

# SAFETY DATA SHEET

according to the OSHA  
Hazard Communication Standard

Version 6.8  
Revision Date 07/10/2026  
Print Date 07/11/2026

## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

Product name : 4-Methoxyphenylacetone nitrile

Product Number : 169986  
Brand : Aldrich  
CAS-No. : 104-47-2

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

Identified uses : Laboratory chemicals, Synthesis of substances

Restrictions on use : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

### 1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-  
527-3887 CHEMTREC (International) 24  
Hours/day; 7 Days/week

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## SECTION 2. HAZARDS IDENTIFICATION

**GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)**

**Hazards for the product as supplied**

Acute toxicity (Oral) : Category 3

Short-term (acute) aquatic hazard : Category 3

Long-term (chronic) aquatic hazard : Category 3

#### Other hazards

None known.

#### GHS label elements

Hazard pictograms :



Signal word : Danger

Hazard statements : H301 Toxic if swallowed.  
H412 Harmful to aquatic life with long lasting effects.

Precautionary statements : **Prevention:**  
P264 Wash skin thoroughly after handling.  
P270 Do not eat, drink or smoke when using this product.  
P273 Avoid release to the environment.  
**Response:**  
P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.  
**Storage:**  
P405 Store locked up.  
**Disposal:**  
P501 Dispose of contents/ container to an approved waste disposal plant.

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### SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 104-47-2

#### Components

| Chemical name              | CAS No./Unique ID | Concentration (% w/w) | Trade secret |
|----------------------------|-------------------|-----------------------|--------------|
| 4-Methoxyphenylacetonitril | 104-47-2*         | >= 90 - <= 100        | -            |

Aldrich - 169986

Page 2 of 13

\* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

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## SECTION 4. FIRST AID MEASURES

|                                                             |                                                                                                                                                                                                                                                                                                                                                           |
|-------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| General advice                                              | : Show this safety data sheet to the doctor in attendance.                                                                                                                                                                                                                                                                                                |
| If inhaled                                                  | : After inhalation: fresh air.                                                                                                                                                                                                                                                                                                                            |
| In case of skin contact                                     | : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.                                                                                                                                                                                                                                                 |
| In case of eye contact                                      | : After eye contact: rinse out with plenty of water. Remove contact lenses.                                                                                                                                                                                                                                                                               |
| If swallowed                                                | : If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible. |
| Most important symptoms and effects, both acute and delayed | : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11                                                                                                                                                                                                                                     |
| Protection of first-aiders                                  | : For personal protection see section 8.                                                                                                                                                                                                                                                                                                                  |
| Notes to physician                                          | : No data available                                                                                                                                                                                                                                                                                                                                       |

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## SECTION 5. FIREFIGHTING MEASURES

|                                       |                                                                                                                          |
|---------------------------------------|--------------------------------------------------------------------------------------------------------------------------|
| Unsuitable extinguishing media        | : For this substance/mixture no limitations of extinguishing agents are given.                                           |
| Specific hazards during fire fighting | : Vapours are heavier than air and may spread along floors.<br><br>Forms explosive mixtures with air on intense heating. |
| Hazardous combustion products         | : Carbon oxides                                                                                                          |

## Nitrogen oxides (NO<sub>x</sub>)

|                                                |                                                                                                                                                                      |
|------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Specific extinguishing methods                 | : No data available                                                                                                                                                  |
| Further information                            | : Suppress (knock down) gases/vapours/mists with a water spray jet.<br>Prevent fire extinguishing water from contaminating surface water or the ground water system. |
| Special protective equipment for fire-fighters | : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.      |

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### SECTION 6. ACCIDENTAL RELEASE MEASURES

|                                                                     |                                                                                                                                                                                                                                                                                                    |
|---------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Personal precautions, protective equipment and emergency procedures | : Advice for non-emergency personnel:<br>Do not breathe vapours, aerosols.<br>Avoid substance contact.<br>Ensure adequate ventilation.<br>Evacuate the danger area, observe emergency procedures, consult an expert.<br>Advice for emergency responders:<br>For personal protection see section 8. |
| Environmental precautions                                           | : Do not let product enter drains.                                                                                                                                                                                                                                                                 |
| Methods and materials for containment and cleaning up               | : Cover drains. Collect, bind, and pump off spills.<br>Observe possible material restrictions (see sections 7 and 10).<br>Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.                                                         |

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### SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

|                                           |                                                                                                                                           |
|-------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Further information on storage conditions | : Tightly closed.<br>Keep in a well-ventilated place.<br>Keep locked up or in an area accessible only to qualified or authorised persons. |
| Storage class                             | : 6.1C, Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects                                       |

Recommended storage temperature : Recommended storage temperature see product label.

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## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

**Engineering measures** : No data available

### Personal protective equipment

Respiratory protection : required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

### Hand protection

Remarks : required

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).  
Safety glasses

Skin and body protection : protective clothing

Hygiene measures : Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : liquid

|                                                     |                                            |
|-----------------------------------------------------|--------------------------------------------|
| Colour                                              | : No data available                        |
| Odour                                               | : No data available                        |
| Odour Threshold<br>pH                               | : No data available<br>: No data available |
| Melting point                                       | : No data available                        |
| Boiling point/boiling range                         | : 547 - 549 °F / 286 - 287 °C              |
| Flash point                                         | : 243 °F / 117 °C<br>DIN 51758             |
| Evaporation rate                                    | : No data available                        |
| Flammability (solid, gas)                           | : No data available                        |
| Flammability (liquids)                              | : No data available                        |
| Burning rate                                        | : No data available                        |
| Upper explosion limit /<br>Upper flammability limit | : 9.4 %(V)                                 |
| Lower explosion limit /<br>Lower flammability limit | : 1.2 %(V)                                 |
| Vapour pressure                                     | : No data available                        |
| Relative vapour density                             | : No data available                        |
| Relative density                                    | : No data available                        |
| Density                                             | : 1.085 g/mL (77 °F / 25 °C)               |
| Water solubility                                    | : No data available                        |
| Partition coefficient: n-<br>octanol/water          | : No data available                        |
| Autoignition temperature                            | : No data available                        |
| Decomposition<br>temperature                        | : No data available                        |
| Viscosity, dynamic                                  | : No data available                        |
| Viscosity, kinematic                                | : No data available                        |

