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

1.1 Product identifiers

Product name: Iron(0) pentacarbonyl
Product Number: 481718
Brand: Aldrich
CAS-No.: 13463-40-6

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses: Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO  63103
UNITED STATES

Telephone: +1 314 771-5765
Fax: +1 800 325-5052

1.4 Emergency telephone

Emergency Phone #: 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Flammable liquids (Category 2), H225
Acute toxicity, Oral (Category 2), H300
Acute toxicity, Inhalation (Category 1), H330
Acute toxicity, Dermal (Category 3), H311

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal Word: Danger

Aldrich - 481718
Hazard statement(s)
- H225: Highly flammable liquid and vapor.
- H300 + H330: Fatal if swallowed or if inhaled.
- H311: Toxic in contact with skin.

Precautionary statement(s)
- P210: Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
- P233: Keep container tightly closed.
- P240: Ground/bond container and receiving equipment.
- P241: Use explosion-proof electrical/ ventilating/ lighting/ equipment.
- P242: Use only non-sparking tools.
- P243: Take precautionary measures against static discharge.
- P260: Do not breathe mist or vapors.
- P264: Wash skin thoroughly after handling.
- P270: Do not eat, drink or smoke when using this product.
- P271: Use only outdoors or in a well-ventilated area.
- P280: Wear protective gloves/ eye protection/ face protection.
- P284: Wear respiratory protection.
- P303 + P361 + P353: IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
- P304 + P340 + P310: IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
- P362: Take off contaminated clothing and wash before reuse.
- P370 + P378: In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
- P403 + P233: Store in a well-ventilated place. Keep container tightly closed.
- P403 + P235: Store in a well-ventilated place. Keep cool.
- P405: Store locked up.
- P501: Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

<table>
<thead>
<tr>
<th>Synonyms</th>
<th>Iron(0) carbonyl</th>
<th>Pentacarbonyliron(0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>C₅FeO₅</td>
<td></td>
</tr>
<tr>
<td>Molecular weight</td>
<td>195.90 g/mol</td>
<td></td>
</tr>
<tr>
<td>CAS-No.</td>
<td>13463-40-6</td>
<td></td>
</tr>
<tr>
<td>EC-No.</td>
<td>236-670-8</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Iron(0) pentacarbonyl</td>
<td>Flam. Liq. 2; Acute Tox. 2;</td>
<td>&lt;= 100 %</td>
</tr>
<tr>
<td></td>
<td>Acute Tox. 1; Acute Tox.</td>
<td></td>
</tr>
</tbody>
</table>
SECTION 4: First aid measures

4.1 Description of first-aid measures

**General advice**
First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

**If inhaled**
After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

**In case of skin contact**
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Call a physician immediately.

**In case of eye contact**
After eye contact: rinse out with plenty of water. Remove contact lenses.

**If swallowed**
If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

4.2 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

4.3 Indication of any immediate medical attention and special treatment needed
No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

**Suitable extinguishing media**
Water Foam Carbon dioxide (CO2) Dry powder

**Unsuitable extinguishing media**
For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Iron oxides
Combustible.
Pay attention to flashback.
Vapors are heavier than air and may spread along floors.
Development of hazardous combustion gases or vapours possible in the event of fire.
Forms explosive mixtures with air at ambient temperatures.

5.3 **Advice for firefighters**
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 **Further information**
Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

### SECTION 6: Accidental release measures

6.1 **Personal precautions, protective equipment and emergency procedures**
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 **Environmental precautions**
Do not let product enter drains. Risk of explosion.

6.3 **Methods and materials for containment and cleaning up**
Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 **Reference to other sections**
For disposal see section 13.

### SECTION 7: Handling and storage

7.1 **Precautions for safe handling**

**Advice on safe handling**
Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

**Advice on protection against fire and explosion**
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

**Hygiene measures**
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 **Conditions for safe storage, including any incompatibilities**

**Storage conditions**
Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

**Storage stability**
Recommended storage temperature

Aldrich - 481718
2 - 8 °C

Storage class
Storage class (TRGS 510): 3: Flammable liquids

7.3 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

8.1 Control parameters

Ingredients with workplace control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Iron(0) pentacarbonyl</td>
<td>13463-40-6</td>
<td>TWA</td>
<td>0.1 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>STEL</td>
<td>0.2 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>0.2 ppm</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ST</td>
<td>0.2 ppm</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PEL</td>
<td>0.1 ppm</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>STEL</td>
<td>0.2 ppm</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
</tbody>
</table>

8.2 Exposure controls

Appropriate engineering controls
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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). Safety glasses

Skin protection
required

Body Protection
Flame retardant antistatic protective clothing.

