

5-Bromo-4-chloro-3-indoxyl- α -D-glucopyranoside \geq 98 %, for biochemistry

article number: **8434** Version: **3.0 en** Replaces version of: 10.01.2022 Version: (2) date of compilation: 14.10.2020 Revision: 02.03.2024

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

1.1 Product identifier

Identification of the substance

Registration number (REACH)

Article number

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It is not required to list the identified uses because the substance is not subject to registration according to REACH (< 1 t/a).

CAS number

Alternative name(s)

Uses advised against:

108789-36-2 X-α-D-qlucoside

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

Relevant identified uses:

Laboratory chemical Laboratory and analytical use

Do not use for private purposes (household). Food, drink and animal feedingstuffs.

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co. KG Schoemperlenstr. 3-5 D-76185 Karlsruhe Germany

Telephone:+49 (0) 721 - 56 06 0 **Telefax:** +49 (0) 721 - 56 06 149 **e-mail:** sicherheit@carlroth.de **Website:** www.carlroth.de

Competent person responsible for the safety data Department Health, Safety and Environment sheet:

e-mail (competent person):

sicherheit@carlroth.de

1.4 Emergency telephone number

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

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

This substance does not meet the criteria for classification in accordance with Regulation No 1272/ 2008/EC.

2.2 Label elements

Labelling according to Regulation (EC) No 1272/2008 (CLP) not required



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2.3 Other hazards

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\ge 0,1\%$.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance Molecular formula Molar mass CAS No $5\text{-}Bromo\text{-}4\text{-}chloro\text{-}3\text{-}indoxyl\text{-}\alpha\text{-}D\text{-}glucopyranoside}$

 $C_{14}H_{15}BrCINO_{6}$

408,6 ^g/_{mol}

108789-36-2

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

No special measures are necessary.

Following inhalation

Provide fresh air.

Following skin contact

Rinse skin with water/shower.

Following eye contact

Rinse cautiously with water for several minutes.

Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

- **4.2** Most important symptoms and effects, both acute and delayed Symptoms and effects are not known to date.
- **4.3** Indication of any immediate medical attention and special treatment needed none



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SECTION 5: Firefighting measures

5.1 Extinguishing media



Suitable extinguishing media

co-ordinate firefighting measures to the fire surroundings! water, foam, dry extinguishing powder, ABC-powder

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible.

Hazardous combustion products

In case of fire may be liberated: Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO₂), Hydrogen chloride (HCl), Hydrogen bromide (HBr)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures



For non-emergency personnel

No special measures are necessary.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains. Take up mechanically.

Advice on how to clean up a spill

Take up mechanically.

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.



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SECTION 7: Handling and storage

- 7.1 Precautions for safe handling
 No special measures are necessary.
 Advice on general occupational hygiene
 Keep away from food, drink and animal feedingstuffs.
- 7.2 Conditions for safe storage, including any incompatibilities

Store in a dry place. Keep in a cool place.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice:

Specific designs for storage rooms or vessels

Recommended storage temperature: -20 °C

7.3 Specific end use(s)

No information available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

This information is not available.

8.2 Exposure controls

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

Skin protection



hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374.

• type of material

NBR (Nitrile rubber)

material thickness

>0,11 mm



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• breakthrough times of the glove material

>480 minutes (permeation: level 6)

• other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Respiratory protection



Respiratory protection necessary at: Dust formation. Particulate filter device (EN 143). P1 (filters at least 80 % of airborne particles, colour code: White).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	solid
Form	powder, crystalline
Colour	whitish
Odour	characteristic
Melting point/freezing point	not determined
Boiling point or initial boiling point and boiling range	674 °C
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	not applicable
Auto-ignition temperature	not determined
Decomposition temperature	not relevant
pH (value)	not applicable
Kinematic viscosity	not relevant
Solubility(ies)	
Water solubility	not determined
Partition coefficient	
Partition coefficient n-octanol/water (log value):	this information is not available
Vapour pressure	not determined



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Density and/or relative density	
Density	1,88 ^g / _{cm³}
Relative vapour density	Information on this property is not available.
Particle characteristics	No data available.
Other safety parameters	
Oxidising properties	none
Other information	
Information with regard to physical hazard classes:	hazard classes acc. to GHS (physical hazards): not relevant
Other safety characteristics:	
Refractive index	1,731

SECTION 10: Stability and reactivity

10.1 Reactivity

9.2

The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: strong oxidiser

10.4 Conditions to avoid

There are no specific conditions known which have to be avoided.

