

ALFAAL09871

## 3-Bromophenyl isothiocyanate

### SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明:  
 Product Description: 3-溴异硫氰酸苯酯  
 3-Bromophenyl isothiocyanate

Cat No. : L09871  
 Synonyms N1-Bromo-3-Isothiocyanato-Benzene.  
 CAS No 2131-59-1  
 Molecular Formula C7 H4 Br N S

Supplier Avocado Research Chemicals Ltd.  
 (Part of Thermo Fisher Scientific)  
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**CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

E-mail address begel.sdsdesk@thermofisher.com

Recommended Use Laboratory chemicals.  
 Uses advised against No Information available

### SECTION 2. HAZARD IDENTIFICATION

**Physical State**  
 Liquid

**Appearance**  
 Yellow

**Odor**  
 No information available

#### Emergency Overview

Harmful if swallowed. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. Harmful if inhaled. May cause respiratory irritation. Moisture sensitive. Lachrymator (substance which increases the flow of tears).

#### Classification of the substance or mixture

Acute Oral Toxicity	Category 4
Acute Dermal Toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 4
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity - (single exposure)	Category 3

#### Label Elements

# SAFETY DATA SHEET

## 3-Bromophenyl isothiocyanate

**Signal Word****Warning****Hazard Statements**

H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation  
H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled

**Precautionary Statements****Prevention**

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray  
P264 - Wash face, hands and any exposed skin thoroughly after handling  
P270 - Do not eat, drink or smoke when using this product  
P271 - Use only outdoors or in a well-ventilated area  
P280 - Wear protective gloves/protective clothing/eye protection/face protection

**Response**

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water  
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing  
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P312 - Call a POISON CENTER or doctor if you feel unwell  
P330 - Rinse mouth  
P362 + P364 - Take off contaminated clothing and wash it before reuse

**Storage**

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

**Disposal**

P501 - Dispose of contents/ container to an approved waste disposal plant

**Physical and Chemical Hazards**

None identified.

**Health Hazards**

Harmful if swallowed. Harmful in contact with skin. Causes skin irritation. Causes serious eye irritation. Harmful if inhaled. May cause respiratory irritation. Lachrymator (substance which increases the flow of tears).

**Environmental hazards**

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants.

**Other Hazards**

Lachrymator (substance which increases the flow of tears)  
This product does not contain any known or suspected endocrine disruptors.

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Component	CAS No	Weight %
3-Bromophenyl isothiocyanate	2131-59-1	97

**SECTION 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.

## 3-Bromophenyl isothiocyanate

**Inhalation**

Remove to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Get medical attention.

**Ingestion**

Do NOT induce vomiting. Call a physician or poison control center immediately.

**Most important symptoms and effects**

. Metabolism may release cyanide, which may result in headache, dizziness, weakness, collapse, unconsciousness, and possible death

**Self-Protection of the First Aider**

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

**Notes to Physician**

Treat symptomatically.

**SECTION 5. FIRE-FIGHTING MEASURES****Suitable Extinguishing Media**

Carbon dioxide (CO<sub>2</sub>). Dry chemical.

**Extinguishing media which must not be used for safety reasons**

No information available.

**Specific Hazards Arising from the Chemical**

Thermal decomposition can lead to release of irritating gases and vapors.

**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.

**SECTION 6. ACCIDENTAL RELEASE MEASURES****Personal Precautions**

Ensure adequate ventilation. Use personal protective equipment as required.

**Environmental Precautions**

Prevent further leakage or spillage if safe to do so.

**Methods for Containment and Clean Up**

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal.

Refer to protective measures listed in Sections 8 and 13.

**SECTION 7. HANDLING AND STORAGE****Handling**

Use only under a chemical fume hood. Wear personal protective equipment/face protection. Avoid contact with skin and eyes. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Wash hands before breaks and immediately after handling the product.

**Storage**

## 3-Bromophenyl isothiocyanate

Keep in a dry, cool and well-ventilated place. Keep container tightly closed.

**Specific Use(s)**

Use in laboratories

**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION****Control Parameters****Exposure Controls****Engineering Measures**

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

**Personal protective equipment**

**Eye Protection** Goggles (European standard - EN 166)

**Hand Protection** Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers	-	EN 374	(minimum requirement)
Neoprene	recommendations			
Natural rubber				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

**Skin and body protection** Wear appropriate protective gloves and clothing to prevent skin exposure

**Respiratory Protection** When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.  
To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

**Large scale/emergency use** Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced  
**Recommended Filter type:** Organic gases and vapours filter Type A Brown conforming to EN14387

**Small scale/Laboratory use** Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.  
**Recommended half mask:-** Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141  
When RPE is used a face piece Fit Test should be conducted

