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.
  - Address: 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.
P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
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
Synonyms:
Iron(0) carbonyl
Pentacarbonyliron(0)

Formula: C₅FeO₅
Molecular weight: 195.90 g/mol
CAS-No.: 13463-40-6
EC-No.: 236-670-8

<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; Acute Tox. 1; Acute Tox.</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

Aldrich - 481718
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
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

<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>0.1 ppm</td>
<td>0.23 mg/m³ USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ST</td>
<td>0.2 ppm</td>
<td>0.45 mg/m³ USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PEL</td>
<td>0.1 ppm</td>
<td>0.8 mg/m³ 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>1.6 mg/m³ 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

- **a)** Appearance  
  Form: clear, liquid
- **b)** Odor  
  No data available
- **c)** Odor Threshold  
  No data available
- **d)** pH  
  No data available
- **e)** Melting point/freezing point  
  Melting point/range: -20 °C (-4 °F) - lit.
- **f)** Initial boiling point and boiling range  
  103 °C 217 °F - lit.
- **g)** Flash point  
  -15 °C (5 °F) - closed cup
- **h)** Evaporation rate  
  No data available
- **i)** Flammability (solid, gas)  
  No data available
- **j)** Upper/lower flammability or explosive limits  
  No data available
- **k)** Vapor pressure  
  53 hPa at 30.3 °C (86.5 °F)  
  47 hPa at 25 °C (77 °F)
- **l)** Vapor density  
  6.76 - (Air = 1.0)
- **m)** Density  
  1.49 g/cm³ at 25 °C (77 °F) - lit.
  Relative density  
  No data available
- **n)** Water solubility  
  No data available
- **o)** Partition coefficient: n-octanol/water  
  No data available
- **p)** Autoignition temperature  
  No data available
- **q)** Decomposition temperature  
  No data available
- **r)** Viscosity  
  No data available
- **s)** Explosive properties  
  No data available
- **t)** Oxidizing properties  
  No data available

### 9.2 Other safety information
Relative vapor density 6.76 - (Air = 1.0)

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

**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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