

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

### 1.1. Product identifier

Product Description: **3-Methylbenzyl isothiocyanate**  
Cat No. : **H54893**  
CAS No 3696-66-0  
Molecular Formula C9 H9 NS

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

Recommended Use Laboratory chemicals.  
Uses advised against No Information available

### 1.3. Details of the supplier of the safety data sheet

Company  
Avocado Research Chemicals Ltd.  
(Part of Thermo Fisher Scientific)  
Shore Road, Heysham  
Lancashire, LA3 2XY,  
United Kingdom  
Office Tel: +44 (0) 1524 850506  
Office Fax: +44 (0) 1524 850608

E-mail address begel.sdsdesk@thermofisher.com

### 1.4. 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

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

#### CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

##### Physical hazards

Based on available data, the classification criteria are not met

##### Health hazards

Acute oral toxicity  
Acute dermal toxicity

Category 4 (H302)  
Category 4 (H312)

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Acute Inhalation Toxicity - Vapors  
Skin Corrosion/Irritation  
Serious Eye Damage/Eye Irritation

Category 4 (H332)  
Category 1 B (H314)  
Category 1 (H318)

## **Environmental hazards**

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

## **2.2. Label elements**



Signal Word

Danger

## **Hazard Statements**

H314 - Causes severe skin burns and eye damage

H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled

## **Precautionary Statements**

P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing

P280 - Wear protective gloves/protective clothing/eye protection/face protection

P301 + P330 + P331 - IF SWALLOWED: Rinse mouth. Do NOT induce vomiting

P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

P310 - Immediately call a POISON CENTER or doctor/physician

P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower

## **2.3. Other hazards**

This product does not contain any known or suspected endocrine disruptors

## **SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS**

### **3.1. Substances**

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
3-Methylbenzyl isothiocyanate	3696-66-0		<=100	Acute Tox. 4 (H302) Acute Tox. 4 (H312) Acute Tox. 4 (H332) Skin Corr. 1B (H314) Eye Dam. 1 (H318)

Full text of Hazard Statements: see section 16

## **SECTION 4: FIRST AID MEASURES**

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## 4.1. Description of first aid measures

<b>General Advice</b>	Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.
<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Call a physician immediately.
<b>Ingestion</b>	Do NOT induce vomiting. Clean mouth with water. Never give anything by mouth to an unconscious person. Call a physician immediately.
<b>Inhalation</b>	If not breathing, give artificial respiration. Remove from exposure, lie down. 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. Call a physician immediately.
<b>Self-Protection of the First Aider</b>	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

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

Causes burns by all exposure routes. Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

## 4.3. Indication of any immediate medical attention and special treatment needed

**Notes to Physician** Treat symptomatically.

## SECTION 5: FIREFIGHTING MEASURES

### 5.1. Extinguishing media

#### **Suitable Extinguishing Media**

CO<sub>2</sub>, dry chemical, dry sand, alcohol-resistant foam.

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

No information available.

### 5.2. Special hazards arising from the substance or mixture

Thermal decomposition can lead to release of irritating gases and vapors. The product causes burns of eyes, skin and mucous membranes.

#### **Hazardous Combustion Products**

None under normal use conditions.

### 5.3. Advice 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

### 6.1. Personal precautions, protective equipment and emergency procedures

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

## **6.2. Environmental precautions**

Should not be released into the environment. See Section 12 for additional Ecological Information.

## **6.3. Methods and material for containment and cleaning up**

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal.

## **6.4. Reference to other sections**

Refer to protective measures listed in Sections 8 and 13.

## **SECTION 7: HANDLING AND STORAGE**

### **7.1. Precautions for safe handling**

Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance.

#### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

### **7.2. Conditions for safe storage, including any incompatibilities**

Corrosives area. Keep containers tightly closed in a dry, cool and well-ventilated place.

**Technical Rules for Hazardous Substances (TRGS) 510**      Class 8A  
**Storage Class (LGK) (Germany)**

### **7.3. Specific end use(s)**

Use in laboratories

## **SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION**

### **8.1. Control parameters**

#### **Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

#### **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

#### **Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)**

No information available

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## Predicted No Effect Concentration (PNEC)

No information available.

## 8.2. Exposure controls

### Engineering Measures

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				

**Skin and body protection** Long sleeved clothing.

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.

