



# MATERIAL SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Date of issue: 02/05/2013

Version 1.0

## SECTION 1. Identification

### Product identifier

Product number	821234
Product name	(4-Methoxyphenyl)acetonitrile for synthesis

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

Identified uses	Chemical for synthesis
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### Details of the supplier of the safety data sheet

Company	EMD Millipore Corporation   290 Concord Road, Billerica, MA 01821, United States of America   SDS Phone Support: +1-978-715-1335   General Inquiries: +1-978-715-4321   Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5)  e-mail: mm_sds@merckgroup.com
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Emergency telephone	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

Acute toxicity, Category 3, Oral, H301

Chronic aquatic toxicity, Category 3, H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

### GHS-Labeling

*Hazard pictograms*



*Signal Word*  
Danger

*Hazard Statements*

H301 Toxic if swallowed.

H412 Harmful to aquatic life with long lasting effects.

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## *Precautionary Statements*

P260 Do not breathe vapors.

P273 Avoid release to the environment.

P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

## **OSHA Hazards**

This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).

## **Other hazards**

None known.

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## **SECTION 3. Composition/information on ingredients**

Formula	4-(CH <sub>3</sub> O)C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> CN	C <sub>9</sub> H <sub>9</sub> NO (Hill)
CAS-No.	104-47-2	
Molar mass	147.18 g/mol	

## **Hazardous ingredients**

*Chemical Name ( Concentration)*

CAS-No.

4-Methoxyphenylacetonitrile ( >= 90 % - <= 100 % )  
104-47-2

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## **SECTION 4. First aid measures**

### **Description of first-aid measures**

#### *Inhalation*

After inhalation: fresh air.

#### *Skin contact*

After skin contact: wash off with plenty of water. Remove contaminated clothing.

#### *Eye contact*

After eye contact: rinse out with plenty of water.

#### *Ingestion*

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.

Never give anything by mouth to an unconscious person.

### **Most important symptoms and effects, both acute and delayed**

Dizziness, Nausea, Vomiting

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.

### **Indication of any immediate medical attention and special treatment needed**

No information available.

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### SECTION 5. Fire-fighting measures

#### Extinguishing media

##### *Suitable extinguishing media*

Water, Carbon dioxide (CO<sub>2</sub>), Foam, Dry powder

##### *Unsuitable extinguishing media*

For this substance/mixture no limitations of extinguishing agents are given.

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

Combustible material, Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapors possible in the event of fire.

Fire may cause evolution of:

nitrogen oxides, Hydrogen cyanide (hydrocyanic acid)

#### Advice for firefighters

##### *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.

##### *Further information*

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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### SECTION 6. Accidental release measures

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

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

#### Environmental precautions

Do not empty into drains.

#### Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7 and 10).

Take up with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

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### SECTION 7. Handling and storage

#### Precautions for safe handling

Observe label precautions.

#### Conditions for safe storage, including any incompatibilities

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Store at +15°C to +25°C (+59°F to +77°F).

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## SECTION 8. Exposure controls/personal protection

### Exposure limit(s)

Contains no substances with occupational exposure limit values.

### Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

### Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

### Hygiene measures

Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance. Work under hood. Do not inhale substance/mixture.

### Eye/face protection

Safety glasses

### Hand protection

Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

### Other protective equipment:

protective clothing

### Respiratory protection

required when vapors/aerosols are generated.

Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

## SECTION 9. Physical and chemical properties

Physical state	liquid
Color	yellow
Odor	weak
Odor Threshold	No information available.
pH	4.5 at 100 g/l 68 °F ( 20 °C) suspension
Melting point	8 °C
Boiling point/boiling range	547 - 549 °F ( 286 - 287 °C) at 1,013 hPa

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Flash point	243 °F ( 117 °C) Method: DIN 51758
Evaporation rate	No information available.
Flammability (solid, gas)	not applicable
Lower explosion limit	1.2 %(V)
Upper explosion limit	9.4 %(V)
Vapor pressure	No information available.
Relative vapor density	No information available.
Relative density	1.085 g/cm <sup>3</sup> at 68 °F ( 20 °C)
Water solubility	0.01 g/l at 68 °F ( 20 °C)
Partition coefficient: n-octanol/water	log Pow: 1.7 (experimental) (Lit.) Bioaccumulation is not expected (log Pow <1).
Autoignition temperature	No information available.
Decomposition temperature	> 662 °F ( > 350 °C)
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Ignition temperature	860 °F ( 460 °C) Method: DIN 51794

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### SECTION 10. Stability and reactivity

#### Reactivity

Forms explosive mixtures with air on intense heating.

