

## MATERIAL SAFETY DATA SHEET

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Version 1.4

## Section 1 - Product and Company Information

Product Name ACETYLFERROCENE, 95%  
Product Number 106860  
Brand ALDRICH

Company Sigma-Aldrich  
Address 3050 Spruce Street  
SAINT LOUIS MO 63103 US

Technical Phone: 800-325-5832  
Fax: 800-325-5052  
Emergency Phone: 314-776-6555

## Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313
ACETYLFERROCENE	1271-55-2	No

Formula C<sub>12</sub>H<sub>12</sub>FeO  
Synonyms Acetoferrocene \* Acetylferrocene \*  
1-Acetylferrocene \* Ferrocene, acetyl- \*  
Ferrocenyl methyl ketone \* Iron,  
(acetylcyclopentadienyl)cyclopentadienyl- \*  
Monacetylferrocene

RTECS Number: OB3700000

## Section 3 - Hazards Identification

## EMERGENCY OVERVIEW

Highly Toxic (USA) Very Toxic (EU).  
Very toxic if swallowed.

## HMIS RATING

HEALTH: 3  
FLAMMABILITY: 0  
REACTIVITY: 0

## NFPA RATING

HEALTH: 3  
FLAMMABILITY: 0  
REACTIVITY: 0

For additional information on toxicity, please refer to Section 11.

## Section 4 - First Aid Measures

## ORAL EXPOSURE

If swallowed, wash out mouth with water provided person is conscious. Call a physician immediately.

## INHALATION EXPOSURE

If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

#### DERMAL EXPOSURE

In case of skin contact, flush with copious amounts of water for at least 15 minutes. Remove contaminated clothing and shoes. Call a physician.

#### EYE EXPOSURE

In case of contact with eyes, flush with copious amounts of water for at least 15 minutes. Assure adequate flushing by separating the eyelids with fingers. Call a physician.

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### Section 5 - Fire Fighting Measures

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#### FLASH POINT

N/A

#### AUTOIGNITION TEMP

N/A

#### FLAMMABILITY

N/A

#### EXTINGUISHING MEDIA

Suitable: Water spray. Carbon dioxide, dry chemical powder, or appropriate foam.

#### FIREFIGHTING

Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.  
Specific Hazard(s): Emits toxic fumes under fire conditions.

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### Section 6 - Accidental Release Measures

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#### PROCEDURE TO BE FOLLOWED IN CASE OF LEAK OR SPILL

Evacuate area.

#### PROCEDURE(S) OF PERSONAL PRECAUTION(S)

Wear self-contained breathing apparatus, rubber boots, and heavy rubber gloves.

#### METHODS FOR CLEANING UP

Sweep up, place in a bag and hold for waste disposal. Avoid raising dust. Ventilate area and wash spill site after material pickup is complete.

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### Section 7 - Handling and Storage

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#### HANDLING

User Exposure: Do not breathe dust. Do not get in eyes, on skin, on clothing. Avoid prolonged or repeated exposure.

#### STORAGE

Suitable: Keep tightly closed.

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### Section 8 - Exposure Controls / PPE

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#### ENGINEERING CONTROLS

Safety shower and eye bath. Use only in a chemical fume hood.

#### PERSONAL PROTECTIVE EQUIPMENT

Respiratory: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN

(EU). 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.

Hand: Compatible chemical-resistant gloves.

Eye: Chemical safety goggles.

#### GENERAL HYGIENE MEASURES

Wash contaminated clothing before reuse. Wash thoroughly after handling.

