Chemical Safety Data Sheet MSDS / SDS

3-FLUORO-4-METHYLBENZENESULFONYL CHLORIDE

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

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

Product identifier

| Product name | : 3-FLUORO-4-METHYLBENZENESULFONYL CHLORIDE | | | |
|---|---|--|--|--|
| CBnumber | : CB6173467 | | | |
| CAS | : 90260-13-2 | | | |
| Synonyms | : 3-Fluoro-4-methylbenzenesulfonyl chloride, 3-fluoro-4-methylbenzene-1-sulfonyl chloride | | | |
| 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

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

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

Continuerinsing.

P310 Immediately call a POISON CENTER or doctor/physician.

P405 Store locked up.

Hazard statements

H314 Causes severe skin burns and eye damage

H318 Causes serious eye damage

SECTION 3: Composition/information on ingredients

Substance

| 4-METHYLBENZENESULFONYL CHLORIDE |
|---|
| nethylbenzenesulfonyl chloride,3-fluoro-4-methylbenzene-1-sulfonyl chloride |
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SECTION 4: First aid measures

Description of first aid measures

General advice

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

lf inhaled

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

In case of skin contact

Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. 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

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, Sulfur oxides, Hydrogen chloride gas, Hydrogen fluoride

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

NFPA 704

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| | 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. <u>mineral oil</u> , ammonia) |
| | REACT | 0 | Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, <u>N2</u>) |
| | SPEC. | | |
| | HAZ. | | |

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. For personal protection see section 8.

Environmental precautions

Do not let product enter drains.

Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. 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

Avoid formation of dust and aerosols.

Provide appropriate exhaust ventilation at places where dust is formed.Normal measures for preventive fire protection.

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. Moisture sensitive.

Specific end use(s)

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

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

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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.

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 EC 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

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 particle respirator type N100 (US) or type P3 (EN 143) 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

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

| Appearance | white solid |
|---|--|
| Odour | No data available |
| Odour Threshold | No data available |
| рН | No data available |
| Melting point/freezing point | Melting point/range: 46 - 50 °C - lit. |
| Initial boiling point and boiling range | No data available |
| Flash point | 110 °C - closed cup |
| Evaporation rate | No data available |
| Flammability (solid, gas) | No data available |
| Upper/lower flammability or explosive | No data available |
| limits | |
| 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

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

Avoid moisture.

Incompatible materials

Strong oxidizing agents

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Sulfur oxides, Hydrogen chloride gas, Hydrogen fluoride Other decomposition products - No data available In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity No data available Skin corrosion/irritation No data available Serious eye damage/eye irritation No data available Respiratory or skin sensitization No data available Germ cell mutagenicity No data available 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. **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** Cough, Shortness of breath, Headache, Nausea, Vomiting

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

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

Other adverse effects

No data available

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 3261 IMDG: 3261 IATA: 3261

UN proper shipping name

ADR/RID: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (3-Fluoro-4-

methylbenzenesulfonyl chloride)

IMDG: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (3-Fluoro-4-

methylbenzenesulfonyl chloride)

IATA: Corrosive solid, acidic, organic, n.o.s. (3-Fluoro-4-methylbenzenesulfonyl chloride)

Transport hazard class(es)

ADR/RID: 8 IMDG: 8 IATA: 8

Packaging group

ADR/RID: II IMDG: II IATA: II

Environmental hazards

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

Special precautions for user

No data available

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

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

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

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/

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

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

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

EC Inventory:Not Listed.

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] ChemlDplus, 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

- [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.