

Chemical Safety Data Sheet MSDS / SDS

1-methyl-3-phenyl-5-[3-(trifluoromethyl)phenyl]-4-pyridone SDS

Revision Date:2024-04-25 Revision Number:1

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

Product name: 1-methyl-3-phenyl-5-[3-(trifluoromethyl)phenyl]-4-pyridone

CAS: 59756-60-4

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.in

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SECTION 2: Hazards identification**Classification of the substance or mixture**

Acute toxicity - Category 3, Dermal

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 2

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

Hazard statement(s)

H311 Toxic in contact with skin

H411 Toxic to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

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

P273 Avoid release to the environment.

Response

P302+P352 IF ON SKIN: Wash with plenty of water/...

P316 Get emergency medical help immediately.

P321 Specific treatment (see ... on this label).

P361+P364 Take off immediately all contaminated clothing and wash it before reuse.

P391 Collect spillage.

Storage

P405 Store locked up.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	1-methyl-3-phenyl-5-[3-(trifluoromethyl)phenyl]-4-pyridone
Common names and synonyms:	1-methyl-3-phenyl-5-[3-(trifluoromethyl)phenyl]-4-pyridone
CAS number:	59756-60-4
EC number:	261-916-6
Concentration:	100%

SECTION 4: First aid measures**Description of necessary first-aid measures****If inhaled**

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

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

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms/effects, acute and delayed

no data available

Indication of immediate medical attention and special treatment needed, if necessary**Absorption, Distribution and Excretion**

In a rat metabolism study/... Preliminary study: Group A, 2 male (M)/2 female (F) exposed to a single oral dose of [14C]fluridone (...radiopurity 99.8%; for test solutions [14C]fluridone was mixed w/[12C]fluridone, ...100% purity; test substance was suspended in

1% sodium carboxymethyl cellulose [CMC]) at ~10 mg/kg. Group B, 1M/1F exposed to a single oral dose at ~1000 mg/kg. Urine, feces and cage rinses were collected daily for 7 days (because expired (trapped) $^{14}\text{CO}_2$ accounted for <1% of the dose after 24 hr, further $^{14}\text{CO}_2$ measurements were discontinued). Definitive study: Group C, vehicle controls, 2M/2F exposed to a single oral dose of 1% CMC. Group D, 5M/5F exposed to a single oral dose at ~7.4 mg/kg. Group E, 7M/7F exposed to ~10 mg/kg unlabeled fluridone once daily for 14 days, then 5M/5F exposed on day 15 to ~10 mg/kg [^{14}C]fluridone. Group F, 5M/5F exposed to a single oral dose at ~900 mg/kg. ...Clinical signs (lack of mobility, abnormal and rapid head movement, squinting, loss of balance and cage biting) occurred only at the HD (Groups B and F), clearing within 24 hr. Results, Group A: by 7 days, 12.52%/12.89% (M/F) was excreted in urine and 72.76%/81.79% in feces. Group B: by 7 days 4.83%/3.43% was excreted in urine and 86.43%/86.31% in feces. Group D: by 24 hr 11.14%/10.44% was excreted in urine and 72.46%/77.72% in feces. By 7 days 11.61%/10.93% was excreted in urine and 79.19%/84.62% in feces. Combined excretion (including cage rinse) by 7 days was 92.93%/98.74%. Group E: by 24 hr 9.54%/8.51% was excreted in urine and 70.69%/69.90% in feces. By 7 days 10.11%/9.14% was excreted in urine and 79.80%/81.79% in feces. Combined excretion (including cage rinse) by 7 days was 92.81%/94.21%. Group F: by 24 hr 2.40%/2.43% was excreted in urine and 27.16%/27.18% in feces (thus, a relative delay in fecal excretion at the HD). By 7 days 8.30%/8.07% was excreted in urine and 91.58%/90.09% in feces. Combined excretion (including cage rinse) by 7 days was 101.02%/99.62%. Total tissue residues were always <1% of the dose (Groups D-F). Under all conditions, highest tissue levels occurred in the liver. The major metabolites were a variety of polar and non-polar compounds resulting from aromatic hydroxylations and heteroaromatic N-demethylation. The parent compound was the primary fecal component over the 1st 72 hr.

SECTION 5: Firefighting measures

Suitable extinguishing media

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

Specific hazards arising from the chemical

no data available

Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

Environmental precautions

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

Methods and materials for containment and cleaning up

If a spill occurs, clean it up promptly. Don't wash it away. Instead, sprinkle the spill with sawdust, vermiculite, or kitty litter. Sweep it into a plastic garbage bag, and dispose of it as directed on the pesticide product label.

