

SAFETY DATA SHEETS

According to the UN GHS revision 9

Version: 1.0
Creation Date: July 15, 2019
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SECTION 1: Identification

1.1 GHS Product identifier

Product name Ferrocene

1.2 Other means of identification

Product number -

Other names Di(cyclopentadienyl)iron; dicyclopentadienyl;
Dicyclopentadienyl Iron

1.3 Recommended use of the chemical and restrictions on use

Identified uses Industrial and scientific research use.

Uses advised against no data available

1.4 Supplier's details

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1.5 Emergency phone number

Emergency phone number +86-4000-6969-66

Service hours Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT
+8 hours).

SECTION 2: Hazard identification

2.1 Classification of the substance or mixture

Flammable solids, Category 1

Acute toxicity - Category 4, Oral

Acute toxicity - Category 4, Inhalation

Reproductive toxicity, Category 1B

Specific target organ toxicity – repeated exposure, Category 2

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

2.2 GHS label elements, including precautionary statements

Pictogram(s)





Signal word	Danger
Hazard statement(s)	H228 Flammable solid H302+H332 Harmful if swallowed or if inhaled H361 Suspected of damaging fertility or the unborn child H373 May cause damage to organs through prolonged or repeated exposure H410 Very toxic to aquatic life with long lasting effects
Precautionary statement(s)	
Prevention	P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. P240 Ground and bond container and receiving equipment. P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment. P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/... P264 Wash ... thoroughly after handling. P270 Do not eat, drink or smoke when using this product. P261 Avoid breathing dust/fume/gas/mist/vapours/spray. P271 Use only outdoors or in a well-ventilated area. P203 Obtain, read and follow all safety instructions before use. P260 Do not breathe dust/fume/gas/mist/vapours/spray. P273 Avoid release to the environment.
Response	P370+P378 In case of fire: Use ... to extinguish. P301+P317 IF SWALLOWED: Get medical help. P330 Rinse mouth. P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing. P317 Get medical help. P318 IF exposed or concerned, get medical advice. P319 Get medical help if you feel unwell. 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.

2.3 Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
Ferrocene	Ferrocene	102-54-5	203-039-3	100%

SECTION 4: First-aid measures

4.1 Description of necessary first-aid measures

If inhaled

Fresh air, rest.

Following skin contact

Rinse and then wash skin with water and soap.

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth.

4.2 Most important symptoms/effects, acute and delayed

Exposure Routes: inhalation, ingestion, skin and/or eye contact Symptoms: Possible irritation eyes, skin, respiratory system Target Organs: Eyes, skin, respiratory system, liver, blood, reproductive system (NIOSH, 2016)

4.3 Indication of immediate medical attention and special treatment needed, if necessary

Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for shock and treat if necessary. For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with normal saline during transport. Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool. Iron and related compounds

SECTION 5: Fire-fighting measures

5.1 Suitable extinguishing media

Fires involving this material can be controlled with a dry chemical, carbon dioxide or Halon extinguisher. (NTP, 1992)

5.2 Specific hazards arising from the chemical

Flash point data for this chemical are not available. It is probably combustible. (NTP, 1992)

5.3 Special protective actions for fire-fighters

Use water spray, powder, alcohol-resistant foam, carbon dioxide.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting.

6.2 Environmental precautions

Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Personal protection: particulate filter respirator adapted to the airborne concentration of the substance.

6.3 Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

NO open flames. 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.

7.2 Conditions for safe storage, including any incompatibilities

Separated from strong oxidants.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

TLV: (as Fe): 10 mg/m³, as TWA

Biological limit values

no data available

8.2 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.

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

Eye/face protection

Wear safety goggles.

Skin protection

Protective gloves.

Respiratory protection

Use local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state	Solid. Crystalline.
Colour	Orange.
Odour	Camphor-like
Melting point/freezing point	> 172.5 - < 174 °C.
Boiling point or initial boiling point and boiling range	249 °C. Atm. press.:1 atm.
Flammability	Combustible Solid
Lower and upper explosion limit/flammability limit	no data available
Flash point	113°C(lit.)
Auto-ignition temperature	> 400 °C. Remarks:At atm. press. of 1.0 atm.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	less than 0.1 mg/mL at 70° F (NTP, 1992)
Partition coefficient n-octanol/water	log Pow = 3.711. Temperature:22 °C.
Vapour pressure	0.007 kPa. Temperature:40 °C.;0.34 kPa. Temperature:100 °C.
Density and/or relative density	1.49 g/cm ³ . Temperature:25 °C.
Relative vapour density	no data available
Particle characteristics	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

On combustion, forms toxic fumes. Reacts violently with ammonium perchlorate and tetranitromethane. Reacts with mercury (II) nitrate.

10.2 Chemical stability

Unusually stable

10.3 Possibility of hazardous reactions

FIRE HAZARD: Moderate FERROCENE reacts violently with tetranitromethane. (NTP, 1992). Contact of tetranitromethane with ferrocene under various conditions leads to violent explosion, [Trans. Met. Chem., 1979, 4, 207-208].

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Reacts violently with /Ammonium perchlorate/.

10.6 Hazardous decomposition products

When heated to decomposition it emits acrid smoke and irritating fumes.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 - rat - 1 320 mg/kg bw.
- Inhalation: no data available
- Dermal: LD50 - rat (male/female) - > 3 000 mg/kg bw.

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

no data available

Reproductive toxicity

no data available

STOT-single exposure

May cause mechanical irritation.

STOT-repeated exposure

no data available

Aspiration hazard

Evaporation at 20°C is negligible; a harmful concentration of airborne particles can, however, be reached quickly when dispersed.

SECTION 12: Ecological information

12.1 Toxicity

- Toxicity to fish: LC50 - *Leuciscus idus melanotus* - 24.5 mg/L - 48 h.
- Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - ca. 2.5 mg/L - 24 h.
- Toxicity to algae: EC50 - *Desmodesmus subspicatus* (previous name: *Scenedesmus subspicatus*) - 1.03 mg/L - 72 h.
- Toxicity to microorganisms: NOEC - *Pseudomonas putida* - > 87.6 mg/L - 6 h.

12.2 Persistence and degradability

no data available

12.3 Bioaccumulative potential

no data available

12.4 Mobility in soil

no data available

12.5 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 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

14.1 UN Number

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.) IATA: Not dangerous goods. (For reference only, please check.)

14.2 UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.) IATA: Not dangerous goods. (For reference only, please check.)

14.3 Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.) IATA: Not dangerous goods. (For reference only, please check.)

14.4 Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.) IATA: Not dangerous goods. (For reference only, please check.)

14.5 Environmental hazards

ADR/RID: Yes

IMDG: Yes

IATA: Yes

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

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

Chemical name	Common names and synonyms	CAS number	EC number
Ferrocene	Ferrocene	102-54-5	203-039-3
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.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Listed.
Korea Existing Chemicals List (KECL)			Listed.

SECTION 16: Other information

Information on revision

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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/>

Any questions regarding this SDS, Please send your inquiry to sds@xixisys.com

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