N-Benzylcupreinium Chloride

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Version:	2
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SECTION 1. Id	entification of the subs	tance/mixtu	re and of the company/und	ertaking
	identifier		e and of the company/and	
Product form		: Substance		
Substance name		: N-Benzylcupr	einium Chloride	
IUPAC name		: (2S,4S,5R)-1-Benzyl-2-((R)-hydroxy(6-hydroxyquinolin-4-yl)methyl)-5-vinylquinuclidin-1-ium chloride		
EC no		: -		
CAS No		: 2023817-94-7		
Formula		: C26H29CIN20	02	
Synonyms : Cinchonanium, 6',9-dihydroxy-1-(phenylmethyl)-, chloride (1:1), (8α,9R)-; Cinchonanium, 9- hydroxy-6'-hydroxy-1-(phenylmethyl)-,chloride, (8α,9R); 1-Benzylcupreinium chloride; (8alpha,9R)-1-Benzyl-9-hydroxy-6'-hydroxycinchonan-1-ium chloride; (8alpha,9R)-1-benzyl-6'- hydroxycinchonan-1-ium-9-ol chloride; (8S,9R)-N-Benzylcupreinium chloride				
1.2. Relevant	t identified uses of the substa	ance or mixture	and uses advised against	
1.2.1. Relevant	t identified uses			
Main use category		: Industrial use	Professional use.	
Use of the substand	ce/mixture	: Phase transfe	r catalyst	
1.2.2. Uses adv	vised against			
No additional inform	nation available			
1.3. Details o	of the supplier of the safety d	ata sheet		
Manufacturer/Supplier Buchler GmbH Harxbuetteler Straße 3 38110 Braunschweig - Germany T +49 5307 9310 - <u>www.buchler-gmbh.com</u> - <u>info@buchler-gmbh.com</u>				
Safety data sheet:	DLAC Dienstleistungsagentur (	Chemie GmbH, E	-Mail: <u>sds@dlac-gmbh.de</u>	
1.4. Emerger	ncy telephone number			
Country	Organisation/Company		Address	Emergency number
		Harxbütteler Str. 3 38110 Braunschweig, Germany	+49 1791437208 (German/English) (Mo-Fr 8:00-16:00)	
SECTION 2: Hazards identification				
2.1. Classification of the substance or mixture				
<b>Classification acc</b>	ording to Regulation (EC) No	. 1272/2008 [CL	.P]	
Acute toxicity (oral), Category 4 H302				
Skin corrosion/irritation, Category 2 H315				
Sensitisation - Skin, Category 1A H317				
Serious eye damage/eye irritation, Category 2 H319				
Specific target orga	an toxicity - Single exposure, Ca	ategory 3, Respi	ratory tract irritation H335	

Full text of H statements: see section 16

Adverse physicochemical, human health and environmental effects

Harmful if swallowed. Causes skin irritation. May cause an allergic skin reaction. Causes serious eye irritation. May cause respiratory irritation.

Harmful if swallowed. Causes skin irrita	ation. May cause an allergic skin reaction. Causes serious eye irritation. May cause respiratory ir
2.2. Label elements	
Labelling according to Regulation (E	EC) No. 1272/2008 [CLP]
Hazard pictograms (CLP)	GHS07
Signal word (CLP)	: Warning
Hazard statements (CLP)	<ul> <li>H302 - Harmful if swallowed</li> <li>H315 - Causes skin irritation</li> <li>H317 - May cause an allergic skin reaction</li> <li>H319 - Causes serious eye irritation</li> <li>H335 - May cause respiratory irritation</li> </ul>
15.04.2025	EN (English)

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Precautionary statements (CLP)       : P261 - Avoid breathing dust         P280 - Wear protective gloves, protective clothing, eye protection         P312 - Call a POISON CENTER, doctor if you feel unwell         P333+P313 - If skin irritation or rash occurs: Get medical advice/attention		ion	

