

---

**1. PRODUCT AND COMPANY IDENTIFICATION****1.1 Product identifiers**

Product name : 3,7-Dimethyl-2,6-octadienenitrile

Product Number : W512508  
Brand : Aldrich

CAS-No. : 5146-66-7

**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Identified uses : Laboratory chemicals, Manufacture of substances

**1.3 Details of the supplier of the safety data sheet**Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USATelephone : +1 800-325-5832  
Fax : +1 800-325-5052**1.4 Emergency telephone number**

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

---

**2. HAZARDS IDENTIFICATION****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Acute toxicity, Inhalation (Category 1), H330

Acute aquatic toxicity (Category 2), H401

Chronic aquatic toxicity (Category 2), H411

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

Hazard statement(s)

H330 : Fatal if inhaled.

H411 : Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P260 : Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.

P271 : Use only outdoors or in a well-ventilated area.

P273 : Avoid release to the environment.

P284 : Wear respiratory protection.

P304 + P340 : IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

P310 : Immediately call a POISON CENTER or doctor/ physician.

P320 : Specific treatment is urgent (see supplemental first aid instructions on this label).

|             |   |
|-------------|---|
| P391        | Collect spillage.   |
| P403 + P233 | Store in a well-ventilated place. Keep container tightly closed.    |
| 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

---

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

|                  |   |                                   |
|------------------|---|-----------------------------------|
| Formula          | : | C <sub>10</sub> H <sub>15</sub> N |
| Molecular Weight | : | 149.23 g/mol                      |
| CAS-No.          | : | 5146-66-7                         |
| EC-No.           | : | 225-918-0                         |

No ingredients are hazardous according to OSHA criteria.

No components need to be disclosed according to the applicable regulations.

For the full text of the H-Statements mentioned in this Section, see Section 16.

---

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

#### In case of eye contact

Flush eyes with water as a precaution.

#### If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

---

## 5. FIREFIGHTING MEASURES

### 5.1 Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides, nitrogen oxides (NO<sub>x</sub>), Hydrogen cyanide (hydrocyanic acid)

### 5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

### 5.4 Further information

no data available

---

## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

For personal protection see section 8.

## 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

## 6.3 Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

## 6.4 Reference to other sections

For disposal see section 13.

---

## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.  
Normal measures for preventive fire protection.  
For precautions see section 2.2.

### 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

---

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

#### Personal protective equipment

##### Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

##### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

##### Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

##### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

---

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |               |                                |
|---------------|--------------------------------|
| a) Appearance | Form: liquid<br>Colour: yellow |
|---------------|--------------------------------|

|   |  |
|---|--|
| b) Odour  | no data available  |
| c) Odour Threshold                              | no data available  |
| d) pH   | no data available  |
| e) Melting point/freezing point                 | Melting point/range: < -30 °C (< -22 °F)                           |
| f) Initial boiling point and boiling range      | 110 °C (230 °F) at 1.7 hPa (1.3 mmHg) - lit.                       |
| g) Flash point                                  | 113 °C (235 °F) - closed cup                                       |
| h) Evaporation rate                             | no data available  |
| i) Flammability (solid, gas)                    | no data available  |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 5.5 %(V)<br>Lower explosion limit: 0.7 %(V) |
| k) Vapour pressure                              | no data available  |
| l) Vapour density                               | no data available  |
| m) Relative density                             | 0.853 g/cm <sup>3</sup> at 25 °C (77 °F)                           |
| n) Water solubility                             | no data available  |
| o) Partition coefficient: n-octanol/water       | log Pow: 3.47  |
| p) Auto-ignition 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**  
no data available

---

**10. STABILITY AND REACTIVITY**

**10.1 Reactivity**

no data available

**10.2 Chemical stability**

Stable under recommended storage conditions.

**10.3 Possibility of hazardous reactions**

no data available

**10.4 Conditions to avoid**

no data available

**10.5 Incompatible materials**

Strong oxidizing agents, Strong acids, Strong bases, Strong oxidizing agents, Strong reducing agents

**10.6 Hazardous decomposition products**

Other decomposition products - no data available

In the event of fire: see section 5

---

## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - rat - 3,100 mg/kg

LC50 Inhalation - rat - 4 h - > 5.2 mg/l

Dermal: no data available

no data available

#### Skin corrosion/irritation

no data available

#### Serious eye damage/eye irritation

no data available

#### Respiratory or skin sensitisation

no data available

#### Germ cell mutagenicity

In vitro tests showed mutagenic effects In vitro tests showed mutagenic effects which were not observed with in vivo test.

#### Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component 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 identified as a carcinogen or potential carcinogen by OSHA.

#### Reproductive toxicity

##### Specific target organ toxicity - single exposure

no data available

##### Specific target organ toxicity - repeated exposure

no data available

#### Aspiration hazard

no data available

#### Additional Information

RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

---

## 12. ECOLOGICAL INFORMATION

### 12.1 Toxicity

no data available

Toxicity to daphnia and other aquatic invertebrates EC50 - Daphnia magna (Water flea) - 7.66 mg/l - 48 h

### 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 Other adverse effects**  
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.  
Toxic to aquatic life.

---

## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

#### Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

#### Contaminated packaging

Dispose of as unused product.

---

## 14. TRANSPORT INFORMATION

### DOT (US)

Not dangerous goods

### IMDG

UN number: 3082      Class: 9      Packing group: III      EMS-No: F-A, S-F  
Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (3,7-Dimethylocta-2,6-dienenitrile)  
Marine pollutant: Marine pollutant

### IATA

UN number: 3082      Class: 9      Packing group: III  
Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (3,7-Dimethylocta-2,6-dienenitrile)

### Further information

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids.

---

## 15. REGULATORY INFORMATION

### SARA 302 Components

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

### SARA 313 Components

SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

### SARA 311/312 Hazards

No SARA Hazards

### Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

### Pennsylvania Right To Know Components

|                                   | CAS-No.   | Revision Date |
|-----------------------------------|-----------|---------------|
| 3,7-Dimethylocta-2,6-dienenitrile | 5146-66-7 |               |

### New Jersey Right To Know Components

|                                   | CAS-No.   | Revision Date |
|-----------------------------------|-----------|---------------|
| 3,7-Dimethylocta-2,6-dienenitrile | 5146-66-7 |               |

### California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

---

## 16. OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3.

|      |  |
|------|--|
| H330 | Fatal if inhaled.                                |
| H401 | Toxic to aquatic life.                           |
| H411 | Toxic to aquatic life with long lasting effects. |

### HMIS Rating

|                        |   |
|------------------------|---|
| Health hazard:         | 1 |
| Chronic Health Hazard: |   |
| Flammability:          | 1 |
| Physical Hazard        | 0 |

### NFPA Rating

|                    |   |
|--------------------|---|
| Health hazard:     | 0 |
| Fire Hazard:       | 1 |
| Reactivity Hazard: | 0 |

### Further information

Copyright 2014 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only. 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](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

### Preparation Information

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

Version: 5.3

Revision Date: 07/09/2014

Print Date: 11/16/2018