SECTION 7: Handling and storage

Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Keep away from children. Store in original container. Do Not contaminate water, food, feed by storage or disposal.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state: White to light yellow solid

Colour: White crystalline solid

Odour: no data available

Melting point/freezing point: 154-155°C

Boiling point or initial boiling point and boiling range: 444.4°C at 760 mmHg

Flammability: no data available

Lower and upper explosion limit/flammability limit: no data available

Flash point: 222.6°C

Auto-ignition temperature: no data available

Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	Solubility in methanol, chloroform, diethyl ether: >10 g/L; in ethyl acetate: >5 g/L; in hexane: <0.5 g/L
Partition coefficient n-octanol/water:	log Kow = 1.87 at pH 7, 25 deg C
Vapour pressure:	0.013 mPa (9.8X10-8 mm Hg) at 25 deg C
Density and/or relative density:	1.274 g/cm ³
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

Stable to hydrolysis at pH 3-9.

Possibility of hazardous reactions

no data available

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits toxic vapors of /nitrogen oxides, hydrogen fluoride/ ...

SECTION 11: Toxicological information**Acute toxicity**

Oral: LD50 Rat oral >10,000 mg/kg

Inhalation: no data available

Dermal: LD50 Rabbit percutaneous >5000 mg/kg

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

Cancer Classification: Group E Evidence of Non-carcinogenicity for Humans

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information**Toxicity**

Toxicity to fish: LC50 /*Oncorhynchus mykiss*/ (Rainbow Trout) 11.7 mg/L/ 96 hr /Conditions of bioassay not specified in source examined

Toxicity to daphnia and other aquatic invertebrates: EC50 *Daphnia magna* (Water flea; intoxication, immobilization) 3.6 ppm/48 hr (95% confidence interval: 3.2-4.0 ppm); static /formulated product/[USEPA, Office of Pesticide Programs; Pesticide Ecotoxicity Database (2000) on 1-Methyl-3-phenyl-5-

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: A half-life of 12 months was reported for fluridone in sediment under laboratory conditions and 17 weeks under field conditions(1). Fluridone was reported to dissipate with average half-lives of 20 days and 3 months in pond water and in pond hydrosol, respectively(2). A half-life of 4 days was observed for fluridone after treatment in a pond(3). A half-life of 1 year or more was observed for fluridone in hydrosols(3). Photodegradation was found to be the major degradation pathway of fluridone in aquatic systems under actual-use conditions(1). In field studies using different soil types, <10% of the originally applied fluridone was found after 220 days in Miller clay and 20% was found remaining after 385 days in Lufkin fine sandy loam soil(4). In laboratory studies, fluridone persistence in non-sterilized soils after 210 days was 62, 44, 10, and 5% in Lufkin fine sandy loam, Miller clay, Hidalgo sandy clay loam, and Brennan fine sandy loam, respectively(4). In Miller clay and Lufkin fine sandy loam no difference was observed in the rate of fluridone degradation between sterilized and non-sterilized samples; however, noticeable differences in degradation were observed between sterilized and non-sterilized Brennan fine sandy loam and Hidalgo sandy clay loam(4). A half-life of 360 days was reported in aerobic soil(5).

Bioaccumulative potential

BCF values ranging from 0 to 91 have been reported for fluridone in various fish(1-4). According to a classification scheme(5), BCF values of <30 are low, and from 30 to 100 are moderate.

Mobility in soil

Koc values for fluridone measured in 6 soils were reported to range from 350 to 2,462(1-3). According to a classification scheme(4), these Koc values suggest that fluridone is expected to have low to slight mobility in soil. The pKa of fluridone is 12.3(5), indicating that this compound will primarily exist in the protonated form in the environment and cations generally adsorb more strongly to organic carbon and clay than their neutral counterparts(6).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN3077 (For reference only, please check.)

IMDG: UN3077 (For reference only, please check.)

IATA: UN3077 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (For reference only, please check.)

IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (For reference only, please check.)

IATA: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 9 (For reference only, please check.)

IMDG: 9 (For reference only, please check.)

IATA: 9 (For reference only, please check.)

Packing group, if applicable

ADR/RID: III (For reference only, please check.)

IMDG: III (For reference only, please check.)

IATA: III (For reference only, please check.)

Environmental hazards

ADR/RID: Yes

IMDG: Yes

IATA: Yes

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Not Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Not Listed.

Korea Existing Chemicals List (KECL)

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

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

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

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

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

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

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

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

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

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

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any