### P337+P313 - If eye irritation persists: Get medical advice/attention P403+P233 - Store in a well-ventilated place. Keep container tightly closed

#### 2.3. **Other hazards**

No additional information available

SECTION 3: Composition/information on ingredients			
3.1. Substances			
Substance name : N-Benzylcupreinium Chloride			
EC No : -			
CAS No : 2023817-94-7			
Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
N-Benzylcupreinium Chloride	(CAS No) 2023817-94-7	≤ 100	Acute Tox. 4 (Oral), H302 Skin Irrit. 2. H315

### 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	<ul> <li>Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or doctor/physician if you feel unwell.</li> </ul>
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. If eye irritation persists: Get medical advice/attention.
First-aid measures after ingestion	: Rinse mouth. Drink water as a precaution. Call a POISON CENTER or doctor/physician if you feel unwell.
4.2. Most important symptoms and effe	cts, both acute and delayed
Symptoms/injuries	<ul> <li>Signs of cinchonism: Neurotoxic effects (e.g. headache, tinnitus, visual disturbances, confusion), gastrointestinal disorders (e.g. nausea, vomiting, diarrhoea), exanthema and haematological disorders.</li> </ul>
Symptoms/injuries after inhalation	: May cause respiratory irritation.
Symptoms/injuries after skin contact	: Causes skin irritation. May cause an allergic skin reaction.
Symptoms/injuries after eye contact	: Causes serious eye irritation.
Symptoms/injuries after ingestion	: Harmful if swallowed.
4.3. Indication of any immediate medic	al attention and special treatment needed
Treat symptomatically.	
<b>SECTION 5: Firefighting measures</b>	
5.1. Extinguishing media	
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.

#### 5.2. Special hazards arising from the substance or mixture

Hazardous decomposition products in case of	: Carbon oxides (CO, CO <sub>2</sub> ). Nitrogen oxides.
fire	

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5.3.	Advice for firefighters	
Firefightin	ng instructions	: Use water spray or fog for cooling exposed containers. Prevent fire-fighting water from entering environment.
Protection	n during firefighting	: Use a self-contained breathing apparatus and also a protective suit (EN 469).
SECTIC	ON 6: Accidental release mea	asures
6.1.	Personal precautions, protective e	quipment and emergency procedures
General n	neasures	: 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	
Emergeno	cy procedures	: Only qualified personnel equipped with suitable protective equipment may intervene.
6.1.2.	For emergency responders	
Protective	e equipment	: Use personal protective equipment as required. Wear suitable respiratory equipment in case of insufficient ventilation.
6.2.	Environmental precautions	
Prevent e	entry to sewers and public waters. Not	fy authorities if the substance enters sewers or public waters.
6.3.	Methods and material for containm	ent and cleaning up
Methods 1	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	
Concernir	ng personal protective equipment to u	se, see section 8. Concerning disposal elimination after cleaning, see section 13.
SECTIO	ON 7: Handling and storage	
7.1.	Precautions for safe handling	
Precautio	ns for safe handling	: Provide local exhaust or general room ventilation. Avoid breathing dust. Avoid contact with skin and eyes. Keep container closed when not in use.
Hygiene r	neasures	: 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, includ	ing any incompatibilities
Storage c	conditions	: Store in original container. Store tightly closed in a dry and cool place. Keep out of direct sunlight. Protect from moisture.
Prohibitio	ns on mixed storage	: Keep away from food, drink and animal feedingstuffs.
7.3.	Specific end use(s)	
No additio	onal information available	
SECTIC	ON 8: Exposure controls/pers	sonal protection
8.1.	Control parameters	
	onal information available	

#### 8.2. **Exposure controls**

### Appropriate engineering controls:

Use adequate ventilation. Avoid dust formation.

