

SAFETY DATA SHEET

Creation Date 29-Mar-2010

Revision Date 25-Dec-2021

Revision Number 5

1. Identification

Product Name 5-Bromo-4-chloro-3-indolyl- β -D-glucuronide cyclohexylammonium salt hydrate

Cat No. : AC331190000; AC331190250; AC331191000

Synonyms X-Gluc

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No.**US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification

Classification under 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

This chemical is not considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Label Elements

None required

Hazards not otherwise classified (HNOC)

None identified

3. Composition/Information on Ingredients

Component	CAS No	Weight %
5-Bromo-4-chloro-3-indolyl-beta-D-glucuronide cyclohexylammonium salt hydrate	NA	>95
.beta.-D-Glucopyranosiduronic acid, 5-bromo-4-chloro-1H-indol-3-yl, compound with cyclohexanamine (1:1)	114162-64-0	-

4. First-aid measures

Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. Get medical attention immediately if symptoms occur.
Inhalation	Remove to fresh air. Get medical attention immediately if symptoms occur.
Ingestion	Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.
Most important symptoms and effects	None reasonably foreseeable.
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray, carbon dioxide (CO ₂), dry chemical, alcohol-resistant foam.
Unsuitable Extinguishing Media	No information available
Flash Point	No information available
Method -	No information available
Autoignition Temperature	No information available
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NO_x).

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health	Flammability	Instability	Physical hazards
0	1	1	N/A

6. Accidental release measures

Personal Precautions	Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.
Environmental Precautions	Should not be released into the environment.
Methods for Containment and Clean Up	Sweep up and shovel into suitable containers for disposal. Avoid dust formation.

7. Handling and storage

Handling	Wear personal protective equipment/face protection. Ensure adequate ventilation. Avoid contact with skin, eyes or clothing. Avoid ingestion and inhalation. Avoid dust formation.
Storage.	Keep containers tightly closed in a dry, cool and well-ventilated place. Protect from direct sunlight. Keep under nitrogen. To maintain product quality: Store in freezer. Incompatible Materials. Strong oxidizing agents.

8. Exposure controls / personal protection

<u>Exposure Guidelines</u>	This product does not contain any hazardous materials with occupational exposure limitsestablished by the region specific regulatory bodies.
Engineering Measures	None under normal use conditions.
<u>Personal Protective Equipment</u>	
Eye/face Protection	Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
Skin and body protection	Wear appropriate protective gloves and clothing to prevent skin exposure.
Respiratory Protection	No protective equipment is needed under normal use conditions.
Hygiene Measures	Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State	Solid
Appearance	White
Odor	No information available
Odor Threshold	No information available
pH	No information available
Melting Point/Range	230 °C / 446 °F
Boiling Point/Range	No information available
Flash Point	No information available
Evaporation Rate	Not applicable
Flammability (solid,gas)	No information available
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	Not applicable
Specific Gravity	No information available
Solubility	Soluble in water
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	Not applicable

Molecular Formula
Molecular Weight

C₁₄ H₁₃ Br Cl N O₇ · C₆ H₁₃ N · x H₂ O
521.79

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Air sensitive. Light sensitive.
Conditions to Avoid	Incompatible products. Excess heat. Avoid dust formation. Exposure to light. Exposure to air.
Incompatible Materials	Strong oxidizing agents
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO ₂), Nitrogen oxides (NO _x)
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information	No acute toxicity information is available for this product
Oral LD50	Based on ATE data, the classification criteria are not met. ATE > 2000 mg/kg.
Dermal LD50	Based on ATE data, the classification criteria are not met. ATE > 2000 mg/kg.
Mist LC50	Based on ATE data, the classification criteria are not met. ATE > 5 mg/l.

Component Information	
Toxicologically Synergistic Products	No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation	No information available
Sensitization	No information available
Carcinogenicity	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
5-Bromo-4-chloro-3-indolyl-beta-D-glucuronide cyclohexylammonium salt hydrate	NA	Not listed	Not listed	Not listed	Not listed	Not listed
.beta.-D-Glucopyranosiduronic acid, 5-bromo-4-chloro-1H-indol-3-yl, compound with cyclohexanamine (1:1)	114162-64-0	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects	No information available
Reproductive Effects	No information available.
Developmental Effects	No information available.
Teratogenicity	No information available.
STOT - single exposure	None known
STOT - repeated exposure	None known

Aspiration hazard No information available

Symptoms / effects, both acute and delayed No information available

Endocrine Disruptor Information No information available

Other Adverse Effects The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

Do not empty into drains.

Persistence and Degradability Soluble in water Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its water solubility.

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT Not regulated

TDG Not regulated

IATA Not regulated

IMDG/IMO Not regulated

15. Regulatory information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
5-Bromo-4-chloro-3-indolyl-beta-D-glucuronide cyclohexylammonium salt hydrate	NA	-	-	-
.beta.-D-Glucopyranosiduronic acid, 5-bromo-4-chloro-1H-indol-3-yl, compound with cyclohexanamine (1:1)	114162-64-0	X	ACTIVE	PMN

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TSCA 12(b) - Notices of Export Not applicable

International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
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**5-Bromo-4-chloro-3-indolyl-β-D-glucuronide
cyclohexylammonium salt hydrate**

Revision Date 25-Dec-2021

5-Bromo-4-chloro-3-indolyl-beta-D-glucuronide cyclohexylammonium salt hydrate	NA	-	-	-	-	-	-	-	-	-
.beta.-D-Glucopyranosiduronic acid, 5-bromo-4-chloro-1H-indol-3-yl, compound with cyclohexanamine (1:1)	114162-64-0	-	X	-	-	-	-	-	X	-

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

U.S. Federal Regulations

SARA 313	Not applicable
SARA 311/312 Hazard Categories	See section 2 for more information
CWA (Clean Water Act)	Not applicable
Clean Air Act	Not applicable
OSHA - Occupational Safety and Health Administration	Not applicable
CERCLA	Not applicable

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations Not applicable

U.S. Department of Transportation

Reportable Quantity (RQ):	N
DOT Marine Pollutant	N
DOT Severe Marine Pollutant	N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH

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

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
5-Bromo-4-chloro-3-indolyl-beta-D-glucuronide cyclohexylammonium salt hydrate	NA	Not applicable	Not applicable	Not applicable	Not applicable
.beta.-D-Glucopyranosiduronic acid, 5-bromo-4-chloro-1H-indol-3-yl, compound with	114162-64-0	Not applicable	Not applicable	Not applicable	Not applicable

cyclohexanamine (1:1)					
Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
5-Bromo-4-chloro-3-indolyl-beta-D-glucuronide cyclohexylammonium salt hydrate	NA	Not applicable	Not applicable	Not applicable	Not applicable
.beta.-D-Glucopyranosiduronic acid, 5-bromo-4-chloro-1H-indol-3-yl, compound with cyclohexanamine (1:1)	114162-64-0	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

Prepared By Regulatory Affairs
Thermo Fisher Scientific
Email: EMSDS.RA@thermofisher.com

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Revision Date 25-Dec-2021
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Revision Summary This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS