

## SAFETY DATA SHEET

Version 6.8  
Revision Date 08/07/2024  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : Cycloheptatriene, 95%

Product Number : C99205  
Brand : Aldrich

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

**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 liquids (Category 2), H225  
Acute toxicity, Oral (Category 3), H301  
Acute toxicity, Dermal (Category 3), H311  
Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319

Aldrich - C99205

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Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335  
Short-term (acute) aquatic hazard (Category 3), H402  
Long-term (chronic) aquatic hazard (Category 3), H412

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 Statements

H225	Highly flammable liquid and vapor.
H301 + H311	Toxic if swallowed or in contact with skin.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H412	Harmful to aquatic life with long lasting effects.

Precautionary Statements

P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P261	Avoid breathing mist or vapors.
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.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
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

Component		Classification	Concentration
<b>1,3,5-cycloheptatriene</b>			
CAS-No.	544-25-2	Flam. Liq. 2; Acute Tox. 3; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H225, H301, H311, H315, H319, H335	>= 90 - <= 100 %
EC-No.	208-866-3		
<b>butyl hydroxytoluene (BHT)</b>			
CAS-No.	128-37-0	Aquatic Acute 1; Aquatic Chronic 1; H400, H410 M-Factor - Aquatic Acute: 1 - Aquatic Chronic: 1	>= 0.1 - < 1 %
EC-No.	204-881-4		
Registration			
number	01-2119565113-46-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

No data available

#### 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

No data available

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

Carbon oxides

Carbon oxides

Mixture with combustible ingredients.

#### 5.3 Advice for firefighters

No data available

#### 5.4 Further information

No data available

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## SECTION 6: Accidental release measures

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

For personal protection see section 8.

### 6.2 Environmental precautions

No data available

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

No data available

### 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

For precautions see section 2.2.

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

No data available

### 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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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
butyl hydroxytoluene (BHT)	128-37-0	TWA	2 mg/m <sup>3</sup>	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen		
		TWA	10 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		PEL	10 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

### 8.2 Exposure controls

#### Personal protective equipment

##### 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: Fluorinated rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 30 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, 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 EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

### **Control of environmental exposure**

Prevent product from entering drains.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

- |   |                   |
|---|-------------------|
| a) Appearance                                   | Form: liquid      |
| b) Odor   | No data available |
| c) Odor Threshold                               | No data available |
| d) pH   | No data available |
| e) Melting point/freezing point                 | No data available |
| f) Initial boiling point and boiling range      | No data available |
| g) Flash point                                  | 5 °C (41 °F)      |
| 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	No data available
t) Oxidizing properties	No data available

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

No data available

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Mixture

#### Acute toxicity

Oral: No data available

Acute toxicity estimate Oral - 100.6 mg/kg

(Calculation method)

Inhalation: No data available

Dermal: No data available

Acute toxicity estimate Dermal - 301.61 mg/kg

(Calculation method)

**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 may cause respiratory irritation.

**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.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

**Components**

**1,3,5-cycloheptatriene**

**Acute toxicity**

Acute toxicity estimate Oral - 100.1 mg/kg

(Expert judgment)

Inhalation: Irritating to respiratory system.

Acute toxicity estimate Dermal - 300.1 mg/kg  
(Expert judgment)

**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**

May cause respiratory irritation.

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**butyl hydroxytoluene (BHT)**

**Acute toxicity**

LD50 Oral - Rat - male and female - > 6,000 mg/kg

(OECD Test Guideline 401)

Inhalation: No data available

LD50 Dermal - Rat - male and female - > 2,000 mg/kg

(OECD Test Guideline 402)

**Skin corrosion/irritation**

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

**Serious eye damage/eye irritation**

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

**Respiratory or skin sensitization**

Patch test: - In vitro study

Result: negative

Remarks: (ECHA)



**Germ cell mutagenicity**

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Remarks: (ECHA)

Test Type: In vitro mammalian cell gene mutation test

Test system: rat hepatocytes

Result: negative

Remarks: (ECHA)

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary cells

Result: negative

Remarks: (ECHA)

Species: Mouse - male and female - Bone marrow

Result: negative

Remarks: (ECHA)

Species: Rat - male - Bone marrow

Result: negative

Remarks: (ECHA)

**Carcinogenicity**

This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

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**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

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**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

#### 1,3,5-cycloheptatriene

No data available

#### butyl hydroxytoluene (BHT)

Toxicity to fish	semi-static test LC50 - Danio rerio (zebra fish) - > 0.57 mg/l - 96 h (Directive 67/548/EEC, Annex V, C.1.)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 0.48 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Desmodesmus subspicatus (green algae) - > 0.4 mg/l - 72 h (Regulation (EC) No. 440/2008, Annex, C.3)
Toxicity to bacteria	static test EC50 - activated sludge - > 10,000 mg/l - 3 h (OECD Test Guideline 209)
Toxicity to fish(Chronic toxicity)	NOEC - Oryzias latipes - 0.053 mg/l - 30 d (OECD Test Guideline 210)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	EC50 - Daphnia magna (Water flea) - 0.096 mg/l - 21 d (OECD Test Guideline 211)

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

No data available

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## SECTION 14: Transport information

### DOT (US)

UN number: 2603    Class: 3 (6.1)    Packing group: II  
Proper shipping name: Cycloheptatriene  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

UN number: 2603    Class: 3 (6.1)    Packing group: II    EMS-No: F-E, S-D  
Proper shipping name: CYCLOHEPTATRIENE

### IATA

UN number: 2603    Class: 3 (6.1)    Packing group: II  
Proper shipping name: Cycloheptatriene

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## SECTION 15: Regulatory information

### CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

### SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

### SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

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

**SARA 311/312 Hazards** : Fire Hazard  
Acute Health Hazard

**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.

### US State Regulations

#### Massachusetts Right To Know

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

#### Maine Chemicals of High Concern

Product does not contain any listed chemicals

#### Vermont Chemicals of High Concern

Product does not contain any listed chemicals

## **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

### **The ingredients of this product are reported in the following inventories:**

TSCA : Product contains substance(s) not listed on TSCA inventory.

### **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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## **SECTION 16: Other information**

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

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