# **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)<sub>5</sub>

Pentacarbonyliron **Brand Name:** Chemical name (IUPAC): Pentacarbonyliron

CAS number(s): 13463-40-6 EC number: 236-670-8 Molecular formula: C<sub>5</sub>FeO<sub>5</sub>

Structure:

$$\begin{array}{c} O & \\ O & \\ O & \\ O & \\ \end{array}$$

## **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.



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# **Physical/Chemical Properties**

Property	Value
Form	Substance
Physical state	Liquid
Color	Colorless to yellow
Odor	Musty
Density	1.46 g/cm <sup>3</sup> @ 20°C
Melting / boiling point	-20°C / 103°C
Flammability	No data available
Explosive properties	Lower: 3.7%; Upper: 12.5% in air @ 25°C
Self-ignition temperature	49°C
Vapor pressure	35 hPa @ 20°C
Molecular weight	195.9 g/mol
Water solubility	Insoluble in water @ 20°C
Flash point	-15°C
Octanol-water partition coefficient (LogPow)	3.0

## **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**

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

# **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**

Effect Assessment	Result
Aquatic Toxicity	Minimally toxic to aquatic life

Fate and behavior	
Biodegradation	No data available
Bioaccumulation potential	No data available
PBT / vPvB conclusion	Not considered to be PBT or vPvB

#### **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

Mexico - Occupational Exposure Limits (OELs)

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 + 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**

Ashland Inc. 5200 Blazer Parkway Dublin, Ohio 43017 http://www.ashland.com/contact

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#### **Additional Information**

For more information on GHS, visit <a href="http://www.osha.gov/dsg/hazcom/ghsguideoct05.pdf">http://www.osha.gov/dsg/hazcom/ghsguideoct05.pdf</a> or <a href="http://live.unece.org/trans/danger/publi/ghs/ghs\_welcome\_e.html">http://live.unece.org/trans/danger/publi/ghs/ghs\_welcome\_e.html</a>.

Ashland product stewardship summaries are located at <a href="http://www.ashland.com/stewardship">http://www.ashland.com/stewardship</a>

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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.