5-Bromo-4-chloro-3-indolyl-beta-D-glucopyranoside (X-Glu)

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830

Date of issue: 9/2/2019 Version: 1.0

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

1.1. Product identifier

Product form	: Substance
Substance name	: 5-Bromo-4-chloro-3-indolyl-beta-D-glucopyranoside (X-Glu)
IUPAC name	: (2S,3R,4S,5S,6R)-2-[(5-bromo-4-chloro-1H-indol-3-yl)oxy]-6-(hydroxymethyl)oxane-3,4,5-triol
EC-No.	: 239-603-0
CAS-No.	: 15548-60-4
Product code	: 36247440
Formula	: C14H15BrClNO6
Product group	: Raw material

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

1.2.1. Relevant identified uses

Main use category	: Laboratory use,Industrial use,Professional use
Industrial/Professional use spec	: For professional use only
Use of the substance/mixture	: For analytical purposes Scientific research and development Not for human consumption or veterinary purposes.

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Supplier

Scafell Organics
Molekula Ltd
Lingfield Way
Darlington - England
T +44 (0) 1949 823777 / +44 (0) 7590 545705
info@molekula.com / kbowen@molekula.com - www.molekula.com

1.4. Emergency telephone number

Emergency number : +44 (0) 7590 545705

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

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

Not classified

Adverse physicochemical, human health and environmental effects

No additional information available

2.2. Label elements

Not classified.

2.3. Other hazards

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

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

SECTION 3: Composition/information on ingredients

3.1. Substances

Name	Product identifier	%
5-Bromo-4-chloro-3-indolyl-beta-D-glucopyranoside (X-Glu)	(CAS-No.) 15548-60-4 (EC-No.) 239-603-0	100

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general : If possible show this sheet, if not available show packaging or label. Never give anything by mouth to an unconscious person. Do not leave affected person unattended.

First-aid measures after inhalation	: If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing. Give oxygen or artificial respiration if necessary. If breathing difficulties persist : Get medical advice/attention.
First-aid measures after skin contact	: After contact with skin, take off immediately all contaminated clothing, and wash immediately with plenty of water. Do not remove clothing if it sticks to the skin. If irritation persists, consult a doctor.
First-aid measures after eye contact	: Rinse immediately with plenty of water. 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 out with water. Do not induce vomiting. Get medical advice/attention.

4.2. Most important symptoms and effects, both acute and delayed

Symptoms/effects	: Not expected to present a significant hazard under anticipated conditions of normal use.
Symptoms/effects after inhalation	: Dust of the product, if present, may cause respiratory irritation after an excessive inhalation exposure.
Symptoms/effects after skin contact	: Dust may cause irritation in skin folds or by contact in combination with tight clothing.
Symptoms/effects after eye contact	: May cause eye irritation. redness, itching, tears.
Symptoms/effects after ingestion	: May cause irritation to the digestive tract. Abdominal pain, nausea.

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	: Foam. Dry powder. Carbon dioxide. Water spray. Sand.
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, CO2). hydrogen bromide. hydrogen chloride. Nitrogen oxides.

5.3. Advice for firefighters

Precautionary measures fire	: Keep container tightly closed and away from heat, sparks and flame. Keep away from combustible materials.
Firefighting instructions	: Use water spray or fog for cooling exposed containers. Exercise caution when fighting any chemical fire. Prevent fire fighting water from entering the environment.
Protection during firefighting	: Do not enter fire area without proper protective equipment, including respiratory protection.
Other information	: Warn all persons of toxic hazard.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures	: Isolate from fire, if possible, without unnecessary risk. Avoid dust formation. No flames, no sparks. Eliminate all sources of ignition.

6.1.1. For non-emergency personnel

Protective equipment	: Wear recommended personal protective equipment.
Emergency procedures	: Evacuate unnecessary personnel. Mark out the contaminated area with signs and prevent access to unauthorized personnel. Do not touch or walk on the spilled product. Avoid contact with skin, eyes and clothing.
Measures in case of dust release	: Keep upwind. Avoid creating or spreading dust. Ventilate the area thoroughly, especially low lying areas (basements, workpits etc).

6.1.2. For emergency responders

Protective equipment	: Equip cleanup crew with proper protection. Use self-contained breathing apparatus and chemically protective clothing.
Emergency procedures	: Ventilate area.

6.2. Environmental precautions

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

6.3. Methods and material for containment and cleaning up

Methods for cleaning up	: On land, sweep or shovel into suitable containers. Shovel or sweep up and put in a closed container for disposal.

6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling	: Avoid creating or spreading dust. Provide local exhaust or general room ventilation.
Hygiene measures	: Take off immediately all contaminated clothing and wash it before reuse. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Do not eat, drink or smoke when using this product.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures	: Ensure adequate ventilation, especially in confined areas.
Storage conditions	: Keep only in the original container in a cool, well ventilated place away from : Heat sources, Direct sunlight. Keep container closed when not in use.
Incompatible products	: Strong oxidizing agents.
Incompatible materials	: Sources of ignition. Direct sunlight. Heat sources.
Heat and ignition sources	: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
Storage area	: Store at -20°C. Store in a dry place. Store in a closed container.

7.3. Specific end use(s)

For analytical purposes. Scientific research and development. Not for human consumption or veterinary purposes.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Exposure controls

Appropriate engineering controls:

Handle in accordance with good industrial hygiene and safety procedures.

Personal protective equipment:

Avoid all unnecessary exposure.

