N-[3,5-bis(trifluoromethyl)benzyl]-N'-[3-(trifluoromethyl)benzyl]-cupreinium Bromide

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Replaces version: -

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

1.1. Product identifier

Product form : Substance
Substance name : N-[3,5-bis(trifluoromethyl)benzyl]-N'-[3-(trifluoromethyl)benzyl]-cupreinium Bromide
IUPAC name : (1S,2S,4S,5R)-1-(3,5-bis(trifluoromethyl)benzyl)-2-((R)-hydroxy(6-hydroxy-1-(3-(trifluoromethyl)benzyl)quinolin-1-ium-4-yl)methyl)-5-vinylquinuclidin-1-ium bromide
EC no : -
CAS No : -
Formula : $C_{36}H_{33}F_9N_2O_2 \cdot 2Br$
Synonyms : (8α,9R)-6′,9-dihydroxy-1-[3,5-bis(trifluoromethyl)benzyl]-1′-[[3-(trifluoromethyl)phenyl]methyl]-Cinchonanium bromide

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 synthesis development
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 - 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	BUCHLER GmbH (A member of the FAGUS Group)	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

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

Acute toxicity (oral), Category 2 H300

Full text of H statements: see section 16

Adverse physicochemical, human health and environmental effects

Fatal if swallowed.

2.2. Label elements

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

Hazard pictograms (CLP) :



GHS06

Signal word (CLP) : Danger
Hazard statements (CLP) : H300 - Fatal if swallowed.
Precautionary statements (CLP) : P264 - Wash hands thoroughly after handling.
P270 - Do not eat, drink or smoke when using this product.
P301+P310 - IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P330 - Rinse mouth.
P405 - Store locked up.
P501 - Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation.

2.3. Other hazards

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

Substance name : N-[3,5-bis(trifluoromethyl)benzyl]-N'-[3-(trifluoromethyl)benzyl]-cupreinium Bromide

EC No : -

CAS No : -

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
N-[3,5-bis(trifluoromethyl)benzyl]-N'-[3-(trifluoromethyl)benzyl]-cupreinium Bromide	(CAS No) - (EC No) -	≤ 100	Acute Tox. 2 (Oral), H300

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.

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 water as a precaution. IF SWALLOWED: Immediately call a POISON CENTER/ doctor.

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 ingestion : Fatal 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 : 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 fire : Carbon oxides (CO, CO_2). 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. For further information refer to section 8: "Exposure controls/personal protection".

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. Wear personal protective equipment. Avoid dust formation. Do not breathe dust. Avoid contact with skin and eyes.

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. Store locked up.

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

N-[3,5-bis(trifluoromethyl)benzyl]-N'-[3-(trifluoromethyl)benzyl]-cupreinium Bromide (-)		
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)

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 / EN ISO 16321).

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, powder
Colour	:	Off-white
Odour	:	No data available
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	:	Not applicable
Flash point	:	Not applicable
Auto-ignition temperature	:	Not applicable
Decomposition temperature	:	Not applicable
pH	:	No data available
Kinematic viscosity	:	Not applicable
Solubility	:	No data available
Partition coefficient n-octanol/water (log value)	:	-0.5524 (QSAR)
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

9.2.1. Information with regard to physical hazard classes

Explosive properties	:	The substance is not explosive.
Oxidising properties	:	The substance has no oxidising properties.

9.2.2. Other safety characteristics

Molecular mass	:	856.47 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

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: Fatal if swallowed.

N-[3,5-bis(trifluoromethyl)benzyl]-N'-[3-(trifluoromethyl)benzyl]-cupreinium Bromide (-)	
LD50 oral	26.57 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
Respiratory or skin sensitisation	:	Not classified Based on available data, the classification criteria are not met
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 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

N-[3,5-bis(trifluoromethyl)benzyl]-N'-[3-(trifluoromethyl)benzyl]-cupreinium Bromide (-)	
Log Pow	-0.5524 (QSAR via EpiSuite KOWWIN)

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 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 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)	:	UN 1544
UN-No. (IMDG)	:	UN 1544
UN-No. (IATA)	:	UN 1544

