

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

### 1.1. Product identifier

Product Description:	<b>4-Methoxybenzotrile</b>
Cat No. :	<b>A15945</b>
Synonyms	4-Methoxybenzotrile
CAS No	874-90-8
Molecular Formula	C8 H7 N O
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

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Acute oral toxicity  
Acute dermal toxicity  
Acute Inhalation Toxicity - Dusts and Mists

Category 4 (H302)  
Category 4 (H312)  
Category 4 (H332)

**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

Warning

### Hazard Statements

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

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water

P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell

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

## 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
Benzonitrile, 4-methoxy-	874-90-8	EEC No. 212-871-6	99	Acute Tox. 4 (H302) Acute Tox. 4 (H312) Acute Tox. 4 (H332)

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

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medical attention.

## **Skin Contact**

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention.

## **Ingestion**

Clean mouth with water. Get medical attention.

## **Inhalation**

Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention.

## **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**

No information available.

## **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**

Water spray. Carbon dioxide (CO<sub>2</sub>). Dry chemical. Chemical 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**

Nitrogen oxides (NO<sub>x</sub>), Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Hydrogen cyanide (hydrocyanic acid).

### **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.

## **SECTION 6: ACCIDENTAL RELEASE MEASURES**

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

Ensure adequate ventilation.

### **6.2. Environmental precautions**

See Section 12 for additional Ecological Information.

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

Sweep up and shovel into suitable containers for disposal. Do not let this chemical enter the environment.

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

Refer to protective measures listed in Sections 8 and 13.

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## SECTION 7: HANDLING AND STORAGE

### 7.1. Precautions for safe handling

Avoid contact with skin and eyes. Do not breathe dust. 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

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

**Technical Rules for Hazardous Substances (TRGS) 510**      Class 11  
**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

List source(s): **UK** - EH40/2005 Work Exposure Limits, Fourth edition. Published 2020.

Component	The United Kingdom	European Union	Ireland
Benzonitrile, 4-methoxy-	STEL: 15 mg/m <sup>3</sup> 15 min TWA: 5 mg/m <sup>3</sup> 8 hr Skin		

#### 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

#### Predicted No Effect Concentration (PNEC)

No information available.

### 8.2. Exposure controls

#### Engineering Measures

Ensure adequate ventilation, especially in confined areas.

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

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## 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 recommendations	-	EN 374	(minimum requirement)
Neoprene				
Natural rubber				
PVC				

### Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

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

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:** 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

### Environmental exposure controls

No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

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

#### Physical State

Powder Solid

#### Appearance

Beige

#### Odor

Odorless

#### Odor Threshold

No data available

#### Melting Point/Range

57 - 60 °C / 134.6 - 140 °F

#### Softening Point

No data available

#### Boiling Point/Range

256 - 257 °C / 492.8 - 494.6 °F @ 765 mmHg

#### Flammability (liquid)

Not applicable

Solid

#### Flammability (solid,gas)

No information available

#### 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

Not applicable

Solid

#### Water Solubility

Soluble

#### Solubility in other solvents

No information available

#### Partition Coefficient (n-octanol/water)

#### Vapor Pressure

No data available

#### Density / Specific Gravity

No data available

#### Bulk Density

No data available

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Vapor Density	Not applicable	Solid
Particle characteristics	No data available	

## 9.2. Other information

Molecular Formula	C8 H7 N O
Molecular Weight	133.15
Evaporation Rate	Not applicable - Solid

## SECTION 10: STABILITY AND REACTIVITY

**10.1. Reactivity** None known, based on information available

**10.2. Chemical stability** Stable under normal conditions.

### 10.3. Possibility of hazardous reactions

**Hazardous Polymerization** No information available.  
**Hazardous Reactions** No information available.

**10.4. Conditions to avoid** Incompatible products.

**10.5. Incompatible materials** Strong oxidizing agents. Strong acids. Strong bases.

**10.6. Hazardous decomposition products** Nitrogen oxides (NO<sub>x</sub>). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Hydrogen cyanide (hydrocyanic acid).

## SECTION 11: TOXICOLOGICAL INFORMATION

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

#### Product Information

<b>(a) acute toxicity;</b>	
Oral	Category 4
Dermal	Category 4
Inhalation	Category 4
<b>(b) skin corrosion/irritation;</b>	No data available
<b>(c) serious eye damage/irritation;</b>	No data available
<b>(d) respiratory or skin sensitization;</b>	
Respiratory	No data available
Skin	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

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(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;	Not applicable Solid
Other Adverse Effects	The toxicological properties have not been fully investigated.
Symptoms / effects,both acute and delayed	No information available.

## 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.

**12.2. Persistence and degradability**  
**Persistence** Soluble in water, Persistence is unlikely, based on information available.

**12.3. Bioaccumulative potential** Bioaccumulation is unlikely

**12.4. Mobility in soil** The product is water soluble, and may spread in water systems Will likely be mobile in the environment due to its water solubility. Highly mobile in soils

**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** 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





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Benzotrile, 4-methoxy-	874-90-8	X	ACTIVE	-	X	X	X	X
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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)
Benzotrile, 4-methoxy-	874-90-8	-	-	-

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
Benzotrile, 4-methoxy-	874-90-8	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)

## 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

### Legend

CAS - Chemical Abstracts Service

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

EINECS/ELINCS - European Inventory of Existing Commercial Chemical

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Substances/EU List of Notified Chemical Substances

**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**ENCS** - Japanese Existing and New Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**TWA** - Time Weighted Average

**ACGIH** - American Conference of Governmental Industrial Hygienists

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

**DNEL** - Derived No Effect Level

Predicted No Effect Concentration (PNEC)

**RPE** - Respiratory Protective Equipment

**LD50** - Lethal Dose 50%

**LC50** - Lethal Concentration 50%

**EC50** - Effective Concentration 50%

**NOEC** - No Observed Effect Concentration

**POW** - Partition coefficient Octanol:Water

**PBT** - Persistent, Bioaccumulative, Toxic

**vPvB** - very Persistent, very Bioaccumulative

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

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

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

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

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

**ATE** - Acute Toxicity Estimate

**BCF** - Bioconcentration factor

**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

25-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.**

## 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**