#### Chemical stability

Sensitive to air.

#### Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents, strong reducing agents, Strong acids, strong alkalis

#### Conditions to avoid

Strong heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

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## Incompatible materials

no information available

## Hazardous decomposition products

in the event of fire: See section 5.

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## SECTION 11. Toxicological information

### Information on toxicological effects

#### *Likely route of exposure*

Eye contact, Skin contact

#### *Acute oral toxicity*

LD50 rat: 100 - 215 mg/kg (External MSDS)

absorption

#### *Acute inhalation toxicity*

Symptoms: Cough, Shortness of breath

#### *Skin irritation*

rabbit

Result: No irritation

OECD Test Guideline 404

#### *Eye irritation*

rabbit

Result: No eye irritation

OECD Test Guideline 405

#### *Specific target organ systemic toxicity - single exposure*

The substance or mixture is not classified as specific target organ toxicant, single exposure.

#### *Specific target organ systemic toxicity - repeated exposure*

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

#### *Aspiration hazard*

Regarding the available data the classification criteria are not fulfilled.

### Carcinogenicity

IARC	No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
OSHA	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.
NTP	No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
ACGIH	No ingredient of this product present at levels greater than or

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equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

### Further information

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

*Toxicity to fish*

LC50 *Leuciscus idus* (Golden orfe): 100 mg/l; 96 h (External MSDS)

### Persistence and degradability

*Biodegradability*

Partially biodegradable.

### Bioaccumulative potential

*Partition coefficient: n-octanol/water*

log Pow: 1.7

(experimental)

(Lit.) Bioaccumulation is not expected (log Pow <1).

### Mobility in soil

No information available.

### Other adverse effects

*Additional ecological information*

Discharge into the environment must be avoided.

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## SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

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## SECTION 14. Transport information

### Land transport (DOT)

UN number	UN 3276
Proper shipping name	NITRILES, TOXIC, LIQUID, N.O.S. ( 4-METHOXYPHENYLACETONITRILE)
Class	6.1
Packing group	III
Environmentally hazardous	--

### Air transport (IATA)

UN number	UN 3276
Proper shipping name	NITRILES, LIQUID, TOXIC, N.O.S. ( 4-METHOXYPHENYLACETONITRILE)
Class	6.1
Packing group	III
Environmentally hazardous	--
Special precautions for user	no

### Sea transport (IMDG)

UN number	UN 3276
Proper shipping name	NITRILES, TOXIC, LIQUID, N.O.S. ( 4-METHOXYPHENYLACETONITRILE)
Class	6.1
Packing group	III
Environmentally hazardous	--
Special precautions for user	yes
EmS	F-A S-A

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## SECTION 15. Regulatory information

### United States of America

#### OSHA Hazards

Toxic by ingestion

This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS, and may deviate from the GHS information on the label and in section 2.

#### SARA 311/312 Hazards

Acute Health Hazard

#### SARA 313

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.



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## SARA 302

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

## Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

## Massachusetts Right To Know

Remarks

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

## Pennsylvania Right To Know

*Ingredients*

4-Methoxyphenylacetonitrile

## New Jersey Right To Know

*Ingredients*

4-Methoxyphenylacetonitrile

## Notification status

TSCA:

On TSCA Inventory

DSL:

This product contains one or several components listed in the Canadian NDSL.

*Ingredients*

4-Methoxyphenylacetonitrile

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## SECTION 16. Other information

### Training advice

Provide adequate information, instruction and training for operators.

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

H301

Toxic if swallowed.

H412

Harmful to aquatic life with long lasting effects.

### Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at [www.wikipedia.org](http://www.wikipedia.org).

Date of issue:02/05/2013

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The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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