

Safety Data Sheet

according to Regulation (EU) 2020/878

BUCHLER

A Member of the FAGUS Group

Trade name: **N-Benzylquininium Chloride**

Date of issue: 28.09.2022

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 : N-Benzylquininium Chloride
IUPAC name : (2S,4S,5R)-1-Benzyl-2-((R)-hydroxy(6-methoxyquinolin-4-yl)methyl)-5-vinylquinuclidin-1-ium chloride
EC no : 614-029-7
CAS No : 67174-25-8
Formula : C27H31ClN2O2
Synonyms : QUIBEC; Cinchonanium, 9-hydroxy-6'-methoxy-1-(phenylmethyl)-,chloride, (8 α ,9R); 1-benzylquininium chloride; (8 α ,9R)-1-Benzyl-9-hydroxy-6'-methoxycinchonan-1-ium chloride; (8 α ,9R)-1-benzyl-6'-methoxycinchonan-1-ium-9-ol chloride; (8S,9R)-N-Benzylquininium chloride

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 : 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 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

Skin corrosion/irritation, Category 2 H315

Sensitisation - Skin, Category 1A H317

Serious eye damage/eye irritation, Category 2 H319

Specific target organ toxicity - Single exposure, Category 3, Respiratory 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.

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

Safety Data Sheet

according to Regulation (EU) 2020/878

BUCHLER

A Member of the FAGUS Group

Trade name: **N-Benzylquininium Chloride**

Date of issue: 28.09.2022

Revision date: -

Version: 1

Replaces version: -

H315 - Causes skin irritation
H317 - May cause an allergic skin reaction
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation

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
- 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-Benzylquininium Chloride
EC No : 614-029-7
CAS No : 67174-25-8

| Name | Product identifier | % | Classification according to Regulation (EC) No. 1272/2008 [CLP] |
|----------------------------|--|-------|--|
| N-Benzylquininium Chloride | (CAS No) 67174-25-8 (EC No) 614-029-7 | ≤ 100 | Acute Tox. 4 (Oral), H302 Skin Irrit. 2, H315 Skin Sens. 1A, H317 Eye Irrit. 2, H319 STOT SE 3, H335 |

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. Call a POISON CENTER or doctor/physician if you feel unwell.

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 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 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 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.

Safety Data Sheet

according to Regulation (EU) 2020/878

BUCHLER

A Member of the FAGUS Group

Trade name: N-Benzylquininium Chloride

Date of issue: 28.09.2022

Revision date: -

Version: 1

Replaces version: -

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.

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 the 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 breathing 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 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.

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). 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:

Safety Data Sheet

according to Regulation (EU) 2020/878

BUCHLER

A Member of the FAGUS Group

Trade name: **N-Benzylquininium Chloride**

Date of issue: 28.09.2022

Revision date: -

Version: 1

Replaces version: -

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, 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 |
| pH | : 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

| | |
|----------------------|--|
| Explosive properties | : The substance is not explosive. |
| Oxidising properties | : The substance has no oxidising properties. |
| Molecular mass | : 451 g/mol |

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.

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.

SECTION 11: Toxicological information

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

Acute toxicity : Oral: Harmful if swallowed.

N-Benzylquininium Chloride (67174-25-8)

| | |
|-----------|----------------------------------|
| LD50 oral | 624.48 mg/kg (QSAR via T.E.S.T.) |
|-----------|----------------------------------|

Safety Data Sheet

according to Regulation (EU) 2020/878

BUCHLER

A Member of the FAGUS Group

Trade name: N-Benzylquininium Chloride

Date of issue: 28.09.2022

Revision date: -

Version: 1

Replaces version: -

| | |
|--|--|
| 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 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 |

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

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 |

Safety Data Sheet

according to Regulation (EU) 2020/878

BUCHLER

A Member of the FAGUS Group

Trade name: N-Benzylquininium Chloride

Date of issue: 28.09.2022

Revision date: -

Version: 1

Replaces version: -

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

N-Benzylquininium Chloride is not on the REACH Candidate List

N-Benzylquininium Chloride 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 : -

Review : -

Abbreviations and acronyms:

Safety Data Sheet

according to Regulation (EU) 2020/878

BUCHLER

A Member of the FAGUS Group

Trade name: **N-Benzylquininium Chloride**

Date of issue: 28.09.2022

Revision date: -

Version: 1

Replaces version: -

| | |
|-------|--|
| 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 |
| 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)

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.