

## SAFETY DATA SHEET

Version 6.0

Revision Date 05/28/2017

Print Date 09/23/2019

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1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : 2-Chloro-2,4,6-cycloheptatrien-1-one

Product Number : 669571

Brand : Aldrich

CAS-No. : 3839-48-3

## 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 Street  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

## 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887

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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)**

Acute toxicity, Oral (Category 4), H302

Skin corrosion (Category 1B), H314

Serious eye damage (Category 1), H318

Respiratory sensitisation (Category 1), H334

Skin sensitisation (Category 1), H317

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)

H302

Harmful if swallowed.

H314

Causes severe skin burns and eye damage.

H317

May cause an allergic skin reaction.

H334

May cause allergy or asthma symptoms or breathing difficulties if inhaled.

Precautionary statement(s)	
P260	Do not breathe dust or mist.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P272	Contaminated work clothing should not be allowed out of the workplace.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P285	In case of inadequate ventilation wear respiratory protection.
P301 + P312	IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.
P301 + P330 + P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310	Immediately call a POISON CENTER/doctor.
P321	Specific treatment (see supplemental first aid instructions on this label).
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P363	Wash contaminated clothing before reuse.
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

Lachrymator.

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Synonyms : 2-Chlorocycloheptatrienone  
2-Chlorotropone

Formula : C<sub>7</sub>H<sub>5</sub>ClO  
Molecular weight : 140.57 g/mol  
CAS-No. : 3839-48-3

#### Hazardous components

Component	Classification	Concentration
<b>2-Chloro-2,4,6-cycloheptatrien-1-one</b>		
	Acute Tox. 4; Skin Corr. 1B; Eye Dam. 1; Resp. Sens. 1; Skin Sens. 1; H302, H314, H317, H334	<= 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

Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Consult a physician.

**In case of eye contact**

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician. Continue rinsing eyes during transport to hospital.

**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

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**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, Hydrogen chloride gas

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**5.4 Further information**

No data available

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**6. ACCIDENTAL RELEASE MEASURES****6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.  
For personal protection see section 8.

**6.2 Environmental precautions**

Do not let product enter drains.

**6.3 Methods and materials for containment and cleaning up**

Pick up and arrange disposal without creating dust. Sweep up and shovel. 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 formation of dust and aerosols.  
Provide appropriate exhaust ventilation at places where dust is formed. 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.

Moisture sensitive. Store under inert gas. Keep in a dry place.

**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.

#### Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

#### Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industria situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

#### 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 (EN 143) respirator cartridges as a backup to engineering controls. If th 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

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: Powder with lumps<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            | 63 - 64 °C (145 - 147 °F)                       |
| f) Initial boiling point and boiling range | 95 - 97 °C (203 - 207 °F) at 0.07 hPa           |
| g) Flash point                             | ( )No data available                            |
| 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	No data available
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	log Pow: 1.75
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

No data available

### 10.5 Incompatible materials

Strong oxidizing agents, Water

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen chloride gas

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

Inhalation: No data available(2-Chloro-2,4,6-cycloheptatrien-1-one)

Dermal: No data available(2-Chloro-2,4,6-cycloheptatrien-1-one)

LD50 Intravenous - Mouse - 47 mg/kg(2-Chloro-2,4,6-cycloheptatrien-1-one)

LD50 Subcutaneous - Mouse - 93 mg/kg(2-Chloro-2,4,6-cycloheptatrien-1-one)

#### Skin corrosion/irritation

No data available(2-Chloro-2,4,6-cycloheptatrien-1-one)

#### Serious eye damage/eye irritation

No data available(2-Chloro-2,4,6-cycloheptatrien-1-one)

## **Respiratory or skin sensitisation**

## **Germ cell mutagenicity**

### **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(2-Chloro-2,4,6-cycloheptatrien-1-one)

No data available(2-Chloro-2,4,6-cycloheptatrien-1-one)

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

No data available(2-Chloro-2,4,6-cycloheptatrien-1-one)

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

No data available

### **Aspiration hazard**

No data available(2-Chloro-2,4,6-cycloheptatrien-1-one)

### **Additional Information**

RTECS: GU4025000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.(2-Chloro-2,4,6-cycloheptatrien-1-one)

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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(2-Chloro-2,4,6-cycloheptatrien-1-one)

### **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**

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chem scrubber.

**Contaminated packaging**

Dispose of as unused product.

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

UN number: 3261      Class: 8      Packing group: III  
Proper shipping name: Corrosive solid, acidic, organic, n.o.s. (2-Chloro-2,4,6-cycloheptatrien-1-one)  
Poison Inhalation Hazard: No

**IMDG**

UN number: 3261      Class: 8      Packing group: III      EMS-No: F-A, S-B  
Proper shipping name: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (2-Chloro-2,4,6-cycloheptatrien-1-one)

**IATA**

UN number: 3261      Class: 8      Packing group: III  
Proper shipping name: Corrosive solid, acidic, organic, n.o.s. (2-Chloro-2,4,6-cycloheptatrien-1-one)

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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**

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-Chloro-2,4,6-cycloheptatrien-1-one	3839-48-3	

**New Jersey Right To Know Components**

	CAS-No.	Revision Date
2-Chloro-2,4,6-cycloheptatrien-1-one	3839-48-3	

**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.**

H302	Harmful if swallowed.
H314	Causes severe skin burns and eye damage.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.

**HMIS Rating**

Health hazard:	3
Chronic Health Hazard:	*
Flammability:	0
Physical Hazard	0

**NFPA Rating**

Health hazard: 3

Fire Hazard: 0

Reactivity Hazard: 0

**Further information**

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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

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