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

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
- 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

Aldrich - C99205
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

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

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,3,5-cycloheptatriene</td>
<td>Flam. Liq. 2; Acute Tox. 3; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H225, H301, H311, H315, H319, H335</td>
<td>&gt;= 90 - &lt;= 100 %</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>544-25-2</td>
<td></td>
</tr>
<tr>
<td>EC-No.</td>
<td>208-866-3</td>
<td></td>
</tr>
</tbody>
</table>

| butyl hydroxytoluene (BHT)       | Aquatic Acute 1; Aquatic Chronic 1; H400, H410 M-Factor - Aquatic Acute: 1 - Aquatic Chronic: 1 | >= 0.1 - < 1 %    |
| CAS-No.                          | 128-37-0                                            |                   |
| 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

**General advice**
First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

**If inhaled**
After inhalation: fresh air.

**In case of skin contact**
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Call a physician immediately.

**In case of eye contact**
After eye contact: rinse out with plenty of water. Call an ophthalmologist. Remove contact lenses.

**If swallowed**
If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

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**
- 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
- Carbon oxides
- Mixture with combustible ingredients.
- Pay attention to flashback.
- Vapors are heavier than air and may spread along floors.
- Development of hazardous combustion gases or vapours possible in the event of fire.
- Forms explosive mixtures with air at ambient temperatures.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Remove container from danger zone and cool with water. 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: Do not breathe vapors, aerosols. 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 carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

**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**  
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.  
For precautions see section 2.2.

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

**Storage conditions**  
Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

**Storage stability**  
Recommended storage temperature 2 - 8 °C

**Storage class**  
Storage class (TRGS 510): 3: Flammable liquids

### 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>butyl hydroxytoluene (BHT)</td>
<td>128-37-0</td>
<td>TWA</td>
<td>2 mg/m3</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Remarks Not classifiable as a human carcinogen</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>10 mg/m3</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PEL</td>
<td>10 mg/m3</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
</tbody>
</table>

**8.2 Exposure controls**

**Appropriate engineering controls**  
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face 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 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.

**Body Protection**
Flame retardant antistatic protective clothing.

**Respiratory protection**
Recommended Filter type: Filter type ABEK
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 vapours/aerosols 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: 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

SECTION 10: Stability and reactivity

10.1 Reactivity
Vapors may form explosive mixture with air.

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
Warming.
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
Acute toxicity estimate Oral - 100.6 mg/kg
(Calculation method)
Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.
Symptoms: Possible symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages: damage of respiratory tract
Dermal: No data available
Acute toxicity estimate Dermal - 301.61 mg/kg
(Calculation method)

Skin corrosion/irritation
Remarks: Mixture causes skin irritation.

Serious eye damage/eye irritation
Remarks: Mixture causes serious eye irritation.

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
11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. Other dangerous properties cannot 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
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

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

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

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

Toxicity to bacteria static test EC50 - activated sludge - > 10,000 mg/l - 3 h
(OECD Test Guideline 209)

Toxicity to NOEC - Oryzias latipes - 0.053 mg/l - 30 d
SECTON 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: 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
- Proper shipping name: CYCLOHEPTATRIENE
- EMS-No: F-E, S-D

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

SECTION 15: Regulatory information

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

**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.

SECTION 16: Other information

Further information
The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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. Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only. 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 misbranding@sial.com.

Version: 6.6  Revision Date: 11/27/2023  Print Date: 01/06/2024