The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

SAFETY DATA SHEET

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

1.1 Product identifiers

- **Product name**: Triirondodecacarbonyl
- **Product Number**: 381411
- **Brand**: Aldrich
- **CAS-No.**: 17685-52-8

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 solids (Category 1), H228
- Acute toxicity, Oral (Category 4), H302
- Acute toxicity, Inhalation (Category 4), H332
- Specific target organ toxicity - single exposure (Category 1), Eyes, H370

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

SECTION 3: Composition/information on ingredients

3.2 Mixtures
Synonyms : tri-Irondodecacarbonyl
Molecular weight : 503.66 g/mol

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>tri-Irondodecacarbonyl</td>
<td>Flam. Sol. 1; Acute Tox. 4; H228, H302, H332</td>
<td>&gt;= 90 - &lt;= 100 %</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>17685-52-8</td>
<td></td>
</tr>
<tr>
<td>EC-No.</td>
<td>241-668-5</td>
<td></td>
</tr>
</tbody>
</table>

| Methanol        | Flam. Liq. 2; Acute Tox. 3; STOT SE 1; H225, H301, H331, H311, H370 | >= 1 - < 5 % |
| CAS-No.         | 67-56-1             |               |
| EC-No.          | 200-659-6           |               |
| Index-No.       | 603-001-00-X        |               |
| Registration number | 01-2119433307-44-XXXX |               |

For the full text of the H-Statements mentioned in this Section, see Section 16.
SECTION 4: First aid measures

4.1 Description of first-aid measures

**General advice**
Show this material safety data sheet to the doctor in attendance.

**If inhaled**
After inhalation: fresh air. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately call in physician.

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

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

**If swallowed**
After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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
Mixture with combustible ingredients.
Vapors are heavier than air and may spread along floors.
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

5.4 Further information

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: Avoid inhalation of dusts. 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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

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.

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
Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Storage conditions
Tightly closed. Keep away from heat and sources of ignition.

Storage stability
Recommended storage temperature
2 - 8 °C

Storage class
Storage class (TRGS 510): 4.1B: Flammable solid hazardous materials

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>
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</thead>
<tbody>
<tr>
<td>Methanol</td>
<td>67-56-1</td>
<td>TWA</td>
<td>200 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>STEL</td>
<td>250 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ST</td>
<td>250 ppm 325 mg/m³</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>200 ppm 260 mg/m³</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PEL</td>
<td>200 ppm 260 mg/m³</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
<tr>
<td></td>
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<td></td>
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<td></td>
<td></td>
<td>USA. Table Z-1-A Limits for Air Contaminants (1989 vacated values)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>USA. Table Z-1-A Limits for Air Contaminants (1989 vacated values)</td>
</tr>
</tbody>
</table>

### Biological occupational exposure limits

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Parameters</th>
<th>Value</th>
<th>Biological specimen</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol</td>
<td>67-56-1</td>
<td>Methanol</td>
<td>15 mg/l</td>
<td>Urine</td>
<td>ACGIH - Biological Exposure Indices (BEI)</td>
</tr>
</tbody>
</table>

**8.2 Exposure controls**

**Appropriate engineering controls**
Change contaminated clothing. Preventive skin protection recommended. Wash hands 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**
Handle with impervious gloves.

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

**Full contact**
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatril® L

**Splash contact**
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatril® L

**Body Protection**
Flame retardant antistatic protective clothing.

**Respiratory protection**
required when dusts 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>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>a) Appearance</td>
<td>Form: powder</td>
</tr>
<tr>
<td></td>
<td>Color: black</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: 165 °C (329 °F) - lit.</td>
</tr>
<tr>
<td>f) Initial boiling point and boiling range</td>
<td>No data available</td>
</tr>
<tr>
<td>g) Flash point</td>
<td>9.7 °C (49.5 °F) - closed cup</td>
</tr>
<tr>
<td>h) Evaporation rate</td>
<td>No data available</td>
</tr>
</tbody>
</table>

Aldrich - 381411
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

9.2 Other safety information
No data available

SECTION 10: Stability and reactivity

10.1 Reactivity
The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

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
no information available

10.5 Incompatible materials
Strong oxidizing agents

10.6 Hazardous decomposition products
In the event of fire: see section 5
SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity
Oral: No data available

Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation
No data available

Serious eye damage/eye irritation
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
Mixture causes damage to organs. - Eyes

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

11.2 Additional Information
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.
Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.

