Product Stewardship Summary
Iron Pentacarbonyl

General Statement
Iron pentacarbonyl is used as a starting material in organic synthesis and industrial processes. Iron pentacarbonyl is a high hazard material. However, the risk of adverse health effects associated with occupational use of this chemical is low if proper precautions are followed.

Chemical Identity

Name: Pentacarbonyliron; Iron carbonyl (Fe(CO)₅)
Brand Name: Pentacarbonyliron
Chemical name (IUPAC): Pentacarbonyliron
CAS number(s): 13463-40-6
EC number: 236-670-8
Molecular formula: C₅FeO₅

Uses and Applications
Pentacarbonyl iron is used as a starting material in organic synthesis and industrial processes, commonly used to make purified iron powder or other complex iron compounds. Ashland sells both purified Pentacarbonyl iron as well as its purified decomposition product, iron powder.
Physical/Chemical Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Form</td>
<td>Substance</td>
</tr>
<tr>
<td>Physical state</td>
<td>Liquid</td>
</tr>
<tr>
<td>Color</td>
<td>Colorless to yellow</td>
</tr>
<tr>
<td>Odor</td>
<td>Musty</td>
</tr>
<tr>
<td>Density</td>
<td>1.46 g/cm³ @ 20°C</td>
</tr>
<tr>
<td>Melting / boiling point</td>
<td>-20°C / 103°C</td>
</tr>
<tr>
<td>Flammability</td>
<td>No data available</td>
</tr>
<tr>
<td>Explosive properties</td>
<td>Lower: 3.7%; Upper: 12.5% in air @ 25°C</td>
</tr>
<tr>
<td>Self-ignition temperature</td>
<td>49°C</td>
</tr>
<tr>
<td>Vapor pressure</td>
<td>35 hPa @ 20°C</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>195.9 g/mol</td>
</tr>
<tr>
<td>Water solubility</td>
<td>Insoluble in water @ 20°C</td>
</tr>
<tr>
<td>Flash point</td>
<td>-15°C</td>
</tr>
<tr>
<td>Octanol-water partition coefficient (LogP&lt;sub&gt;ow&lt;/sub&gt;)</td>
<td>3.0</td>
</tr>
</tbody>
</table>

Exposure, Hazard and Safety Assessment

The following section describes possible exposures scenarios and hazards associated with Iron pentacarbonyl. The exposure assessment describes both the amount of and the frequency with which a chemical substance reaches a person, a population of people, or the environment. Hazard refers to the inherent properties of a substance that make it capable of causing harm to human health or the environment. The safety assessment reports the possibility of a harmful event arising from exposure to a chemical or physical agent under specific conditions. Just because a substance may possess potentially harmful properties does not mean that it automatically poses a risk. It is not possible to make that determination without understanding the exposure.

Human Health Effects

Human Exposure Assessment

**Consumer:** Iron pentacarbonyl is used as a starting material in organic synthesis and industrial processes. Consumers are unlikely to come into contact with this substance outside of an accidental release or exposure.

**Worker:** In the industrial setting, Iron pentacarbonyl is manufactured and handled in closed processes as much as possible, which ensures that worker exposure is minimized. The proper administrative and engineering controls, good housekeeping, and use of personal protective equipment during loading, unloading, sampling or during maintenance operations is crucial to minimize potential exposures to Iron pentacarbonyl.
Human Hazard Assessment

<table>
<thead>
<tr>
<th>Effect Assessment</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acute Toxicity</td>
<td>Iron pentacarbonyl is potentially fatal if swallowed or inhaled, and is highly toxic in contact with the skin.</td>
</tr>
<tr>
<td>Oral / inhalation / dermal</td>
<td></td>
</tr>
<tr>
<td>Irritation / corrosion</td>
<td>Based on available data, Iron pentacarbonyl is not expected to be irritating to the skin, eyes, or respiratory tract</td>
</tr>
<tr>
<td>Skin / eye / respiratory tract</td>
<td></td>
</tr>
<tr>
<td>Sensitization</td>
<td>Based on available data, Iron pentacarbonyl is not expected to be a skin sensitizer</td>
</tr>
<tr>
<td>Toxicity after repeated exposure</td>
<td>Long term, repeat inhalation exposure to Iron pentacarbonyl may cause respiratory irritation and lung damage</td>
</tr>
<tr>
<td>Oral / inhalation / dermal</td>
<td></td>
</tr>
<tr>
<td>Genotoxicity / Mutagenicity</td>
<td>Based on available data, Iron pentacarbonyl is not expected to be mutagenic or genotoxic</td>
</tr>
<tr>
<td>Carcinogenicity</td>
<td>Based on available data, Iron pentacarbonyl is not expected to be carcinogenic</td>
</tr>
<tr>
<td>Toxicity for reproduction</td>
<td>Based on available data, Iron pentacarbonyl is not expected to be a reproductive toxicant.</td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Human Health Safety Assessment

**Consumer:** Despite a high hazard profile, consumer exposure to Iron pentacarbonyl is not expected and therefore negligible, and thus the risk to human health is expected to be low.