10.5 Incompatible materials

There is no additional information.

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

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

Classification according to GHS (1272/2008/EC, CLP)

This substance does not meet the criteria for classification in accordance with Regulation No 1272/ 2008/EC.

Acute toxicity

Shall not be classified as acutely toxic.

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.



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Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

• If swallowed

Data are not available.

• If in eyes

Data are not available.

• If inhaled

Data are not available.

• If on skin

Data are not available.

Other information

Health effects are not known. This information is based upon the present state of our knowledge.

11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of \ge 0,1%.

11.3 Information on other hazards

There is no additional information.



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SECTION 12: Ecological information

12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

12.2 Persistence and degradability

Theoretical Oxygen Demand (without nitrification): 1,077 $^{mg}/_{mg}$ Theoretical Oxygen Demand (with nitrification): 1,233 $^{mg}/_{mg}$ Theoretical Carbon Dioxide: 1,508 $^{mg}/_{mg}$

12.3 Bioaccumulative potential

Data are not available.

12.4 Mobility in soil

Data are not available.

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of $\ge 0,1\%$.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods



Consult the appropriate local waste disposal expert about waste disposal.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions. Non-contaminated packages may be recycled.



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SECTION 14: Transport information

- 14.1 UN number or ID number
- 14.2 UN proper shipping name
- 14.3 Transport hazard class(es)
- 14.4 Packing group
- 14.5 Environmental hazards

not subject to transport regulations

not assigned

none

not assigned

non-environmentally hazardous acc. to the dangerous goods regulations

- **14.6** Special precautions for user There is no additional information.
- **14.7** Maritime transport in bulk according to IMO instruments The cargo is not intended to be carried in bulk.
- 14.8 Information for each of the UN Model Regulations

International Maritime Dangerous Goods Code (IMDG) - Additional information Not subject to IMDG.

International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information Not subject to ICAO-IATA.

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

Relevant provisions of the European Union (EU)

Restrictions according to REACH, Annex XVII not listed

List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list Not listed.

Seveso Directive

2012/18/EU (Seveso III)			
Νο	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the ap- plication of lower and upper-tier re- quirements	Notes
	not assigned		

Deco-Paint Directive

ľ	ndustrial Emissions Directive (IED)	
	VOC content	0 %

VOC content	0 %
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Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Water Framework Directive (WFD)

List of pollutants (WFD)

Name of substance	Name acc. to inventory	CAS No	Listed in	Remarks
5-Bromo-4-chloro-3-indoxyl-α-D- glucopyranoside	Organohalogen compounds and substances which may form such compounds in the aquatic envir- onment		a)	

Legend

a) Indicative list of the main pollutants

Regulation on the marketing and use of explosives precursors

not listed

Regulation on drug precursors

not listed

Regulation on substances that deplete the ozone layer (ODS)

not listed

Regulation concerning the export and import of hazardous chemicals (PIC)

not listed

Regulation on persistent organic pollutants (POP)

not listed

Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

National inventories

Country	Inventory	Status
TW	TCSI	substance is listed
Logond		

Legend TCSI

SI Taiwan Chemical Substance Inventory

15.2 Chemical safety assessment

No Chemical Safety Assessment has been carried out for this substance.



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SECTION 16: Other information

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety- relev- ant
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of ≥ 0,1%.	yes
14.8	Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional in- formation: Not subject to ADR, RID and ADN.		yes

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concern- ing the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
DGR	Dangerous Goods Regulations (see IATA/DGR)
ED	Endocrine disruptor
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Na- tions
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SVHC	Substance of Very High Concern
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative

Key literature references and sources for data

Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures. Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU.

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.