

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

### 1.1. Product identifier

|                           |  |
|---------------------------|--|
| Product Description:      | <b>3,4-Dimethoxyphenylacetonitrile</b>           |
| Cat No. :                 | <b>A12003</b>                                    |
| Synonyms                  | Veratryl cyanide; Homoveratronicitrile           |
| CAS No                    | 93-17-4  |
| Molecular Formula         | C <sub>10</sub> H <sub>11</sub> N O <sub>2</sub> |
| 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.<br>(Part of Thermo Fisher Scientific)<br>Shore Road, Heysham<br>Lancashire, LA3 2XY,<br>United Kingdom<br>Office Tel: +44 (0) 1524 850506<br>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 3 (H301)  
Category 3 (H311)  
Category 3 (H331)

## **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**

H301 + H311 + H331 - Toxic if swallowed, in contact with skin or if inhaled

## **Precautionary Statements**

P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician  
P280 - Wear protective gloves/protective clothing/eye protection/face protection  
P312 - Call a POISON CENTER or doctor if you feel unwell  
P302 + P350 - IF ON SKIN: Gently wash with plenty of soap and water  
P304 + P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position 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 |
|---------------------------------|---------|-------------------|----------|---|
| 3,4-Dimethoxyphenylacetonitrile | 93-17-4 | EEC No. 202-225-1 | > 99     | Acute Tox. 3 (H301)<br>Acute Tox. 3 (H311)<br>Acute Tox. 3 (H331)                       |

REACH registration number

-

Full text of Hazard Statements: see section 16

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

### **4.1. Description of first aid measures**

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|   |  |
|---|--|
| <b>Eye Contact</b>                        | Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes.   |
| <b>Skin Contact</b>                       | Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes.  |
| <b>Ingestion</b>                          | Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Drink plenty of water. If possible drink milk afterwards.         |
| <b>Inhalation</b>                         | Remove from exposure, lie down. Remove to fresh air.   |
| <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**

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. 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**

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.

### **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

Ensure adequate ventilation.

#### 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 container tightly closed in a dry and well-ventilated place.

Technical Rules for Hazardous Substances (TRGS) 510 Class 6.1C  
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):

| Component                       | The United Kingdom   | European Union | Ireland |
|---------------------------------|--|----------------|---------|
| 3,4-Dimethoxyphenylacetonitrile | STEL: 15 mg/m <sup>3</sup> 15 min<br>TWA: 5 mg/m <sup>3</sup> 8 hr<br>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)

See values below.

| Component   | Fresh water           | Fresh water sediment            | Water Intermittent   | Microorganisms in sewage treatment | Soil (Agriculture)           |
|---|-----------------------|---------------------------------|----------------------|------------------------------------|------------------------------|
| 3,4-Dimethoxyphenylacetonitrile<br>93-17-4 (> 99) | PNEC =<br>0.09988mg/L | PNEC = 1.09mg/kg<br>sediment dw | PNEC =<br>0.9988mg/L | PNEC = 2.3mg/L                     | PNEC =<br>0.159mg/kg soil dw |

| Component                | Marine water | Marine water sediment | Marine water intermittent | Food chain | Air |
|--------------------------|--------------|-----------------------|---------------------------|------------|-----|
| 3,4-Dimethoxyphenylaceto | PNEC =       | PNEC =                |                           |            |     |

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|                             |              |                           |  |  |  |
|-----------------------------|--------------|---------------------------|--|--|--|
| nitrile<br>93-17-4 ( > 99 ) | 0.009988mg/L | 0.109mg/kg<br>sediment dw |  |  |  |
|-----------------------------|--------------|---------------------------|--|--|--|

## 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

### Personal protective equipment

#### Eye Protection

Wear safety glasses with side shields (or goggles) Goggles (European standard - EN 166)

#### Hand Protection

Protective gloves

| Glove material    | Breakthrough time                 | Glove thickness | EU standard | Glove comments        |
|-------------------|-----------------------------------|-----------------|-------------|-----------------------|
| Disposable gloves | See manufacturers recommendations | -               | EN 374      | (minimum requirement) |

#### 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

Wear a NIOSH/MSHA or European Standard EN 149 approved full-facepiece airline respirator in the positive pressure mode with emergency escape provisions. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

#### Large scale/emergency use

In case of insufficient ventilation, wear suitable respiratory equipment

#### 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. 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            | Solid                           |                                   |
| Appearance                | White                           |                                   |
| Odor                      | Odorless                        |                                   |
| Odor Threshold            | No data available               |                                   |
| Melting Point/Range       | 62 - 65 °C / 143.6 - 149 °F     |                                   |
| Softening Point           | No data available               |                                   |
| Boiling Point/Range       | 171 - 178 °C / 339.8 - 352.4 °F | @ 10 mmHg                         |
| Flammability (liquid)     | Not applicable                  | Solid                             |
| Flammability (solid,gas)  | No information available        |                                   |
| Explosion Limits          | No data available               |                                   |
| Flash Point               | 250 °C / 482 °F                 | Method - No information available |
| Autoignition Temperature  | 360 °C / 680 °F                 |                                   |
| Decomposition Temperature | No data available               |                                   |
| pH                        | No information available        |                                   |
| Viscosity                 | No data available               |                                   |

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|   |                               |
|---|-------------------------------|
| Water Solubility                        | Insoluble                     |
| 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             |
| Vapor Density                           | No data available (Air = 1.0) |
| Particle characteristics                | No data available             |

## 9.2. Other information

|                   |              |
|-------------------|--------------|
| Molecular Formula | C10 H11 N O2 |
| Molecular Weight  | 177.2        |

## 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. Excess heat.

### 10.5. Incompatible materials

Strong oxidizing agents. Strong acids. Strong bases.