Aldrich - 169986

Page 6 of 13

|                          |                     |
|--------------------------|---------------------|
| Flow time                | : No data available |
| Explosive properties     | : No data available |
| Oxidizing properties     | : No data available |
| Molecular weight         | : 147.17 g/mol      |
| Particle characteristics |                     |
| Particle size            | : No data available |

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## SECTION 10. STABILITY AND REACTIVITY

|                                    |                                                                                                                                                 |
|------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| Reactivity                         | : Forms explosive mixtures with air on intense heating.<br><br>A range from approx. 15 Kelvin below the flash point is to be rated as critical. |
| Chemical stability                 | : The product is chemically stable under standard ambient conditions (room temperature) .                                                       |
| Possibility of hazardous reactions | : No data available                                                                                                                             |
| Conditions to avoid                | : Strong heating.                                                                                                                               |
| Incompatible materials             | : No data available                                                                                                                             |
| Hazardous decomposition products   | : In the event of fire: see section 5                                                                                                           |

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## SECTION 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - 100 - 215 mg/kg

Remarks: (External MSDS)

Oral: absorption

Symptoms: Cough, Shortness of breath

Dermal: No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

(OECD Test Guideline 404)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

**Respiratory or skin sensitization**

No data available

**Germ cell mutagenicity**

No data available

**Carcinogenicity**

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

RTECS: AM0810000

Treat as cyanide poisoning., Always have on hand a cyanide first-aid kit, together with proper instructions., Nausea, Vomiting, Diarrhoea, Headache, Dizziness, Rash, Cyanosis

After absorption:

Dizziness

Nausea

Vomiting

Other information

The following applies to cyanogen compounds/ nitriles in general: utmost caution! Release of hydrocyanic acid is possible - blockade of cellular respiration. Cardiovascular disorders, dyspnoea, unconsciousness.

Further data:

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

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## SECTION 12. ECOLOGICAL INFORMATION

### Ecotoxicity

#### Components:

##### **4-Methoxyphenylacetoneitrile:**

Toxicity to fish : LC50 (Leuciscus idus (Golden orfe)): 100 mg/l  
Exposure time: 96 h  
Remarks: (External MSDS)

### Ecotoxicology Assessment

Chronic aquatic toxicity : Harmful to aquatic life with long lasting effects.

### Persistence and degradability

#### Components:

##### **4-Methoxyphenylacetoneitrile:**

Biodegradability : Result: Partially biodegradable.

### Bioaccumulative potential

No data available

### Mobility in soil

No data available

### Other adverse effects

#### Components:

##### **4-Methoxyphenylacetoneitrile:**

Additional ecological information : Discharge into the environment must be avoided.

### Endocrine disrupting properties

No data available

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## SECTION 13. DISPOSAL CONSIDERATIONS

### Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## SECTION 14. TRANSPORT INFORMATION

### International Regulations

**IATA-DGR**

UN/ID No. : UN 3276  
Proper shipping name : Nitriles, liquid, toxic, n.o.s.  
(4-Methoxyphenylacetonitrile)  
Class : 6.1  
Packing group : III  
Labels : Division 6.1 - Toxic substances  
Packing instruction (cargo : 663  
aircraft)  
Packing instruction : 655  
(passenger aircraft)

**IMDG-Code**

UN number : UN 3276  
Proper shipping name : NITRILES, LIQUID, TOXIC, N.O.S.  
(4-Methoxyphenylacetonitrile)  
Class : 6.1  
Packing group : III  
Labels : 6.1  
EmS Code : F-A, S-A  
Marine pollutant : no

**Transport in bulk according to IMO instruments**

Not applicable for product as supplied.

**National Regulations****49 CFR**

UN/ID/NA number : UN 3276  
Proper shipping name : Nitriles, liquid, toxic, n.o.s.  
(4-Methoxyphenylacetonitrile)  
Class : 6.1  
  
Packing group : III  
Labels : Division 6.1 - Toxic substances  
ERG Code : 151  
Marine pollutant : no  
Poison Inhalation Hazard : No

**Special precautions for user**

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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**SECTION 15. REGULATORY INFORMATION****CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

**SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

## **SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : Acute Health Hazard

**SARA 313** : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

## **US State Regulations**

### **Massachusetts Right To Know**

No components are subject to the Massachusetts Right to Know Act.

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No components are subject to the Massachusetts Right to Know Act.

### **Pennsylvania Right To Know**

4-Methoxyphenylacetonitrile 104-47-2

### **Pennsylvania Right To Know**

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### **Maine Chemicals of High Concern**

Product does not contain any listed chemicals

### **Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

### **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

### **New Jersey Right To Know**

4-Methoxyphenylacetonitrile 104-47-2

### **The components of this product are reported in the following inventories:**

US TSCA : All substances listed as active on the TSCA inventory

### **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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## **SECTION 16. OTHER INFORMATION**

### **Full text of other abbreviations**

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response,

Aldrich - 169986

Page 11 of 13

Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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