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#### Section 9 - Physical/Chemical Properties

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Appearance	Physical State: Solid Form: Fine crystals	
Property	Value	At Temperature or Pressure
Molecular Weight	228.07 AMU	
pH	N/A	
BP/BP Range	N/A	
MP/MP Range	82 °C	
Freezing Point	N/A	
Vapor Pressure	N/A	
Vapor Density	N/A	
Saturated Vapor Conc.	N/A	
SG/Density	N/A	
Bulk Density	N/A	
Odor Threshold	N/A	
Volatile%	N/A	
VOC Content	N/A	
Water Content	N/A	
Solvent Content	N/A	
Evaporation Rate	N/A	
Viscosity	N/A	
Surface Tension	N/A	
Partition Coefficient	N/A	
Decomposition Temp.	N/A	
Flash Point	N/A	
Explosion Limits	N/A	
Flammability	N/A	
Autoignition Temp	N/A	
Refractive Index	N/A	
Optical Rotation	N/A	
Miscellaneous Data	N/A	
Solubility	N/A	

N/A = not available

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#### Section 10 - Stability and Reactivity

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##### STABILITY

Stable: Stable.

Materials to Avoid: Strong oxidizing agents, Strong reducing agents.

##### HAZARDOUS DECOMPOSITION PRODUCTS

Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide, Iron oxides.

##### HAZARDOUS POLYMERIZATION

Section 11 - Toxicological Information

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ROUTE OF EXPOSURE

Skin Contact: May cause skin irritation.  
Skin Absorption: May be harmful if absorbed through the skin.  
Eye Contact: May cause eye irritation.  
Inhalation: Material may be irritating to mucous membranes and upper respiratory tract. May be harmful if inhaled.  
Ingestion: May be fatal if swallowed.

SIGNS AND SYMPTOMS OF EXPOSURE

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

TOXICITY DATA

Oral  
Rat  
25 mg/kg  
LD50  
Remarks: Behavioral:Somnolence (general depressed activity).  
Vascular:Regional or general arteriolar or venous dilation.  
Lungs, Thorax, or Respiration:Dyspnea.

Oral  
Mouse  
50 mg/kg  
LD50  
Remarks: Behavioral:Tremor. Behavioral:Somnolence (general depressed activity). Vascular:Regional or general arteriolar or venous dilation.

Intraperitoneal  
Mouse  
25 MG/KG  
LD50  
Remarks: Skin and Appendages: Other: Hair. Behavioral:Tremor.  
Gastrointestinal:Changes in structure or function of salivary glands.

Intravenous  
Mouse  
75 MG/KG  
LD50

Skin  
Mammal  
23.3 mg/kg  
LD50

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Section 12 - Ecological Information

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No data available.

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Section 13 - Disposal Considerations

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APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

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. Observe all federal, state, and local environmental regulations.

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## Section 14 - Transport Information

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### DOT

Proper Shipping Name: Toxic solids, organic, n.o.s.  
UN#: 2811  
Class: 6.1  
Packing Group: Packing Group II  
Hazard Label: Toxic substances.  
PIH: Not PIH

### IATA

Proper Shipping Name: Toxic solid, organic, n.o.s.  
IATA UN Number: 2811  
Hazard Class: 6.1  
Packing Group: II

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## Section 15 - Regulatory Information

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### EU ADDITIONAL CLASSIFICATION

Symbol of Danger: T+  
Indication of Danger: Very toxic.  
R: 28  
Risk Statements: Very toxic if swallowed.  
S: 28-36/37-45  
Safety Statements: After contact with skin, wash immediately with plenty of water. Wear suitable protective clothing and gloves. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

### US CLASSIFICATION AND LABEL TEXT

Indication of Danger: Highly Toxic (USA) Very Toxic (EU).  
Risk Statements: Very toxic if swallowed.  
Safety Statements: After contact with skin, wash immediately with plenty of water. Wear suitable protective clothing and gloves. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

### UNITED STATES REGULATORY INFORMATION

SARA LISTED: No  
TSCA INVENTORY ITEM: Yes Yes

### CANADA REGULATORY INFORMATION

WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.  
DSL: No  
NDSL: Yes

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## Section 16 - Other Information

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### DISCLAIMER

For R&D use only. Not for drug, household or other uses.

### WARRANTY

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

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