### 10.6. Hazardous decomposition products

Nitrogen oxides (NOx). 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 | No acute toxicity information is available for this product |
|---------------------|---|

#### (a) acute toxicity;

|            |                   |
|------------|-------------------|
| Oral       | No data available |
| Dermal     | No data available |
| Inhalation | No data available |

| Component                       | LD50 Oral | LD50 Dermal               | LC50 Inhalation             |
|---------------------------------|-----------|---------------------------|-----------------------------|
| 3,4-Dimethoxyphenylacetonitrile | -         | LD50 > 2000 mg/kg ( Rat ) | LC50 > 5.5 mg/L ( Rat ) 4 h |

|                                |                   |
|--------------------------------|-------------------|
| (b) skin corrosion/irritation; | No data available |
|--------------------------------|-------------------|

|                                    |                   |
|------------------------------------|-------------------|
| (c) serious eye damage/irritation; | No data available |
|------------------------------------|-------------------|

|  |  |
|--|--|
| (d) respiratory or skin sensitization; |  |
|--|--|

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

|  |                          |
|--|--------------------------|
| <u>12.2. Persistence and degradability</u> | No information available |
|--|--------------------------|

|  |                          |
|--|--------------------------|
| <u>12.3. Bioaccumulative potential</u> | No information available |
|--|--------------------------|

|                               |                          |
|-------------------------------|--------------------------|
| <u>12.4. Mobility in soil</u> | No information available |
|-------------------------------|--------------------------|

|   |                                   |
|---|-----------------------------------|
| <u>12.5. Results of PBT and vPvB assessment</u> | 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

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## SECTION 13: DISPOSAL CONSIDERATIONS

### 13.1. Waste treatment methods

|  |   |
|--|---|
| <b>Waste from Residues/Unused Products</b> | Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification. |
| <b>Contaminated Packaging</b>              | Empty remaining contents. Dispose of in accordance with local regulations. Do not re-use empty containers.  |
| <b>European Waste Catalogue (EWC)</b>      | According to the European Waste Catalog, Waste Codes are not product specific, but application specific.  |
| <b>Other Information</b>                   | Waste codes should be assigned by the user based on the application for which the product was used.   |

## SECTION 14: TRANSPORT INFORMATION

### IMDG/IMO

|   |                              |
|---|------------------------------|
| <b>14.1. UN number</b>                  | UN2811                       |
| <b>14.2. UN proper shipping name</b>    | Toxic solid, organic, n.o.s. |
| <b>14.3. Transport hazard class(es)</b> | 6.1                          |
| <b>14.4. Packing group</b>              | III                          |

### ADR

|   |                              |
|---|------------------------------|
| <b>14.1. UN number</b>                  | UN2811                       |
| <b>14.2. UN proper shipping name</b>    | Toxic solid, organic, n.o.s. |
| <b>14.3. Transport hazard class(es)</b> | 6.1                          |
| <b>14.4. Packing group</b>              | III                          |

### IATA

|   |                               |
|---|-------------------------------|
| <b>14.1. UN number</b>                  | UN2811                        |
| <b>14.2. UN proper shipping name</b>    | TOXIC SOLID, ORGANIC, N.O.S.* |
| <b>14.3. Transport hazard class(es)</b> | 6.1                           |
| <b>14.4. Packing group</b>              | III                           |

|  |                                  |
|--|----------------------------------|
| <b>14.5. Environmental hazards</b>                                   | No hazards identified            |
| <b>14.6. Special precautions for user</b>                            | No special precautions required. |
| <b>14.7. Maritime transport in bulk according to IMO instruments</b> | 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)



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| Component                       | CAS No  | EINECS    | ELINCS | NLP | IECSC | TCSI | KECL | ENCS | ISHL |
|---------------------------------|---------|-----------|--------|-----|-------|------|------|------|------|
| 3,4-Dimethoxyphenylacetonitrile | 93-17-4 | 202-225-1 | -      | -   | -     | X    | -    | X    | X    |

| Component                       | CAS No  | TSCA | TSCA Inventory notification - Active-Inactive | DSL | NDSL | AICS | NZIoC | PICCS |
|---------------------------------|---------|------|---|-----|------|------|-------|-------|
| 3,4-Dimethoxyphenylacetonitrile | 93-17-4 | -    | -   | -   | -    | -    | -     | X     |

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) |
|---------------------------------|---------|---|---|---|
| 3,4-Dimethoxyphenylacetonitrile | 93-17-4 | -   | -   | -   |

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 |
|---------------------------------|---------|---|--|
| 3,4-Dimethoxyphenylacetonitrile | 93-17-4 | 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

See table for values

| Component                       | Germany - Water Classification (AwSV) | Germany - TA-Luft Class |
|---------------------------------|---------------------------------------|-------------------------|
| 3,4-Dimethoxyphenylacetonitrile | WGK1                                  |                         |

## 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

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H331 - Toxic if inhaled

## 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

**Key literature references and sources for data**

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

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

**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)

## 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

**Revision Date**

04-Feb-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**