Materials for protective clothing:

Wear suitable protective clothing, gloves and eye/face protection

Hand protection:

The protective gloves to be used must comply with the specifications of the regulation 2016/425 and the resultant standard EN 374

Type	Material	Permeation	Thickness (mm)	Penetration	Standard
Disposable gloves	Nitrile rubber (NBR)	6 (> 480 minutes)	0.11		EN 374

Eye protection:

Emergency eye wash fountains should be available in the immediate vicinity of any potential exposure. Use eye protection according to EN 166, designed to protect against powders and dusts.

Type	Use	Characteristics	Standard
Safety glasses	Fine dust, Dust	With side shields	EN 166

Skin and body protection:

Emergency safety showers should be available in the immediate vicinity of any potential exposure. Keep suitable chemically resistant protective clothing readily available for emergency use

Type	Standard
Long sleeved protective clothing	EN ISO 13982

Respiratory protection:

No respiratory protection needed under normal use conditions. [In case of inadequate ventilation] wear respiratory protection.

Device	Filter type	Condition	Standard
Dust mask	Type P1	Dust protection	EN 14387

Other information:

Do not eat, drink or smoke during use.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Solid
Appearance	: Crystalline powder.
Molecular mass	: 408.63 g/mol
Colour	: light yellow. White to off-white.
Odour	: No data available.
Odour threshold	: No data available
pH	: No data available
Relative evaporation rate (butylacetate=1)	: No data available

Melting point	: 249 - 251 °C
Freezing point	: No data available
Boiling point	: No data available
Flash point	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Flammability (solid, gas)	: Non flammable.
Vapour pressure	: No data available
Relative vapour density at 20 °C	: No data available
Relative density	: No data available
Solubility	: No data available
Log Pow	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidising properties	: No data available
Explosive limits	: No data available

9.2. Other information
No additional information available

SECTION 10: Stability and reactivity
10.1. Reactivity
The product is non-reactive under normal conditions of use, storage and transport.
10.2. Chemical stability
Stable under recommended handling and storage conditions (see section 7).
10.3. Possibility of hazardous reactions
No dangerous reactions known under normal conditions of use.
10.4. Conditions to avoid
Protect from sunlight. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
10.5. Incompatible materials
Strong oxidizers.
10.6. Hazardous decomposition products
No hazardous decomposition products known at room temperature. Thermal decomposition generates : Carbon oxides (CO, CO2). Nitrogen oxides. hydrogen bromide. hydrogen chloride.

SECTION 11: Toxicological information
11.1. Information on toxicological effects
Acute toxicity (oral)	: Not classified
Acute toxicity (dermal)	: Not classified
Acute toxicity (inhalation)	: Not classified
Skin corrosion/irritation	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Serious eye damage/irritation	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Respiratory or skin sensitisation	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Germ cell mutagenicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Carcinogenicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Reproductive toxicity	: Not classified
Additional information	: Based on available data, the classification criteria are not met
STOT-single exposure	: Not classified
Additional information	: Based on available data, the classification criteria are not met
STOT-repeated exposure	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Aspiration hazard	: Not classified
Additional information	: Based on available data, the classification criteria are not met
Potential adverse human health effects and symptoms	: Based on available data, the classification criteria are not met.

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity : Not classified

Chronic aquatic toxicity : Not classified

12.2. Persistence and degradability

5-Bromo-4-chloro-3-indolyl-beta-D-glucopyranoside (X-Glu) (15548-60-4)	
Persistence and degradability	No data available.

12.3. Bioaccumulative potential

5-Bromo-4-chloro-3-indolyl-beta-D-glucopyranoside (X-Glu) (15548-60-4)	
Bioaccumulative potential	No data available.

12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

5-Bromo-4-chloro-3-indolyl-beta-D-glucopyranoside (X-Glu) (15548-60-4)
This substance/mixture does not meet the PBT criteria of REACH regulation, annex XIII
This substance/mixture does not meet the vPvB criteria of REACH regulation, annex XIII

12.6. Other adverse effects

Additional information : Avoid release to the environment.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Product/Packaging disposal recommendations : Dispose in a safe manner in accordance with local/national regulations.

Ecology - waste materials : Avoid release to the environment.

SECTION 14: Transport information

In accordance with ADR / RID / IMDG / IATA / ADN

ADR	IMDG	IATA	ADN	RID
14.1. UN number				
Not regulated	Not regulated	Not regulated	Not regulated	Not regulated
14.2. UN proper shipping name				
Not regulated	Not regulated	Not regulated	Not regulated	Not regulated
14.3. Transport hazard class(es)				
Not regulated	Not regulated	Not regulated	Not regulated	Not regulated
14.4. Packing group				
Not regulated	Not regulated	Not regulated	Not regulated	Not regulated
14.5. Environmental hazards				
Not regulated	Not regulated	Not regulated	Not regulated	Not regulated
No supplementary information available				

14.6. Special precautions for user

Overland transport

Not regulated

Transport by sea

Not regulated

Air transport

Not regulated

Inland waterway transport

Not regulated

Rail transport

Not regulated

14.7. Transport in bulk according to Annex II of Marpol and the IBC Code

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

No REACH Annex XVII restrictions

5-Bromo-4-chloro-3-indolyl-beta-D-glucopyranoside (X-Glu) is not on the REACH Candidate List

Directive 2012/18/EU (SEVESO III)

15.1.2. National regulations

No additional information available

15.2. Chemical safety assessment

No chemical safety assessment has been carried out for the substance or the mixture by the supplier

SECTION 16: Other information

Data sources	: 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.
Other information	: None.

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.