14.2. UN proper shipping name

Proper Shipping Name (ADR)	:	ALKALOIDS, SOLID, N.O.S. (N-[3,5-bis(trifluoromethyl)benzyl]-N'-[3-(trifluoromethyl)benzyl]-cupreinium Bromide)
Proper Shipping Name (IMDG)	:	ALKALOIDS, SOLID, N.O.S. (N-[3,5-bis(trifluoromethyl)benzyl]-N'-[3-(trifluoromethyl)benzyl]-cupreinium Bromide)
Proper Shipping Name (IATA)	:	Alkaloids, solid, n.o.s. (N-[3,5-bis(trifluoromethyl)benzyl]-N'-[3-(trifluoromethyl)benzyl]-cupreinium Bromide)
Transport document description (ADR)	:	UN 1544 ALKALOIDS, SOLID, N.O.S. (N-[3,5-bis(trifluoromethyl)benzyl]-N'-[3-(trifluoromethyl)benzyl]-cupreinium Bromide), 6.1, II, (D/E)
Transport document description (IMDG)	:	UN 1544 ALKALOIDS, SOLID, N.O.S. (N-[3,5-bis(trifluoromethyl)benzyl]-N'-[3-(trifluoromethyl)benzyl]-cupreinium Bromide), 6.1, II
Transport document description (IATA)	:	UN 1544 Alkaloids, solid, n.o.s. (N-[3,5-bis(trifluoromethyl)benzyl]-N'-[3-(trifluoromethyl)benzyl]-cupreinium Bromide), 6.1, II

14.3. Transport hazard class(es)

ADR

Transport hazard class(es) (ADR)	:	6.1
Danger labels (ADR)	:	6.1

:



IMDG

Transport hazard class(es) (IMDG)	:	6.1
Danger labels (IMDG)	:	6.1

:



IATA

Transport hazard class(es) (IATA)	:	6.1
Hazard labels (IATA)	:	6.1

:



14.4. Packing group

Packing group (ADR) : II
Packing group (IMDG) : II
Packing group (IATA) : II

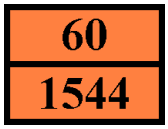
14.5. Environmental hazards

Dangerous for the environment : No
Marine pollutant : No
Other information : No supplementary information available

14.6. Special precautions for user

- Overland transport

Classification code (ADR) : T2
Special provisions (ADR) : 43, 274
Limited quantities (ADR) : 500 g
Excepted quantities (ADR) : E4
Packing instructions (ADR) : P002, IBC08
Special packing provisions (ADR) : B4
Mixed packing provisions (ADR) : MP10
Portable tank and bulk container instructions (ADR) : T3
Portable tank and bulk container special provisions (ADR) : TP33
Tank code (ADR) : SGAH, L4BH
Tank special provisions (ADR) : TU15, TE19
Vehicle for tank carriage : AT
Transport category (ADR) : 2
Special provisions for carriage - Packages (ADR) : V11
Special provisions for carriage - Loading, unloading and handling (ADR) : CV13, CV28
Special provisions for carriage - Operation (ADR) : S9, S19
Hazard identification number (Kemler No.) : 60
Orange plates :



Tunnel restriction code (ADR) : D/E

- Transport by sea

Special provisions (IMDG) : 43, 223, 274
Limited quantities (IMDG) : 500 g
Excepted quantities (IMDG) : E4
Packing instructions (IMDG) : P002
IBC packing instructions (IMDG) : IBC08
IBC special provisions (IMDG) : B4, B21
Tank instructions (IMDG) : T3
Tank special provisions (IMDG) : TP33
EmS-No. (Fire) : F-A
EmS-No. (Spillage) : S-A
Stowage category (IMDG) : A

- Air transport

PCA Excepted quantities (IATA) : E4
PCA Limited quantities (IATA) : Y644

PCA limited quantity max net quantity (IATA)	:	1kg
PCA packing instructions (IATA)	:	669
PCA max net quantity (IATA)	:	25kg
CAO packing instructions (IATA)	:	676
CAO max net quantity (IATA)	:	100kg
Special provisions (IATA)	:	A3, A5, A6, A801
ERG code (IATA)	:	6L

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).

POP Regulation (Persistent Organic Pollutants)

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

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: 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:

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. 2 (Oral)	Acute toxicity (oral), Category 2
H300	Fatal if swallowed.

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.