

ALFAAL09756

## 1,4-Phenylene diisothiocyanate

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

**产品说明:**  
**Product Description:** 1, 4-亚苯基二异硫氰酸酯  
 1,4-Phenylene diisothiocyanate

**Cat No. :** L09756  
**Synonyms** 1,4-Diisothiocyanatobenzene; Bitoscanate; Phenylene Thiocyanate.  
**CAS No** 4044-65-9  
**Molecular Formula** C8 H4 N2 S2

**Supplier** Avocado Research Chemicals Ltd.  
 (Part of Thermo Fisher Scientific)  
 Shore Road, Heysham  
 Lancashire, LA3 2XY,  
 United Kingdom  
 Office Tel: +44 (0) 1524 850506  
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**Emergency Telephone Number** For information **US** call: 001-800-227-6701 / **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

**E-mail address** begel.sdsdesk@thermofisher.com

**Recommended Use** Laboratory chemicals.  
**Uses advised against** No Information available

### SECTION 2. HAZARD IDENTIFICATION

**Physical State**  
Powder Solid

**Appearance**  
Light yellow

**Odor**  
No information available

#### Emergency Overview

Toxic if swallowed. Causes skin irritation. Causes serious eye irritation. May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause respiratory irritation. Very toxic to aquatic life with long lasting effects. Moisture sensitive.

#### Classification of the substance or mixture

Acute Oral Toxicity	Category 3
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Respiratory Sensitization	Category 1
Specific target organ toxicity - (single exposure)	Category 3
Acute aquatic toxicity	Category 1
Chronic aquatic toxicity	Category 1

#### Label Elements

## 1,4-Phenylene diisothiocyanate



## Signal Word

Danger

## Hazard Statements

H301 - Toxic if swallowed  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled  
H335 - May cause respiratory irritation  
H410 - Very toxic to aquatic life with long lasting effects

## 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  
P284 - In case of inadequate ventilation wear respiratory protection

## Response

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  
P330 - Rinse mouth  
P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor  
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water  
P332 + P313 - If skin irritation occurs: Get medical advice/attention  
P337 + P313 - If eye irritation persists: Get medical advice/attention  
P342 + P311 - If experiencing respiratory symptoms: Call a POISON CENTER or doctor  
P362 + P364 - Take off contaminated clothing and wash it before reuse

## Storage

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed  
P405 - Store locked up

## Disposal

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

## Physical and Chemical Hazards

None identified.

## Health Hazards

Toxic if swallowed. Causes skin irritation. Causes serious eye irritation. May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause respiratory irritation.

## Environmental hazards

Very toxic to aquatic life with long lasting effects. Is not likely mobile in the environment due its low water solubility. Spillage unlikely to penetrate soil.

## Other Hazards

This product does not contain any known or suspected endocrine disruptors.

## SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
Bitoscanate	4044-65-9	>95

**SECTION 4. FIRST AID MEASURES****General Advice**

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

**Eye Contact**

In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

**Skin Contact**

Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.

**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. Immediate medical attention is required.

**Ingestion**

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

**Most important symptoms and effects**

None reasonably foreseeable. May cause allergy or asthma symptoms or breathing difficulties if inhaled. Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing

**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**

Water spray, carbon dioxide (CO<sub>2</sub>), dry chemical, alcohol-resistant foam.

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

No information available.

**Specific Hazards Arising from the Chemical**

Do not allow run-off from fire-fighting to enter drains or water courses.

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

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

Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas.

**Environmental Precautions**

Do not flush into surface water or sanitary sewer system. Do not allow material to contaminate ground water system. Prevent product from entering drains. Local authorities should be advised if significant spillages cannot be contained.

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**Methods for Containment and Clean Up**

Sweep up and shovel into suitable containers for disposal. Avoid dust formation.

Refer to protective measures listed in Sections 8 and 13.

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

Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Avoid dust formation. Use only under a chemical fume hood. Do not breathe (dust, vapor, mist, gas). Do not ingest. If swallowed then seek immediate medical assistance.

**Storage**

Keep container tightly closed in a dry and well-ventilated place. Store under an inert atmosphere.

**Specific Use(s)**

Use in laboratories

**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION****Control Parameters****Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

**Exposure Controls****Engineering Measures**

Ventilation systems. 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** Long sleeved clothing

**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

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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:** Particulates filter conforming to EN 143

**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:-** Particle filtering: EN149:2001  
 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**

Prevent product from entering drains. Do not allow material to contaminate ground water system. Local authorities should be advised if significant spillages cannot be contained.

**SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES**

<b>Appearance</b>	Light yellow	
<b>Physical State</b>	Powder Solid	
<b>Odor</b>	No information available	
<b>Odor Threshold</b>	No data available	
<b>pH</b>	No information available	
<b>Melting Point/Range</b>	129 - 133 °C / 264.2 - 271.4 °F	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	No information available	
<b>Flash Point</b>	No information available	<b>Method -</b> No information available
<b>Evaporation Rate</b>	Not applicable	Solid
<b>Flammability (solid,gas)</b>	No information available	
<b>Explosion Limits</b>	No data available	
<b>Vapor Pressure</b>	No data available	
<b>Vapor Density</b>	Not applicable	Solid
<b>Specific Gravity / Density</b>	No data available	
<b>Bulk Density</b>	No data available	
<b>Water Solubility</b>	Insoluble	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Component</b>	<b>log Pow</b>	
Bitoscanate	4.67	
<b>Autoignition Temperature</b>	No data available	
<b>Decomposition Temperature</b>	No data available	
<b>Viscosity</b>	Not applicable	Solid
<b>Explosive Properties</b>	No information available	
<b>Oxidizing Properties</b>	No information available	
<b>Molecular Formula</b>	C8 H4 N2 S2	
<b>Molecular Weight</b>	192.27	

**SECTION 10. STABILITY AND REACTIVITY**

<b>Stability</b>	Moisture sensitive.
<b>Hazardous Reactions</b>	None under normal processing.
<b>Hazardous Polymerization</b>	No information available.
<b>Conditions to Avoid</b>	Incompatible products. Exposure to moist air or water.

**Materials to avoid** Oxidizing agent.

**Hazardous Decomposition Products** Thermal decomposition can lead to release of irritating gases and vapors.

## SECTION 11. TOXICOLOGICAL INFORMATION

### Product Information

**(a) acute toxicity;**

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Bitoscanate	230 mg/kg (mouse)		

**(b) skin corrosion/irritation;** Category 2

**(c) serious eye damage/irritation;** Category 2

**(d) respiratory or skin sensitization;**

Respiratory Category 1  
Skin No data available

**(e) germ cell mutagenicity;** No data available

**(f) carcinogenicity;** No data available  
There are no known carcinogenic chemicals in this product

**(g) reproductive toxicity;** No data available

**(h) STOT-single exposure;** Category 3  
**Results / Target organs** Respiratory system

**(i) STOT-repeated exposure;** No data available  
**Target Organs** No information available.

**(j) aspiration hazard;** Not applicable  
Solid

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

**Symptoms / effects, both acute and delayed** Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing

## SECTION 12. ECOLOGICAL INFORMATION

**Ecotoxicity effects** Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment.

Component	Freshwater Fish	Water Flea	Freshwater Algae	Microtox
Bitoscanate		0.077 mg/l/48h (Daphnia magna)		

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**Persistence and Degradability****Persistence**

Insoluble in water, May persist.

**Degradation in sewage treatment plant**

Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

**Bioaccumulative Potential**

May have some potential to bioaccumulate; Product has a high potential to bioconcentrate

Component	log Pow	Bioconcentration factor (BCF)
Bitoscanate	4.67	No data available

**Mobility in soil**

Spillage unlikely to penetrate soil Is not likely mobile in the environment due its low water solubility Is not likely mobile in the environment due its low water solubility and propensity to bind to soil particles

**Endocrine Disruptor Information**

This product does not contain any known or suspected endocrine disruptors

**Persistent Organic Pollutant**

This product does not contain any known or suspected substance

**Ozone Depletion Potential**

This product does not contain any known or suspected substance

**SECTION 13. DISPOSAL CONSIDERATIONS****Waste from Residues/Unused Products**

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. Should not be released into the environment.

**Contaminated Packaging**

Dispose of this container to hazardous or special waste collection point.

**Other Information**

Do not flush to sewer. Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains. Do not let this chemical enter the environment.

**SECTION 14. TRANSPORT INFORMATION****Road and Rail Transport****UN-No**

UN2811

**Proper Shipping Name**

Toxic solid, organic, n.o.s.

**Technical Shipping Name**

Bitoscanate

**Hazard Class**

6.1

**Packing Group**

III

**IMDG/IMO****UN-No**

UN2811

**Proper Shipping Name**

Toxic solid, organic, n.o.s.

**Technical Shipping Name**

Bitoscanate

**Hazard Class**

6.1

**Packing Group**

III

**IATA****UN-No**

UN2811

**Proper Shipping Name**

Toxic solid, organic, n.o.s.

**Technical Shipping Name**

Bitoscanate

**Hazard Class**

6.1

**Packing Group**

III

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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
Bitoscanate	-	-	X	-	223-741-3	X	-	-	-	-	-	-

## National Regulations

## SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department  
 Creation Date 21-Feb-2017  
 Revision Date 22-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.

Chemical incident response training.

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

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer

**PNEC** - Predicted No Effect Concentration

**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)



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**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**