**Worker:** In the industrial setting, Iron pentacarbonyl is manufactured and handled in closed processes as much as possible, which ensures that worker exposure is minimized. Although the hazards are high, good manufacturing processes and industrial hygiene practices will ensure exposure, and thus risk, to workers is low.

Environmental Effects

**Environmental Exposure**
Iron pentacarbonyl is insoluble in water. No data on biodegradation or bioaccumulation is available.

Environmental Hazard Assessment

<table>
<thead>
<tr>
<th>Effect Assessment</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aquatic Toxicity</td>
<td>Minimally toxic to aquatic life</td>
</tr>
</tbody>
</table>

**Fate and behavior**

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Biodegradation</td>
<td>No data available</td>
</tr>
<tr>
<td>Bioaccumulation potential</td>
<td>No data available</td>
</tr>
<tr>
<td>PBT / vPvB conclusion</td>
<td>Not considered to be PBT or vPvB</td>
</tr>
</tbody>
</table>

Environmental Safety Assessment

Iron pentacarbonyl has low aquatic toxicity. If a release into the aquatic environment does occur, Iron pentacarbonyl is anticipated to have a minimal effect as it has shown low toxicity to aquatic organisms.
Risk Management Recommendations

Exposure to Iron pentacarbonyl can be controlled by sufficient ventilation, proper handling and storage techniques, and the use of appropriate personal protective equipment as recommended in the SDS.

Occupational exposure limits include, but are not limited to, the following:

- ACGIH TLV (TWA) 0.1 ppm
- ACGIH TLV (STEL) 0.2 ppm
- NIOSH REL (TWA) 0.1 ppm
- NIOSH STEL 0.2 ppm

Regulatory Agency Review
Iron pentacarbonyl is included on the following lists:

ACGIH - Threshold Limit Values (TLVs)
Alberta - Occupational Exposure Limits (OELs)
Argentina - Occupational Exposure Limits (OELs)
Arizona DOSH - List of Highly Hazardous Chemicals, Toxics and Reactives
Australia - Workplace Exposure Standards
Australian Inventory of Chemical Substances (AICS)
Austria - Occupational Exposure Limits (OELs)
Belgium - Occupational Exposure Limits (OELs)
British Columbia - Occupational Exposure Limits (OELs)
Bulgaria - Occupational Exposure Limits (OELs)
Cal/OSHA - Permissible Exposure Limits for Chemical Contaminants
Colombia - Occupational Exposure Limits (OELs)
Connecticut OSHA - List of Highly Hazardous Chemicals, Toxics and Reactives
Denmark - Occupational Exposure Limits (OELs)
Department of Homeland Security – Chemicals of Interest
DOE Protective Action Criteria (PAC)
Environment Canada - National Pollutant Release Inventory (NPRI) – 2016-2017
EPA - Clean Air Act - Section 112(r) Regulated Chemicals for Accidental Release Prevention
EPA - EPCRA - Section 302 - Extremely Hazardous Substance (EHS) List
EPA - EPCRA - Section 304 - Extremely Hazardous Substance (EHS) Reportable Quantities (RQs)
EPA - EPCRA - Section 313 - Toxic Chemicals
EPA - Office of Pollution Prevention and Toxics (OPPT) High Production Volume (HPV) Program - 1990
EPA - SARA - Section 302A - Extremely Hazardous Substance (EHS) List
EPA - Toxics Release Inventory (TRI) Chemicals
Finland - Occupational Exposure Limits (OELs)
Florida - List of Regulated Toxic Substances and Threshold Quantities (TQs)
France - Occupational Exposure Limits (OELs)
Germany - Occupational Exposure Limits (OELs)
Hawaii - Department of Labor and Industrial Relations - Air Contaminants - Permissible Exposure Limits
Hawaii - State Department of Health - Reportable Quantities
Iceland - Occupational Exposure Limits (OELs)
Indiana OSHA - List of Highly Hazardous Chemicals, Toxics and Reactives
Iowa OSHA - List of Highly Hazardous Chemicals, Toxics and Reactives
Jordan - Occupational Exposure Limits (OELs)
Korea - Occupational Exposure Limits (OELs)
Maryland OSH - List of Highly Hazardous Chemicals, Toxics and Reactives
Massachusetts Department of Public Health - Massachusetts Substance List (MSL)
Massachusetts Toxics Use Reduction Act (TURA)
Mexico - National Inventory of Chemical Substances
Michigan - Exposure Limits for Air Contaminants - Table G-1-A
Mine Safety and Health Administration (MSHA) - Permissible Exposure Limits (PELs)
Minnesota - Department of Labor and Industry - Air Contaminants - Permissible Exposure Limits
Minnesota - List of Hazardous Substances
Nevada OSHA - List of Highly Hazardous Chemicals, Toxics and Reactives
New Jersey - Right to Know List
New Mexico OHSB - List of Highly Hazardous Chemicals, Toxics and Reactives
New Zealand - Inventory of Chemicals (NZIoC)
New Zealand - Workplace Exposure Standards
NIOSH - Recommended Exposure Limits (RELs)
Ontario - Current Occupational Exposure Limits (OELs)
OSHA - List of Highly Hazardous Chemicals, Toxics and Reactives
OSHA - Vacated Permissible Exposure Limits (PELs)
Pennsylvania - Hazardous Substance List
Peru - Occupational Exposure Limits (OELs)
Philippine Inventory of Chemicals and Chemical Substances (PICCS)
Puerto Rico OSHA - List of Highly Hazardous Chemicals, Toxics and Reactives
Rhode Island - Hazardous Substance List
Russia - Occupational Exposure Limits (OELs)
Singapore - Occupational Exposure Limits (OELs)
South Carolina OSH - List of Highly Hazardous Chemicals, Toxics and Reactives
Switzerland - Occupational Exposure Limits (OELs)
Technischen Regeln für Gefahrstoffe (TRGS) - TRGS900
Tennessee OSHA - List of Highly Hazardous Chemicals, Toxics and Reactives
The Netherlands - Occupational Exposure Limits (OELs)
United Kingdom - Occupational Exposure Limits (OELs)
United Kingdom - Workplace Exposure Limits (WELs) – 2011
Utah OSH - List of Highly Hazardous Chemicals, Toxics and Reactives
Vermont - Department of Labor - Air Contaminants - Permissible Exposure Limits
Vermont OSHA - List of Highly Hazardous Chemicals, Toxics and Reactives
Vietnam - Occupational Exposure Limits (OELs)
Virgin Islands DOSH - List of Highly Hazardous Chemicals, Toxics and Reactives
Virginia OSH - List of Highly Hazardous Chemicals, Toxics and Reactives
Washington State - Permissible Exposure Limits (PELs) for Airborne Contaminants
Wyoming OSHA - List of Highly Hazardous Chemicals, Toxics and Reactives