**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

**Environmental exposure controls** No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

### 9.1. Information on basic physical and chemical properties

**Physical State** Liquid

**Appearance** Light brown

**Odor** No information available

**Odor Threshold** No data available

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Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	127 °C / 260.6 °F	
Flammability (liquid)	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Flash Point	No information available	Method - No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	No data available	
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Vapor Pressure	No data available	
Density / Specific Gravity	1.09 g/cm3	@ 20 °C
Bulk Density	Not applicable	Liquid
Vapor Density	No data available	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

## 9.2. Other information

Molecular Formula	C9 H9 NS
Molecular Weight	163.24

## SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity	None known, based on information available
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10.2. Chemical stability	Stable under normal conditions.
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### 10.3. Possibility of hazardous reactions

Hazardous Polymerization	No information available.
Hazardous Reactions	None under normal processing.

10.4. Conditions to avoid	Incompatible products. Excess heat.
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10.5. Incompatible materials	None known.
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10.6. Hazardous decomposition products	None under normal use conditions.
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## SECTION 11: TOXICOLOGICAL INFORMATION

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

#### Product Information

(a) acute toxicity;	
Oral	Category 4
Dermal	Category 4
Inhalation	Category 4

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(b) skin corrosion/irritation; Category 1 B

(c) serious eye damage/irritation; Category 1

(d) respiratory or skin sensitization;

Respiratory

No data available

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; No data available

(i) STOT-repeated exposure; No data available

Target Organs

No information available.

(j) aspiration hazard; No data available

**Symptoms / effects, both acute and delayed**

Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated. Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation.

## 11.2. Information on other hazards

### **Endocrine Disrupting Properties**

Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

## **SECTION 12: ECOLOGICAL INFORMATION**

### 12.1. Toxicity

#### **Ecotoxicity effects**

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

12.2. Persistence and degradability No information available

12.3. Bioaccumulative potential No information available

12.4. Mobility in soil No information available

12.5. Results of PBT and vPvB assessment No data available for assessment.

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## 12.6. Endocrine disrupting properties

### Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

## 12.7. Other adverse effects

### 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

### 13.1. Waste treatment methods

#### 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.

#### Contaminated Packaging

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

#### European Waste Catalogue (EWC)

According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

#### Other Information

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 flush to sewer. Large amounts will affect pH and harm aquatic organisms.

## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

#### 14.1. UN number

UN2922

#### 14.2. UN proper shipping name

Corrosive liquid, toxic, n.o.s.  
(3-Methylbenzyl isothiocyanate)

#### 14.3. Transport hazard class(es)

8

#### Subsidiary Hazard Class

6.1

#### 14.4. Packing group

III

### ADR

#### 14.1. UN number

UN2922

#### 14.2. UN proper shipping name

Corrosive liquid, toxic, n.o.s.  
(3-Methylbenzyl isothiocyanate)

#### 14.3. Transport hazard class(es)

8

#### Subsidiary Hazard Class

6.1

#### 14.4. Packing group

III

### IATA

#### 14.1. UN number

UN2922

#### 14.2. UN proper shipping name

Corrosive liquid, toxic, n.o.s.  
(3-Methylbenzyl isothiocyanate)

#### 14.3. Transport hazard class(es)

8

#### Subsidiary Hazard Class

6.1

#### 14.4. Packing group

III

#### 14.5. Environmental hazards

No hazards identified



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**14.6. Special precautions for user** No special precautions required.

**14.7. Maritime transport in bulk according to IMO instruments** Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

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

#### International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
3-Methylbenzyl isothiocyanate	3696-66-0	-	-	-	-	-	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
3-Methylbenzyl isothiocyanate	3696-66-0	-	-	-	-	-	-	-

**Legend:** X - Listed '-' - Not Listed

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

#### Authorisation/Restrictions according to EU REACH

Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
3-Methylbenzyl isothiocyanate	3696-66-0	-	-	-

#### Seveso III Directive (2012/18/EC)

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
3-Methylbenzyl isothiocyanate	3696-66-0	Not applicable	Not applicable

#### Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

#### Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

#### National Regulations

**UK** - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

#### WGK Classification

Water endangering class = 3 (self classification)

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## 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3

H302 - Harmful if swallowed

H312 - Harmful in contact with skin

H332 - Harmful if inhaled

H314 - Causes severe skin burns and eye damage

H318 - Causes serious eye damage

### 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  
Predicted No Effect Concentration (PNEC)

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

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

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

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

**BCF** - Bioconcentration factor

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

**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

### 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.

### Prepared By

Health, Safety and Environmental Department

### Revision Date

08-Mar-2024

### Revision Summary

New emergency telephone response service provider.

**This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.**

### Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the

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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**