

SAFETY DATA SHEET

Version 6.4
Revision Date 08/24/2022
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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : *p*-Cymene
Product Number : C121452
Brand : Aldrich
Index-No. : 601-094-00-1
CAS-No. : 99-87-6

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 3), H226
Acute toxicity, Inhalation (Category 3), H331
Reproductive toxicity (Category 2), H361
Aspiration hazard (Category 1), H304
Short-term (acute) aquatic hazard (Category 2), H401
Long-term (chronic) aquatic hazard (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) | |
| H226 | Flammable liquid and vapor. |
| H304 | May be fatal if swallowed and enters airways. |
| H331 | Toxic if inhaled. |
| H361 | Suspected of damaging fertility or the unborn child. |
| H411 | Toxic to aquatic life with long lasting effects. |
| Precautionary statement(s) | |
| P201 | Obtain special instructions before use. |
| P202 | Do not handle until all safety precautions have been read and understood. |
| 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. |
| P271 | Use only outdoors or in a well-ventilated area. |
| P273 | Avoid release to the environment. |
| P280 | Wear protective gloves/ protective clothing/ eye protection/ face protection. |
| P301 + P310 | IF SWALLOWED: Immediately call a POISON CENTER/ doctor. |
| P303 + P361 + P353 | IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower. |
| P304 + P340 + P311 | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor. |
| P308 + P313 | IF exposed or concerned: Get medical advice/ attention. |
| P331 | Do NOT induce vomiting. |
| P370 + P378 | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish. |
| P391 | Collect spillage. |
| 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

May form explosive peroxides.

SECTION 3: Composition/information on ingredients

3.1 Substances

| | |
|------------------|---|
| Synonyms | : 1-Isopropyl-4-methylbenzene 4-Isopropyltoluene |
| Formula | : C ₁₀ H ₁₄ |
| Molecular weight | : 134.22 g/mol |
| CAS-No. | : 99-87-6 |
| EC-No. | : 202-796-7 |

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| Component | Classification | Concentration |
|-----------------|--|---------------|
| p-Cymene | | |
| | Flam. Liq. 3; Acute Tox. 3; Repr. 2; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 2; H226, H331, H361, H304, H401, H411 | <= 100 % |

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. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact

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

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

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

Combustible.

Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air at elevated temperatures.
Development of hazardous combustion gases or vapours possible in the event of fire.

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 safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

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

Change contaminated clothing. Preventive skin protection recommended. Wash hands 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 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

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Change contaminated clothing. Preventive skin protection recommended. Wash hands 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

required

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

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, clear Color: colorless |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/freezing point: < -20 °C (< -4 °F) - OECD Test Guideline 102 |
| f) Initial boiling point and boiling range | 176 - 178 °C 349 - 352 °F - lit. |
| g) Flash point | 52 °C (126 °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: 5.6 %(V) Lower explosion limit: 0.7 %(V) |
| k) Vapor pressure | 3.6 hPa at 25 °C (77 °F) - OECD Test Guideline 104 |
| l) Vapor density | No data available |
| m) Density | 0.86 g/cm ³ at 25 °C (77 °F) - lit. |
| Relative density | No data available |
| n) Water solubility | 0.015 g/l at 20 °C (68 °F) - OECD Test Guideline 105 |
| o) Partition coefficient: n-octanol/water | log Pow: 4.8 at ca.20 °C (ca.68 °F) - OECD Test Guideline 117 |
| p) Autoignition temperature | > 400 °C (> 752 °F) at 994 hPa |
| q) Decomposition temperature | No data available |
| r) Viscosity | No data available |
| s) Explosive properties | No data available |
| t) Oxidizing properties | none |

9.2 Other safety information

| | |
|------------------------------|-------------------|
| Solubility in other solvents | Alcohol - soluble |
|------------------------------|-------------------|

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .
Stable under recommended storage conditions.

Test for peroxide formation before distillation or evaporation. Test for peroxide formation or discard after 1 year.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heating.

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

Acute toxicity

LD50 Oral - Rat - male and female - 4,750 mg/kg

LC50 Inhalation - Rat - 4 h - 3 mg/l - vapor

(Acute toxicity estimate)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

LD50 Dermal - Rabbit - > 5,000 mg/kg

Remarks: (ECHA)

No data available

Skin corrosion/irritation

No data available

Skin - reconstructed human epidermis (RhE)

Result: No skin irritation

(OECD Test Guideline 439)

Serious eye damage/eye irritation

Eyes - Humans

Result: No eye irritation

(OECD Test Guideline 492)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative

(OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Chromosome aberration test in vitro

Test system: Human lymphocytes

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster fibroblasts

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

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

Suspected of damaging fertility.

Developmental Toxicity- Rat- male and female- Oral

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

May be fatal if swallowed and enters airways.

11.2 Additional Information

Repeated dose toxicity - Rat - male - Oral - NOAEL (No observed adverse effect level) - 50 mg/kg

Repeated dose toxicity - Rat - male - Inhalation

Remarks: (ECHA)

RTECS: GZ5950000

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

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish static test LC50 - Cyprinodon variegatus (sheepshead minnow) - 48 mg/l - 96 h
(OPPTS 850.1075)

Toxicity to daphnia semi-static test EC50 - Daphnia magna (Water flea) - 3.7 mg/l - 48 h
and other aquatic h
invertebrates (OECD Test Guideline 202)

Toxicity to algae static test EC50 - Scenedesmus capricornutum (fresh water algae) - 4.03 mg/l - 72 h
(OECD Test Guideline 201)

Toxicity to bacteria static test NOEC - activated sludge - 100 mg/l - 28 d

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 14 d
Result: 88 % - Readily biodegradable.
(OECD Test Guideline 301C)

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

SECTION 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.

SECTION 14: Transport information

DOT (US)

UN number: 2046 Class: 3 Packing group: III
Proper shipping name: Cymenes
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 2046 Class: 3 Packing group: III EMS-No: F-E, S-D
Proper shipping name: CYMENES
Marine pollutant : yes

IATA

UN number: 2046 Class: 3 Packing group: III
Proper shipping name: Cymenes

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 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

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