**Regulatory Information / Classification and Labeling**

Under the Globally Harmonized System for classification and labeling (GHS), substances are classified according to their physical, health, and environmental hazards. The hazards are communicated via specific labels and the (Extended) SDS. GHS attempts to standardize hazard communication so that the intended audience (workers, consumers, transport workers, and emergency responders) can better understand the hazards of the chemicals in use.

**GHS Classification:**

Flammable Liquid, Category 1
Acute Toxicity, Category 2 (Oral)
Acute Toxicity, Category 2 (Dermal)
Acute Toxicity, Category 1 (Inhalation)
STOT Repeat Exposure, Category 1

**Hazard Statements:**

H220: Extremely flammable gas
H300: Fatal if swallowed.
H310: Fatal in contact with skin.
H330: Fatal if inhaled.
H372: Causes damage to lungs through prolonged or repeated inhalation exposure

**Signal Word:** DANGER
Precautionary Statements:

P101 If medical advice is needed, have product container or label at hand.
P102 Keep out of reach of children.
P103 Read label before use.
P210: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P260: Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.
P262: Do not get in eyes, on skin, or on clothing.
P231 Handle under inert gas.
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P303+P361+P353 IF ON SKIN (or hair): Remove/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/ P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P361 + P364: Take off immediately all contaminated clothing and wash it 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.
P422 Store contents under inert gas.
P411+P235 Store at temperatures not exceeding 4°C. Keep cool.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.
P280: Wear protective gloves/ eye protection/ face protection.

Hazard Pictograms:

Conclusion

Iron pentacarbonyl is used in numerous chemical synthesis processes. When handled safely and responsibly, the potential for fatal or highly toxic effects can be minimized, allowing workers to safely handle the material.

Contact Information with Company

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Additional Information

For more information on GHS, visit http://www.osha.gov/dsg/hazcom/ghsguideoct05.pdf or http://live.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html.
Ashland product stewardship summaries are located at http://www.ashland.com/stewardship
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REACH registration is specific to Importers/Manufacturers that place the chemical on the EU market, and specific to registered uses. Inclusion on the list of REACH Registered Substances does not automatically imply registration by Ashland.

Inclusion on the New Zealand Inventory of Chemicals applies only to the pure substance listed. The importer of record must determine whether or not their substances are in compliance.