Respiratory protection
required when vapours/aerosols are generated.
Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

**Control of environmental exposure**
Do not let product enter drains. Risk of explosion.

### SECTION 9: Physical and chemical properties

#### 9.1 Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Information</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) Appearance</td>
<td>Form: clear, liquid</td>
</tr>
<tr>
<td>b) Odor</td>
<td>No data available</td>
</tr>
<tr>
<td>c) Odor Threshold</td>
<td>No data available</td>
</tr>
<tr>
<td>d) pH</td>
<td>No data available</td>
</tr>
<tr>
<td>e) Melting point/freezing point</td>
<td>Melting point/range: -20 °C (-4 °F) - lit.</td>
</tr>
<tr>
<td>f) Initial boiling point and boiling range</td>
<td>103 °C 217 °F - lit.</td>
</tr>
<tr>
<td>g) Flash point</td>
<td>-15 °C (5 °F) - closed cup</td>
</tr>
<tr>
<td>h) Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td>i) Flammability (solid, gas)</td>
<td>No data available</td>
</tr>
<tr>
<td>j) Upper/lower flammability or explosive limits</td>
<td>No data available</td>
</tr>
<tr>
<td>k) Vapor pressure</td>
<td>53 hPa at 30.3 °C (86.5 °F)</td>
</tr>
<tr>
<td>l) Vapor density</td>
<td>47 hPa at 25 °C (77 °F)</td>
</tr>
<tr>
<td>m) Density</td>
<td>1.49 g/cm3 at 25 °C (77 °F) - lit.</td>
</tr>
<tr>
<td>Relative density</td>
<td>No data available</td>
</tr>
<tr>
<td>n) Water solubility</td>
<td>No data available</td>
</tr>
<tr>
<td>o) Partition coefficient: n-octanol/water</td>
<td>No data available</td>
</tr>
<tr>
<td>p) Autoignition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>q) Decomposition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>r) Viscosity</td>
<td>No data available</td>
</tr>
<tr>
<td>s) Explosive properties</td>
<td>No data available</td>
</tr>
<tr>
<td>t) Oxidizing properties</td>
<td>No data available</td>
</tr>
</tbody>
</table>

#### 9.2 Other safety information
SECTION 10: Stability and reactivity

10.1 Reactivity
Vapors may form explosive mixture with air.

10.2 Chemical stability
The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid

10.5 Incompatible materials
Strong oxidizing agents, Strong bases, Amines, Halogens

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - 5.1 mg/kg
LC50 Inhalation - 4 h - 0.08 mg/l - vapor

LD50 Dermal - 300 mg/kg
No data available

Skin corrosion/irritation
Remarks: No data available

Serious eye damage/eye irritation
Remarks: 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.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA’s list of regulated carcinogens.

**Reproductive toxicity**
No data available
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

11.2 **Additional Information**
RTECS: NO4900000
Liver injury may occur., Kidney injury may occur., Aspiration or inhalation may cause chemical pneumonitis., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath
Stomach - Irregularities - Based on Human Evidence
Stomach - Irregularities - Based on Human Evidence

**SECTION 12: Ecological information**

12.1 **Toxicity**
No data available

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 **Results of PBT and vPvB assessment**
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 **Endocrine disrupting properties**
No data available

12.7 **Other adverse effects**
No data available
SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

DOT (US)
UN number: 1994  Class: 6.1I (3)  Packing group: I
Proper shipping name: Iron pentacarbonyl
Reportable Quantity (RQ): Poison Inhalation Hazard: Hazard Zone A

IMDG
UN number: 1994  Class: 6.1 (3)  Packing group: I  EMS-No: F-E, S-D
Proper shipping name: IRON PENTACARBONYL

IATA
UN number: 1994  Class: 6.1 (3)
Proper shipping name: Iron pentacarbonyl
IATA Passenger: Not permitted for transport
IATA Cargo: Not permitted for transport

SECTION 15: Regulatory information

SARA 302 Components
Iron(0) pentacarbonyl  CAS-No.  13463-40-6  Revision Date  2007-03-01

SARA 313 Components
The following components are subject to reporting levels established by SARA Title III, Section 313:
Iron(0) pentacarbonyl  CAS-No.  13463-40-6  Revision Date  2007-03-01

SARA 311/312 Hazards
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components
Iron(0) pentacarbonyl  CAS-No.  13463-40-6  Revision Date  2007-03-01

Pennsylvania Right To Know Components
Iron(0) pentacarbonyl  CAS-No.  13463-40-6  Revision Date  2007-03-01
SECTION 16: Other information

Further information
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. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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Version: 8.6 Revision Date: 05/25/2023 Print Date: 07/08/2023