Stomach - Irregularities - Based on Human Evidence

Components

tri-Ironoxidecarbonyl

Acute toxicity
Oral: No data available
Inhalation: No data available  
Dermal: No data available

**Skin corrosion/irritation**  
No data available

**Serious eye damage/eye irritation**  
No data available

**Respiratory or skin sensitization**  
No data available

**Germ cell mutagenicity**  
No data available

**Carcinogenicity**  
No data available

**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

---

**Methanol**

**Acute toxicity**  
Acute toxicity estimate Oral - 100.1 mg/kg  
(Expert judgment)  
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)  
Symptoms: Nausea, Vomiting  
Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l - vapor  
(Expert judgment)  
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)  
Symptoms: Irritation symptoms in the respiratory tract.  
Acute toxicity estimate Dermal - 300.1 mg/kg  
(Expert judgment)  
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

**Skin corrosion/irritation**  
Skin - Rabbit  
Result: No skin irritation  
Remarks: (ECHA)  
Remarks: Drying-out effect resulting in rough and chapped skin.

**Serious eye damage/eye irritation**  
Eyes - Rabbit  
Result: No eye irritation  
Remarks: (ECHA)
Respiratory or skin sensitization
Sensitisation test: - Guinea pig
Result: negative
(OECD Test Guideline 406)

Germ cell mutagenicity
Based on available data the classification criteria are not met.
Test Type: Ames test
Test system: Salmonella typhimurium
Result: negative
Test Type: In vitro mammalian cell gene mutation test
Test system: Chinese hamster lung cells
Result: negative
Method: OECD Test Guideline 474
Species: Mouse - male and female - Bone marrow
Result: negative

Carcinogenicity
Did not show carcinogenic effects in animal experiments.

Reproductive toxicity
Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure
Causes damage to organs. - Eyes, Central nervous system
Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
Acute oral toxicity - Nausea, Vomiting
Acute inhalation toxicity - Irritation symptoms in the respiratory tract.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

SECTION 12: Ecological information

12.1 Toxicity
Mixture
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

Aldrich - 381411
12.7 Other adverse effects
No data available

Components

tri-Irondodecacarbonyl
No data available

Methanol
Toxicity to fish: flow-through test LC50 - Lepomis macrochirus (Bluegill) - 15,400.0 mg/l - 96 h (US-EPA)
Toxicity to daphnia and other aquatic invertebrates: semi-static test EC50 - Daphnia magna (Water flea) - 18,260 mg/l - 96 h (OECD Test Guideline 202)
Toxicity to algae: static test ErC50 - Pseudokirchneriella subcapitata (green algae) - ca. 22,000.0 mg/l - 96 h (OECD Test Guideline 201)
Toxicity to bacteria: static test IC50 - activated sludge - > 1,000 mg/l - 3 h (OECD Test Guideline 209)
Toxicity to fish (Chronic toxicity): NOEC - Oryzias latipes (Orange-red killifish) - 7,900 mg/l - 200 h
Remarks: (External MSDS)

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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)
UN number: 3175 Class: 4.1 Packing group: II
Proper shipping name: Solids containing flammable liquid, n.o.s. (Methanol, tri-Irondodecacarbonyl)
Reportable Quantity (RQ):
 Poison Inhalation Hazard: No

IMDG
UN number: 3175 Class: 4.1 Packing group: II EMS-No: F-A, S-I
Proper shipping name: SOLIDS CONTAINING FLAMMABLE LIQUID, N.O.S. (Methanol, tri-Irondodecacarbonyl)

IATA
Aldrich - 381411
UN number: 3175   Class: 4.1   Packing group: II
Proper shipping name: Solids containing flammable liquid, n.o.s. (Methanol, tri-Irondodecadecarbonyl)

SECTION 15: Regulatory information

SARA 302 Components
This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components
The following components are subject to reporting levels established by SARA Title III, Section 313:

<table>
<thead>
<tr>
<th>Proper shipping name</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol</td>
<td>67-56-1</td>
<td>2007-07-01</td>
</tr>
</tbody>
</table>

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

Massachusetts Right To Know Components

<table>
<thead>
<tr>
<th>Proper shipping name</th>
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</tr>
</thead>
<tbody>
<tr>
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<td>67-56-1</td>
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</table>

Pennsylvania Right To Know Components

<table>
<thead>
<tr>
<th>Proper shipping name</th>
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</tr>
</thead>
<tbody>
<tr>
<td>tri-Irondodecadecarbonyl</td>
<td>17685-52-8</td>
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</tr>
<tr>
<td>Methanol</td>
<td>67-56-1</td>
<td>2007-07-01</td>
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</tbody>
</table>

New Jersey Right To Know Components

<table>
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<tr>
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<tr>
<td>Methanol</td>
<td>67-56-1</td>
<td>2007-07-01</td>
</tr>
</tbody>
</table>

California Prop. 65 Components
, which is/are known to the State of California to cause birth defects or other reproductive harm. For more information go to www.P65Warnings.ca.gov.Methanol

<table>
<thead>
<tr>
<th>Proper shipping name</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
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<tbody>
<tr>
<td>Methanol</td>
<td>67-56-1</td>
<td>2012-03-16</td>
</tr>
</tbody>
</table>
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: 6.4 Revision Date: 02/07/2023 Print Date: 07/08/2023