

according to Regulation UK SI 2019/758 and UK SI 2020/1577 as amended

Creation Date 03-May-2012 Revision Date 23-Jan-2024 Revision Number 3

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

1.1. Product identifier

Product Description: Benzyl isothiocyanate

Cat No. : A15008

Synonyms Isothiocyanic acid benzyl ester

CAS No 622-78-6 EC No 210-753-9 Molecular Formula C8 H7 N S

REACH registration number -

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

Benzyl isothiocyanate

Revision Date 23-Jan-2024

Acute oral toxicity	Category 4 (H302)
Acute dermal toxicity	Category 4 (H312)
Acute Inhalation Toxicity - Vapors	Category 4 (H332)
Skin Corrosion/Irritation	Category 2 (H315)
Serious Eye Damage/Eye Irritation	Category 2 (H319)
Respiratory Sensitization	Category 1 (H334)
Specific target organ toxicity - (single exposure)	Category 3 (H335)

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

H334 - May cause allergy or asthma symptoms or breathing difficulties if inhaled

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

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

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

P332 + P313 - If skin irritation occurs: Get medical advice/attention

P337 + P313 - If eye irritation persists: Get medical advice/attention

2.3. 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

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
Benzene, (isothiocyanatomethyl)-	622-78-6	EEC No. 210-753-9	>95	Resp. Sens. 1 (H334)
				Acute Tox. 4 (H302)
				Acute Tox. 4 (H312)
				Acute Tox. 4 (H332)

Benzyl isothiocyanate		Revision Date 23-Jan-2024

		Skin Irrit. 2 (H315)
		Eye Irrit. 2 (H319)
		STOT SE 3 (H335)

REACH registration number

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of 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.

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

Inhalation 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. Remove to fresh air. Get medical attention. If not

breathing, give artificial respiration.

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.

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

Causes burns by all exposure routes. May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause allergic skin reaction. 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

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

CO₂, 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.

Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO2), Hydrogen cyanide (hydrocyanic acid), Thermal decomposition can lead to release of irritating gases and vapors.

5.3. Advice for firefighters

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

Benzyl isothiocyanate

Revision Date 23-Jan-2024

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

Use personal protective equipment as required. Ensure adequate ventilation. 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. Methods for Containment and Clean Up.

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

Do not get in eyes, on skin, or on clothing. Wear personal protective equipment/face protection. 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.

7.2. Conditions for safe storage, including any incompatibilities

To maintain product quality: Keep refrigerated. Keep in a dry place. Store under an inert atmosphere.

Technical Rules for Hazardous Substances (TRGS) 510 Class 10 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

Benzyl isothiocyanate Revision Date 23-Jan-2024

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

No information available

Predicted No Effect Concentration (PNEC)

No information available.

8.2. 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 Natural rubber Nitrile rubber Neoprene	Breakthrough time See manufacturers recommendations	Glove thickness	EU standard EN 374	Glove comments (minimum requirement)
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 compatability, 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 No protective equipment is needed under normal use conditions.

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

Small scale/Laboratory use Maintain adequate ventilation

Environmental exposure controls No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State Liquid

AppearanceYellowOdorpungent

Odor Threshold No data available
Melting Point/Range No data available
Softening Point No data available

Benzyl isothiocyanate Revision Date 23-Jan-2024

Liquid

Boiling Point/Range 243 °C / 469.4 °F @ 760 mmHg

Flammability (liquid)
Flammability (solid,gas)

No data available
Not applicable

Explosion Limits No data available

Flash Point $> 110 \, ^{\circ}\text{C} \, / > 230 \, ^{\circ}\text{F}$ Method - No information available

Autoignition Temperature
Decomposition Temperature
pH
Viscosity
Water Solubility
Solubility in other solvents
No data available
No information available
No information available
No information available
No information available

Partition Coefficient (n-octanol/water)

Vapor Pressure 0.02 mmHg @ 20 °C

Density / Specific Gravity 1.125

Bulk DensityNot applicableLiquidVapor DensityNo information available(Air = 1.0)

Particle characteristics Not applicable (liquid)

9.2. Other information

Molecular FormulaC8 H7 N SMolecular Weight149.22

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity

None known, based on information available

10.2. Chemical stability

Stable under normal conditions. Moisture sensitive.

10.3. Possibility of hazardous reactions

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous Reactions None under normal processing.

10.4. Conditions to avoid

Incompatible products. Excess heat. Exposure to moist air or water.

10.5. Incompatible materials

Strong oxidizing agents. Acids. Alcohols. Amines.

10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO₂). Hydrogen cyanide (hydrocyanic acid).

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

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

Revision Date 23-Jan-2024 Benzyl isothiocyanate

(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

May cause sensitization by inhalation

(e) germ cell mutagenicity; No data available

No data available (f) carcinogenicity;

There are no known carcinogenic chemicals in this product

No data available (g) reproductive toxicity;

(h) STOT-single exposure; Category 3

Respiratory system. Results / Target organs

(i) STOT-repeated exposure; No data available

No information available. **Target Organs**

(j) aspiration hazard; No data available

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

delayed

Symptoms / effects, both acute and 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.

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 Do not empty into drains.

Component	Microtox	M-Factor
Benzene, (isothiocyanatomethyl)-	EC50 = 0.01 mg/L 15 min	
	EC50 = 0.01 mg/L 30 min	
	EC50 = 0.01 mg/L 5 min	

12.2. Persistence and degradability No information available

12.3. Bioaccumulative potential No information available

Benzyl isothiocyanate Revision Date 23-Jan-2024

12.4. Mobility in soil No information available

12.5. Results of PBT and vPvB

assessment

No data available for assessment.

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 Ozone Depletion Potential This product does not contain any known or suspected substance 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.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO Not regulated

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

14.4. Packing group

ADR Not regulated

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

14.4. Packing group

IATA Not regulated

14.1. UN number

14.2. UN proper shipping name

14.3. Transport hazard class(es)

14.4. Packing group

14.5. Environmental hazardsNo hazards identified

14.6. Special precautions for user No special precautions required.

14.7. Maritime transport in bulk Not applicable, packaged goods

according to IMO instruments

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
Benzene, (isothiocyanatomethyl)-	622-78-6	210-753-9	-	-	X	Χ	-	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Benzene, (isothiocyanatomethyl)-	622-78-6	Х	ACTIVE	-	Х	X	Х	Х

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 Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Benzene, (isothiocyanatomethyl)-	622-78-6	-	-	-

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
Benzene, (isothiocyanatomethyl)-	622-78-6	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)

Benzyl isothiocyanate Revision Date 23-Jan-2024

Component	Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81)	Switzerland - Ordinance on Incentive Taxes on Volatile Organic Compounds (OVOC)	Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure
Benzene, (isothiocyanatomethyl)-	Prohibited and Restricted		
622-78-6 (>95)	Substances		

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

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

Legend

CAS - Chemical Abstracts Service

TSCA - United States Toxic Substances Control Act Section 8(b)

Inventory

EINECS/ELINCS - European Inventory of Existing Commercial Chemical DSL/NDSL - Canadian Domestic Substances List/Non-Domestic

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 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.

Prepared By Health, Safety and Environmental Department

03-May-2012 **Creation Date Revision Date** 23-Jan-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.

Benzyl isothiocyanate Revision Date 23-Jan-2024

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