

## Chemical Safety Data Sheet MSDS / SDS

## 4-Methoxybenzyl cyanide

Revision Date:2025-02-01 Revision Number:1

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

## Product identifier

Product name : 4-Methoxybenzyl cyanide  
CBnumber : CB1192481  
CAS : 104-47-2  
EINECS Number : 203-206-0  
Synonyms : 2-(4-methoxyphenyl)acetonitrile,4-methoxyphenyl

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

## Company Identification

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 400-158-6606

## SECTION 2: Hazards identification

## GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

## Precautionary statements

P405 Store locked up.  
P321 Specific treatment (see ... on this label).  
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.  
P270 Do not eat, drink or smoke when using this product.  
P264 Wash skin thoroughly after handling.  
P264 Wash hands thoroughly after handling.

## Hazard statements

H412 Harmful to aquatic life with long lasting effects  
H402 Harmful to aquatic life  
H301 Toxic if swallowed

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## SECTION 3: Composition/information on ingredients

### Substance

Product name	: 4-Methoxybenzyl cyanide
Synonyms	: 2-(4-methoxyphenyl)acetonitrile, 4-methoxyphenyl
CAS	: 104-47-2
EC number	: 203-206-0
MF	: C <sub>9</sub> H <sub>9</sub> NO
MW	: 147.17

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## SECTION 4: First aid measures

### Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

#### In case of eye contact

Flush eyes with water as a precaution.

#### If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 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

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

No data available

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## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### Special hazards arising from the substance or mixture

Carbon oxides, Nitrogen oxides (NO<sub>x</sub>)

### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

## Further information

No data available

## NFPA 704



**HEALTH 3** Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

**FIRE 1** Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

**REACT 0** Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N2](#))

☐ SPEC.

☐ HAZ.

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

For personal protection see section 8.

### Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

### Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

### Reference to other sections

For disposal see section 13.

## SECTION 7: Handling and storage

### Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. For precautions see section 2.2.

### Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Store in cool place.

### Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## SECTION 8: Exposure controls/personal protection

### control parameter

#### Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

### Exposure controls

#### Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

#### Personal protective equipment

##### Eye/face protection

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

##### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

##### Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

##### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	liquid
Odour	No data available
Odour Threshold	No data available
pH	4.5 (100g/l, H <sub>2</sub> O, 20 °C)suspension

Melting point/freezing point	8 °C
Initial boiling point and boiling range	286 - 287 °C
Flash point	117 °C - DIN 51758
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	Upper explosion limit: 9,4 %(V) Lower explosion limit: 1,2 %(V)
Vapour pressure	No data available
Vapour density	No data available
Relative density	1,085 g/mL at 25 °C
Water solubility	0.01g/l
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

#### Other safety information

No data available

## SECTION 10: Stability and reactivity

#### Reactivity

No data available

#### Chemical stability

Stable under recommended storage conditions.

#### Possibility of hazardous reactions

No data available

#### Conditions to avoid

No data available

#### Incompatible materials

No data available

#### Hazardous decomposition products

Other decomposition products - No data available

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx)

In the event of fire: see section 5

## SECTION 11: Toxicological information

### Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - 100 - 215 mg/kg Remarks: (External MSDS) absorption

#### 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 sensitisation Germ cell mutagenicity 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.

#### Reproductive toxicity

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

Acute inhalation toxicity - Cough, Shortness of breath

#### 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

### Toxicity

#### Toxicity to fish

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

#### Persistence and degradability

Biodegradability Result: - Partially biodegradable.

#### Bioaccumulative potential

#### Mobility in soil

#### Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

#### **Other adverse effects**

Harmful to aquatic life with long lasting effects. Discharge into the environment must be avoided.

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## **SECTION 13: Disposal considerations**

#### **Waste treatment methods**

##### **Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

##### **Contaminated packaging**

Dispose of as unused product.

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## **SECTION 14: Transport information**

#### **UN number**

ADR/RID: 3276 IMDG: 3276 IATA: 3276

#### **UN proper shipping name**

ADR/RID: NITRILES, LIQUID, TOXIC, N.O.S. (4-Methoxyphenylacetoneitrile) IMDG: NITRILES, LIQUID, TOXIC, N.O.S. (4-Methoxyphenylacetoneitrile) IATA: Nitriles, liquid, toxic, n.o.s. (4-Methoxyphenylacetoneitrile)

#### **Transport hazard class(es)**

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

#### **Packaging group**

ADR/RID: III IMDG: III IATA: III

#### **Environmental hazards**

ADR/RID: no IMDG Marine pollutant: no IATA: no

#### **Special precautions for user**

No data available

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## **SECTION 15: Regulatory information**

#### **Safety, health and environmental regulations/legislation specific for the substance or mixture**

## Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

## Measures for Environmental Management of New Chemical Substances

Korea Existing Chemicals List (KECL):Listed. website: <http://ncis.nier.go.kr>

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

EC Inventory:Listed.

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: <https://www.mee.gov.cn/>

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>

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## SECTION 16: Other information

### Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

### References

【1】CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

【2】ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

【3】ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

【4】eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:  
[http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)

【5】ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

【6】Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

【7】HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

【8】IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

【9】IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

【10】Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

### Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.