on persistent organic pollutants).

Ozone Regulation (1005/2009)

Contains no substance(s) listed on the Ozone Depletion list (Regulation EU 1005/2009 on substances that deplete the ozone layer).

Explosives Precursors Regulation (2019/1148)

Contains no substance(s) listed on the Explosives Precursors list (Regulation EU 2019/1148 on the marketing and use of explosives precursors).

Drug Precursors Regulation (273/2004)

Contains no substance(s) listed on the Drug Precursors list (Regulation EC 273/2004 on the manufacture and the placing on market of certain substances used in the illicit manufacture of narcotic drugs and psychotropic substances).

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 : Section 2.3. Other hazards

Section 11.2.1 Endocrine disrupting properties Section 12.6. Endocrine disrupting properties

Section 15.1.1. EU-Regulations

Review :

Abbreviations and acronyms:

abble viations and action yms.		
ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road	
BCF	Bioconcentration factor	
DNEL	Derived-No Effect Level	
EC50	The effective concentration of substance that causes 50 % of the maximum response (Median Effective Concentration)	
IATA	International Air Transport Association	
IMDG	International Maritime Dangerous Goods	
LC50	Lethal Concentration to 50 % of a test population (Median Lethal Concentration)	
LD50	Lethal Dose to 50 % of a test population (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. 1	Sensitisation - Skin, Category 1
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.

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