

## Chemical Safety Data Sheet MSDS / SDS

**4-Iodo-3-(trifluoromethyl)benzonitrile**Revision Date:2023-11-29 Revision Number:1

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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name : 4-Iodo-3-(trifluoromethyl)benzonitrile  
CBnumber : CB01114595  
CAS : 161320-00-9

**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

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**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

**Precautionary statements**

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.  
Continuerinsing.

**Hazard statements**

H302 Harmful if swallowed  
H319 Causes serious eye irritation

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**SECTION 3: Composition/information on ingredients****Substance**

Product name : 4-Iodo-3-(trifluoromethyl)benzonitrile  
Synonyms : 4-iodo-3-(trifluoromethyl)benzonitrile

CAS	: 161320-00-9
MF	: C8H3F3IN
MW	: 297.02

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## SECTION 4: First aid measures

### Description of first aid measures

#### General advice

Show this material 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

After swallowing: immediately make victim drink water (two glasses at most). 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

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

#### Unsuitable extinguishing media

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

### Special hazards arising from the substance or mixture

Carbon oxides Nitrogen oxides (NO<sub>x</sub>) Hydrogen fluoride Hydrogen iodide Combustible.

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

### Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

### 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: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

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. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

### Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### Precautions for safe handling

For precautions see section 2.2.

### Conditions for safe storage, including any incompatibilities

### Storage conditions

Tightly closed. Dry.

### 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

#### Personal protective equipment

##### Eye/face protection

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

##### Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested: KCL 741 Dermatrill? L

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested: KCL 741 Dermatrill? L

### Body Protection

protective clothing

### Respiratory protection

required when dusts 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 P2

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.

### Control of environmental exposure

Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	solid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 92 - 99 °C
Initial boiling point and boiling range	271 °C
Flash point	118 °C
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available
Relative density	No data available
Water solubility	No data available
Partition coefficient: n-octanol/water	log Pow: 3,449

Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
Explosive properties	No data available
Oxidizing properties	No data available

### Other safety information

No data available

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## SECTION 10: Stability and reactivity

### Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### Possibility of hazardous reactions

No data available

### Conditions to avoid

no information available

### Incompatible materials

Strong oxidizing agents

### Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### Information on toxicological effects

#### Acute toxicity

Oral

Inhalation

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

Prolonged or repeated exposure may cause allergic reactions in certain sensitive individuals. The preceding data, or interpretation of data, was determined using Quantitative Structure Activity Relationship (QSAR) modeling.

**Germ cell mutagenicity**

No data available

**Carcinogenicity**

No data available

**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

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## SECTION 12: Ecological information

**Toxicity**

No data available

**Persistence and degradability**

No data available

**Bioaccumulative potential**

No data available

**Mobility in soil**

No data available

**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**

No data available

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## SECTION 13: Disposal considerations

**Waste treatment methods****Product**

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14: Transport information

**UN number**

ADR/RID: - IMDG: - IATA: -

**UN proper shipping name**

ADR/RID: Not dangerous goods IMDG: Not dangerous goods IATA: Not dangerous goods

**Transport hazard class(es)**

ADR/RID: - IMDG: - IATA: -

**Packaging group**

ADR/RID: - IMDG: - IATA: -

**Environmental hazards**

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

**Special precautions for user****Further information**

Not classified as dangerous in the meaning of transport regulations.

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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**

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

EC Inventory:Not Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Not Listed. website: <https://echa.europa.eu/>

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: <https://www.epa.govt.nz/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: <https://emb.gov.ph/>

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: <https://www.epa.gov/>

Vietnam National Chemical Inventory:Not Listed. website: <https://chemicaldata.gov.vn/>

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## SECTION 16: Other information

**Abbreviations and acronyms**

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

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

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

STEL: Short term exposure limit

TWA: Time Weighted Average

## 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.