

SAFETY DATA SHEET

Version 6.7
Revision Date 08/05/2024
Print Date 08/06/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : *p*-Cymene
Product Number : W235601
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
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 3), H226
Acute toxicity, Inhalation (Category 3), H331
Reproductive toxicity (Category 2), H361

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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 Statements

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 Statements

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 : C₁₀H₁₄
Molecular weight : 134.22 g/mol
CAS-No. : 99-87-6
EC-No. : 202-796-7
Index-No. : 601-094-00-1

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

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
Combustible.

5.3 Advice for firefighters

No data available

5.4 Further information

No data available

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.

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

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

No data available

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 | 176 - 178 °C 349 - 352 °F - lit. |

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and boiling range

- | | |
|---|--|
| 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
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SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

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

No data available

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

Acute toxicity estimate Inhalation - 4 h - 3 mg/l - vapor

(Expert judgment)

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

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

Remarks: (ECHA)

No data available

Skin corrosion/irritation

Remarks: 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 and other aquatic invertebrates	semi-static test EC50 - Daphnia magna (Water flea) - 3.7 mg/l - 48 h (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

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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

No data available

SECTION 14: Transport information

DOT (US)

UN number: 2046 Class: 3 Packing group: III
Proper shipping name: Cymenes
Reportable Quantity (RQ):
Marine pollutant: yes 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
Marine pollutant : yes

IATA

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

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.

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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

p-Cymene 99-87-6

Pennsylvania Right To Know

p-Cymene 99-87-6

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 : All substances listed as active on the 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.

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.

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