

## Chemical Safety Data Sheet MSDS / SDS

**3-(Trifluoromethyl)benzoic acid**

Revision Date:2024-12-21 Revision Number:1

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

Product name : 3-(Trifluoromethyl)benzoic acid  
CBnumber : CB1306657  
CAS : 454-92-2  
EINECS Number : 207-230-2  
Synonyms : 3-(Trifluoromethyl)benzoic acid,3-trifluoromethylbenzoate

**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)

**Precautionary statements**

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.  
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.  
Continuerinsing.  
P405 Store locked up.

**Hazard statements**

H335 May cause respiratory irritation  
H319 Causes serious eye irritation  
H315 Causes skin irritation

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

## Substance

Product name	: 3-(Trifluoromethyl)benzoic acid
Synonyms	: 3-(Trifluoromethyl)benzoic acid,3-trifluoromethylbenzoate
CAS	: 454-92-2
EC number	: 207-230-2
MF	: C8H5F3O2
MW	: 190.12

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## SECTION 4: First aid measures

### Description of first aid measures

#### If inhaled

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

#### In case of skin contact

Wash off with soap and plenty of water.

#### 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.

### 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, Hydrogen fluoride

### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### Further information

No data available

### NFPA 704



HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

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

Avoid dust formation. Avoid breathing vapours, mist or gas.

For personal protection see section 8.

### Environmental precautions

No special environmental precautions required.

### Methods and materials for containment and cleaning up

Sweep up and shovel. 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

Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

### Conditions for safe storage, including any incompatibilities

Store in cool place. Keep container tightly closed in a dry and well-ventilated 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

General industrial hygiene practice.

#### 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).

##### 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.

Full contact

Material: Nitrile rubber

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

Material tested: Dermatril? (KCL 740 / Aldrich Z677272, Size M)

Splash contact Material: Nitrile rubber

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

Material tested: Dermatril? (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

##### Body Protection

Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### Respiratory protection

Respiratory protection is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

##### Control of environmental exposure

No special environmental precautions required.

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## SECTION 9: Physical and chemical properties

## Information on basic physicochemical properties

Appearance	beige crystalline
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 104 - 106 °C - lit.
Initial boiling point and boiling range	238,5 °C at 1033 hPa - lit.
Flash point	237-240°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	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

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## 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

Oxidizing agents, Reducing agents, Bases

## Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen fluoride

Other decomposition products - No data available In the event of fire: see section 5

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## SECTION 11: Toxicological information

### Information on toxicological effects

#### Acute toxicity

No data available

#### Skin corrosion/irritation

#### Serious eye damage/eye irritation Respiratory or skin sensitisation

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.

#### 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

#### Additional Information

RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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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

Offer surplus and non-recyclable solutions to a licensed disposal company.

#### Contaminated packaging

Dispose of as unused product.

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## SECTION 14: Transport information

### UN number

ADR/RID: - IMDG: - IATA: -

14.2 UN proper shipping name ADR/RID: Not dangerous goods IMDG: Not dangerous goods IATA: Not dangerous goods

14.3 Transport hazard class(es)

ADR/RID: - IMDG: - IATA: -

14.4 Packaging group

ADR/RID: - IMDG: - IATA: -

14.5 Environmental hazards

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

14.6 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

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

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

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

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

EC Inventory:Listed.

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

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not 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.