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

Product name : 2,4,6-Cycloheptatriene-1-carbonitrile

Product Number : 393320

Brand : Aldrich

CAS-No. : 13612-59-4

**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  
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

**1.4 Emergency telephone number**

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

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

Flammable liquids (Category 4), H227

Acute toxicity, Oral (Category 4), H302

Acute toxicity, Inhalation (Category 4), H332

Acute toxicity, Dermal (Category 4), H312

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 : Warning

Hazard statement(s)

H227

Combustible liquid.

H302 + H312 + H332

Harmful if swallowed, in contact with skin or if inhaled

Precautionary statement(s)

P210

Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

P261

Avoid breathing dust/ fume/ gas/ mist/ vapours/ 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/ protective clothing/ eye protection/ face protection.

P301 + P312

IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you

|   |  |
|---|--|
| P302 + P352<br>P304 + P340                  | feel unwell.<br>IF ON SKIN: Wash with plenty of soap and water.<br>IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.  |
| P312<br>P322<br>P330<br>P363<br>P370 + P378 | Call a POISON CENTER or doctor/ physician if you feel unwell.<br>Specific measures (see supplemental first aid instructions on this label).<br>Rinse mouth.<br>Wash contaminated clothing before reuse.<br>In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction. |
| P403 + P235<br>P501                         | Store in a well-ventilated place. Keep cool.<br>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>8</sub> H <sub>7</sub> N |
| Molecular weight | : 117.15 g/mol                    |
| CAS-No.          | : 13612-59-4                      |

#### Hazardous components

| Component                                    | Classification  | Concentration |
|--|---|---------------|
| <b>2,4,6-Cycloheptatriene-1-carbonitrile</b> |   |               |
|  | Flam. Liq. 4; Acute Tox. 4;<br>H227, H302 + H312 + H332 | <= 100 %      |

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. Move out of dangerous area.

#### 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. Consult a physician.

#### In case of eye contact

Flush eyes with water as a precaution.

#### If swallowed

Do NOT induce vomiting. 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

For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

- 5.2 Special hazards arising from the substance or mixture**  
Carbon oxides, Nitrogen oxides (NOx), Hydrogen cyanide (hydrocyanic acid)
- 5.3 Advice for firefighters**  
Wear self-contained breathing apparatus for firefighting if necessary.
- 5.4 Further information**  
Use water spray to cool unopened containers.

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## 6. ACCIDENTAL RELEASE MEASURES

- 6.1 Personal precautions, protective equipment and emergency procedures**  
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low 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.
- 6.3 Methods and materials for containment and cleaning up**  
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal.
- 6.4 Reference to other sections**  
For disposal see section 13.

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## 7. HANDLING AND STORAGE

- 7.1 Precautions for safe handling**  
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.  
Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.  
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

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## 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**  
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.
- 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.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

|   |  |
|---|--|
| a) Appearance                                   | Form: liquid<br>Colour: light yellow                   |
| b) Odour  | No data available                                      |
| c) Odour Threshold                              | No data available                                      |
| d) pH   | No data available                                      |
| e) Melting point/freezing point                 | No data available                                      |
| f) Initial boiling point and boiling range      | 51 - 53 °C (124 - 127 °F) at 2.0 hPa (1.5 mmHg) - lit. |
| g) Flash point                                  | 85 °C (185 °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) Vapour pressure                              | No data available                                      |
| l) Vapour density                               | No data available                                      |
| m) Relative density                             | 1.017 g/cm <sup>3</sup> at 25 °C (77 °F)               |
| n) Water solubility                             | No data available                                      |
| o) Partition coefficient: n-octanol/water       | No data available                                      |
| 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

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## 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

Heat, flames and sparks.

#### 10.5 Incompatible materials

Strong oxidizing agents

#### 10.6 Hazardous decomposition products

Other decomposition products - No data available

In the event of fire: see section 5

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### 11. TOXICOLOGICAL INFORMATION

#### 11.1 Information on toxicological effects

##### Acute toxicity

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

No data available

##### 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

No data available

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

##### Additional Information

RTECS: Not available

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

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### 12. ECOLOGICAL INFORMATION

#### 12.1 Toxicity

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 Other adverse effects**

No data available

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**13. DISPOSAL CONSIDERATIONS****13.1 Waste treatment methods****Product**

This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company.

**Contaminated packaging**

Dispose of as unused product.

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**14. TRANSPORT INFORMATION****DOT (US)**

NA-Number: 1993

Class: NONE

Packing group: III

Proper shipping name: Combustible liquid, n.o.s. (2,4,6-Cycloheptatriene-1-carbonitrile)

Poison Inhalation Hazard: No

**IMDG**

Not dangerous goods

**IATA**

Not dangerous goods

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**15. REGULATORY INFORMATION****SARA 302 Components**

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

**SARA 313 Components**

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**

Fire Hazard, Acute Health Hazard

**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 |
|---------------------------------------|------------|---------------|
| 2,4,6-Cycloheptatriene-1-carbonitrile | 13612-59-4 |               |

**New Jersey Right To Know Components**

|                                       | CAS-No.    | Revision Date |
|---------------------------------------|------------|---------------|
| 2,4,6-Cycloheptatriene-1-carbonitrile | 13612-59-4 |               |

**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.

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## 16. OTHER INFORMATION

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

|                       |  |
|-----------------------|--|
| Acute Tox.            | Acute toxicity   |
| Flam. Liq.            | Flammable liquids  |
| H227                  | Combustible liquid.                                      |
| H302                  | Harmful if swallowed.                                    |
| H302 + H312 +<br>H332 | Harmful if swallowed, in contact with skin or if inhaled |

### HMIS Rating

|                        |   |
|------------------------|---|
| Health hazard:         | 1 |
| Chronic Health Hazard: |   |
| Flammability:          | 2 |
| Physical Hazard        | 0 |

### NFPA Rating

|                    |   |
|--------------------|---|
| Health hazard:     | 1 |
| Fire Hazard:       | 2 |
| Reactivity Hazard: | 0 |

### Further information

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### Preparation Information

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

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