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

Hazard statement(s)
H228 Flammable solid.
H302 + H332 Harmful if swallowed or if inhaled.
H370 Causes damage to organs (Eyes).

Precautionary statement(s)
P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P240 Ground/bond container and receiving equipment.
P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P260 Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.
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.
P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P307 + P311 IF exposed: Call a POISON CENTER or doctor/ physician.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
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

3.2 Mixtures
Synonyms : tri-Irondodecacarbonyl

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>tri-Irondodecacarbonyl</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CAS-No.</td>
<td>17685-52-8</td>
<td>Flam. Sol. 1; Acute Tox. 4;</td>
</tr>
<tr>
<td>EC-No.</td>
<td>241-668-5</td>
<td>H228, H302, H332 &gt;= 90 - &lt;= 100 %</td>
</tr>
<tr>
<td>Methanol</td>
<td></td>
<td>Flam. Liq. 2; Acute Tox. 3;</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>67-56-1</td>
<td>STOT SE 1; H225, H301,</td>
</tr>
<tr>
<td>EC-No.</td>
<td>200-659-6</td>
<td>H331, H311, H370</td>
</tr>
<tr>
<td>Index-No.</td>
<td>603-001-00-X</td>
<td>Concentration limits:</td>
</tr>
<tr>
<td>Registration number</td>
<td>01-2119433307-44-X</td>
<td>&gt;= 10 %: STOT SE 1, H370; 3 - &lt; 10 %: STOT SE 2, H371;</td>
</tr>
</tbody>
</table>

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>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol</td>
<td>67-56-1</td>
<td>TWA 200 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>STEL 250 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>ST 250 ppm 325 mg/m³</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA 200 ppm 260 mg/m³</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>PEL 200 ppm 260 mg/m³</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Skin C 1,000 ppm</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>STEL 250 ppm 325 mg/m³</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA 200 ppm 260 mg/m³</td>
<td>USA. Table Z-1-A Limits for Air Contaminants (1989 vacated values)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>STEL 250 ppm 325 mg/m³</td>
<td>USA. Table Z-1-A Limits for Air Contaminants (1989 vacated values)</td>
<td></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>

**Remarks**

End of shift (As soon as possible after exposure ceases)
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 EN 16523-1 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**
Recommended Filter type: Filter type P2
The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

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**

a) Appearance  
Form: powder  
Color: black
b) Odor  No data available

c) Odor Threshold  No data available

d) pH  No data available

e) Melting point/freezing point  Melting point/range: 165 °C (329 °F) - lit.

f) Initial boiling point and boiling range  No data available

g) Flash point  9.7 °C (49.5 °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  No data available

l) Vapor density  No data available

m) Density  No data available

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  Not classified as explosive.

t) Oxidizing properties  none

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-Irondodecaboryl

**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

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-Iron dodecacarbonyl)
Reportable Quantity (RQ): Poison Inhalation Hazard: No

IMDG
UN number: 3175   Class: 4.1   Packing group: II
Proper shipping name: SOLIDS CONTAINING FLAMMABLE LIQUID, N.O.S. (Methanol, tri-Iron dodecacarbonyl)

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

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>Component</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>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
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<tbody>
<tr>
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<tr>
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<td>--------------</td>
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</tr>
<tr>
<td>Methanol</td>
<td>67-56-1</td>
<td>2007-07-01</td>
</tr>
<tr>
<td><strong>Pennsylvania Right To Know Components</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>tri-Irondodecacarbonyl</td>
<td>17685-52-8</td>
<td></td>
</tr>
<tr>
<td>Methanol</td>
<td>67-56-1</td>
<td>2007-07-01</td>
</tr>
<tr>
<td><strong>New Jersey Right To Know Components</strong></td>
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</tr>
<tr>
<td>tri-Irondodecacarbonyl</td>
<td>17685-52-8</td>
<td></td>
</tr>
<tr>
<td>Methanol</td>
<td>67-56-1</td>
<td>2007-07-01</td>
</tr>
<tr>
<td><strong>California Prop. 65 Components</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>, which is/are known to the State of California to cause birth defects or other reproductive harm. For more information go to <a href="http://www.P65Warnings.ca.gov">www.P65Warnings.ca.gov</a>.</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.