**Hygiene Measures** Handle in accordance with good industrial hygiene and safety practice.

**Environmental exposure controls** No information available.

**SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES**

<b>Appearance</b>	Yellow	
<b>Physical State</b>	Liquid	
<b>Odor</b>	No information available	
<b>Odor Threshold</b>	No data available	
<b>pH</b>	No information available	
<b>Melting Point/Range</b>	No data available	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	No information available	@ 760 mmHg
<b>Flash Point</b>	> 110 °C / > 230 °F	<b>Method -</b> No information available
<b>Evaporation Rate</b>	No data available	
<b>Flammability (solid,gas)</b>	Not applicable	Liquid
<b>Explosion Limits</b>	No data available	
<b>Vapor Pressure</b>	No data available	
<b>Vapor Density</b>	7.38	(Air = 1.0)
<b>Specific Gravity / Density</b>	No data available	
<b>Bulk Density</b>	Not applicable	Liquid
<b>Water Solubility</b>	No information available	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Autoignition Temperature</b>	No data available	
<b>Decomposition Temperature</b>	No data available	
<b>Viscosity</b>	No data available	
<b>Explosive Properties</b>	No information available	
<b>Oxidizing Properties</b>	No information available	
<b>Molecular Formula</b>	C7 H4 Br N S	
<b>Molecular Weight</b>	214.09	

## SECTION 10. STABILITY AND REACTIVITY

<b>Stability</b>	Moisture sensitive.
<b>Hazardous Reactions</b>	No information available.
<b>Hazardous Polymerization</b>	No information available.
<b>Conditions to Avoid</b>	Excess heat. Incompatible products. Exposure to moist air or water.
<b>Materials to avoid</b>	Acids. Strong oxidizing agents. Strong bases. Alcohols. Amines.
<b>Hazardous Decomposition Products</b>	Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO <sub>2</sub> ). Hydrogen halides. Sulfur oxides.

## SECTION 11. TOXICOLOGICAL INFORMATION

### Product Information

<b>(a) acute toxicity;</b>	
<b>(b) skin corrosion/irritation;</b>	Category 2
<b>(c) serious eye damage/irritation;</b>	Category 2
<b>(d) respiratory or skin sensitization;</b>	
Respiratory	No data available

**SAFETY DATA SHEET**  
**3-Bromophenyl isothiocyanate**

<b>Skin</b>	No data available
<b>(e) germ cell mutagenicity;</b>	No data available
<b>(f) carcinogenicity;</b>	No data available There are no known carcinogenic chemicals in this product
<b>(g) reproductive toxicity;</b>	No data available
<b>(h) STOT-single exposure;</b>	Category 3
<b>Results / Target organs</b>	Respiratory system
<b>(i) STOT-repeated exposure;</b>	No data available
<b>Target Organs</b>	No information available.
<b>(j) aspiration hazard;</b>	No data available
<b>Other Adverse Effects</b>	The toxicological properties have not been fully investigated.
<b>Symptoms / effects,both acute and delayed</b>	Metabolism may release cyanide, which may result in headache, dizziness, weakness, collapse, unconsciousness, and possible death

**SECTION 12. ECOLOGICAL INFORMATION**

<b>Ecotoxicity effects</b>	Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.
<b>Persistence and Degradability</b>	No information available
<b>Bioaccumulative Potential</b>	No information available
<b>Mobility in soil</b>	No information available
<b>Endocrine Disruptor Information</b>	This product does not contain any known or suspected endocrine disruptors
<b>Persistent Organic Pollutant</b>	This product does not contain any known or suspected substance
<b>Ozone Depletion Potential</b>	This product does not contain any known or suspected substance

**SECTION 13. DISPOSAL CONSIDERATIONS**

<b>Waste from Residues/Unused Products</b>	Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.
<b>Contaminated Packaging</b>	Dispose of this container to hazardous or special waste collection point.
<b>Other Information</b>	Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

**SECTION 14. TRANSPORT INFORMATION**

## 3-Bromophenyl isothiocyanate

**Road and Rail Transport** Not Regulated**IMDG/IMO** Not regulated**IATA** Not regulated**Special Precautions for User** No special precautions required**SECTION 15. REGULATORY INFORMATION****International Inventories**

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
3-Bromophenyl isothiocyanate	-	-	X	-	-	-	-	-	-	-	-	-

**National Regulations****SECTION 16. OTHER INFORMATION**

**Prepared By** Health, Safety and Environmental Department  
**Creation Date** 26-Sep-2009  
**Revision Date** 27-Apr-2024  
**Revision Summary** New emergency telephone response service provider.

**Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

**Legend****CAS** - Chemical Abstracts Service**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances**PICCS** - Philippines Inventory of Chemicals and Chemical Substances**IECSC** - Chinese Inventory of Existing Chemical Substances**KECL** - Korean Existing and Evaluated Chemical Substances**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List**ENCS** - Japanese Existing and New Chemical Substances**AICS** - Australian Inventory of Chemical Substances**NZIoC** - New Zealand Inventory of Chemicals**WEL** - Workplace Exposure Limit**ACGIH** - American Conference of Governmental Industrial Hygienists**DNEL** - Derived No Effect Level**TWA** - Time Weighted Average**IARC** - International Agency for Research on Cancer**PNEC** - Predicted No Effect Concentration

## 3-Bromophenyl isothiocyanate

**RPE** - Respiratory Protective Equipment  
**LC50** - Lethal Concentration 50%  
**NOEC** - No Observed Effect Concentration  
**PBT** - Persistent, Bioaccumulative, Toxic

**LD50** - Lethal Dose 50%  
**EC50** - Effective Concentration 50%  
**POW** - Partition coefficient Octanol:Water  
**vPvB** - very Persistent, very Bioaccumulative

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - (Volatile Organic Compound)

**Key literature references and sources for data**

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**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 Safety Data Sheet**