#### Hand protection:

Wear suitable gloves (EN 374). Nitrile rubber. Butyl rubber. 0.4 mm. The exact break trough 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:**

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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 c	hemical properties	
Physical state	: Solid, powder	
Colour	: White - beige	
Odour	: Odourless	
Melting point/freezing point	: No data available	
Boiling point or initial boiling point and boiling range	: No data available	
Flammability	: No data available	
Lower and upper explosion limit	: No data available	
Flash point	: No data available	
Auto-ignition temperature	: No data available	
Decomposition temperature	: No data available	
рН	: 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	: No data available	
Particle characteristics	: No data available	
9.2. Other information		
9.2.1. Information with regard to physical haz	ard classes	
Explosive properties	: The substance is not explosive.	
Oxidising properties	: The substance has no oxidising properties.	
9.2.2. Other safety characteristics		
Molecular mass	: 437 g/mol	
<b>SECTION 10: Stability and reactivity</b>		
10.1. Reactivity		
No dangerous reactions known under normal co	nditions of use.	
10.2. Chemical stability		
Stable under use and storage conditions as reco	mmended in section 7.	
10.3. Possibility of hazardous reactions		
None under normal use.		
10.4. Conditions to avoid		
Direct sunlight. High temperature.		
10.5. Incompatible materials		
Oxidizing agents.		
10.6. Hazardous decomposition products	; ;	
In case of fire: Carbon monoxide. Carbon dioxide. Nitrogen oxides.		
<b>SECTION 11: Toxicological informat</b>	ion	
11.1. Information on hazard classes as de	efined in Regulation (EC) No 1272/2008	
Acute toxicity	: Oral: Harmful if swallowed.	
N Dependeurseinium Obleside (0002047.04.7	n	
N-Benzylcupreinium Chloride (2023817-94-7	]	
LD50 oral	583.04 mg/kg (QSAR via T.E.S.T.)	

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Skin corrosion/irritation	: Causes skin irritation.
Serious eye damage/irritation	: Causes serious eye irritation.
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)	: May cause respiratory irritation.
Specific target organ toxicity (repeated	: Not classified
exposure)	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 has no endocrine disrupting properties.
•	
11.2.2. Other information	
Potential adverse human health effects and	: Signs of cinchonism: Neurotoxic effects (e.g. headache, tinnitus, visual disturbances,
symptoms	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 assessme	
This substance does not meet the PBT- or vPvB	
12.6. Endocrine disrupting properties	. The substance has no and aring discusting presenting
Endocrine disruption for the environment	: The substance has no endocrine disrupting properties.
12.7. Other adverse effects	
No additional information available	
SECTION 13: Disposal consideration	ns
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	<ul> <li>O7 00 00 - WASTES FROM ORGANIC CHEMICAL PROCESSES</li> <li>O7 01 00 - wastes from the manufacture, formulation, supply and use (MFSU) of basic organic chemicals</li> </ul>
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.

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SECTION 14: Transport information	n		
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		
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			
	ng to IMO instruments		
Not applicable			
SECTION 15: Regulatory information			
	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).		
POP Pagulation (Parsistant Organic Pollutants)			

### POP Regulation (Persistent Organic Pollutants)

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

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### Ozone Regulation (2024/590)

Contains no substance(s) listed on the Ozone Depletion list (Regulation EU 2024/590 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: Othe	er 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 e	arlier Versions	: Section 1.1 + 1.4 Section 2.3 Section 11.2 Section 12.6 Section 15.1.1
Abbreviations and acron	iyms:	
ADR	European Agreement concerning the International Carriage of Dangerous Goods by Road	

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)
ΙΑΤΑ	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	
Eye Irrit. 2	Serious eye damage/eye irritation, Category 2	
Skin Irrit. 2	Skin corrosion/irritation, Category 2	
Skin Sens. 1A	Sensitisation - Skin, Category 1A	
STOT SE 3	Specific target organ toxicity — Single exposure, Category 3, Respiratory tract irritation	
H302	Harmful if swallowed	
H315	Causes skin irritation	
H317	May cause an allergic skin reaction	
H319	Causes serious eye irritation	
H335	May cause respiratory irritation	

SDS EU (REACH Annex II)

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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.