

SAFETY DATA SHEET

Version 6.4
Revision Date 08/06/2021
Print Date 06/18/2022**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**Product name : Ocimene
Product Number : W353901
Brand : Aldrich
CAS-No. : 13877-91-3**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 sheetCompany : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATESTelephone : +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
Self-heating chemicals (Category 2), H252
Skin irritation (Category 2), H315
Aspiration hazard (Category 1), H304
Short-term (acute) aquatic hazard (Category 1), H400
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

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Hazard statement(s)	
H226	Flammable liquid and vapor.
H252	Self-heating in large quantities; may catch fire.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H400	Very toxic to aquatic life.
H411	Toxic to aquatic life with long lasting effects.
Precautionary statement(s)	
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P235 + P410	Keep cool. Protect from sunlight.
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.
P264	Wash skin thoroughly after handling.
P273	Avoid release to the environment.
P280	Wear protective gloves/ 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.
P331	Do NOT induce vomiting.
P332 + P313	If skin irritation occurs: 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.
P391	Collect spillage.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P407	Maintain air gap between stacks/ pallets.
P420	Store away from other materials.
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

3.1 Substances

Synonyms	:	3,7-Dimethyl-1,3,6-octatriene 3,7-Dimethyl-1,3,6-octatrien
Formula	:	C ₁₀ H ₁₆
Molecular weight	:	136.23 g/mol
CAS-No.	:	13877-91-3
EC-No.	:	237-641-2

Component	Classification	Concentration
3,7-Dimethylocta-1,3,6-triene		
	Flam. Liq. 3; 2; Skin Irrit. 2; Asp. Tox. 1; Aquatic	<= 100 %

	Acute 1; Aquatic Chronic 2; H226, H252, H315, H304, H400, H411	
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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

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.

In case of eye contact

After eye contact: rinse out with plenty of water. 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 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

Tightly closed. Keep away from heat and sources of ignition.

Storage class

Storage class (TRGS 510): 4.2: Pyrophoric and self-heating hazardous materials

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

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

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 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) at 1,013 hPa - (ECHA)
f) Initial boiling point and boiling range	65 - 66 °C 149 - 151 °F at 17 hPa
g) Flash point	56 °C (133 °F) - closed cup - Regulation (EC) No. 440/2008, Annex, A.9
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	2.2 hPa at 24 °C (75 °F) - OECD Test Guideline 104
l) Vapor density	No data available
m) Density	0.818 g/cm ³ at 20 °C (68 °F) - lit.
Relative density	0.798 at 20 °C (68 °F)

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|---|--|
| n) Water solubility | 0.0145 g/l at 24 °C (75 °F) - OECD Test Guideline 105 - slightly soluble |
| o) Partition coefficient: n-octanol/water | log Pow: 5.4 at 25 °C (77 °F) - OECD Test Guideline 117 |
| p) Autoignition temperature | Self-heating in large quantities; may catch fire. |
| 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

Vapor/air-mixtures are explosive at intense warming.

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

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 - 5,000 mg/kg

(OECD Test Guideline 401)

Inhalation: No data available

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

(OECD Test Guideline 402)

No data available

Skin corrosion/irritation

Skin - human skin

Result: Skin irritation

(OECD Test Guideline 439)

Serious eye damage/eye irritation

Eyes - chicken

Result: No eye irritation

(OECD Test Guideline 438)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative

(OECD Test Guideline 429)

Germ cell mutagenicity

No data available

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

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

No data available

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

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 daphnia and other aquatic invertebrates semi-static test EC50 - *Daphnia magna* (Water flea) - 1.47 mg/l - 48 h
(OECD Test Guideline 202)

Toxicity to algae static test ErC50 - *Pseudokirchneriella subcapitata* (green algae) - 0.342 mg/l - 48 h
(OECD Test Guideline 201)

static test EbC50 - *Pseudokirchneriella subcapitata* (green algae) -

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0.31 mg/l - 48 h
(OECD Test Guideline 201)

static test EC10 - Pseudokirchneriella subcapitata (green algae) -
0.274 mg/l - 48 h
(OECD Test Guideline 201)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
Result: 73 % - Readily biodegradable.
(OECD Test Guideline 310)

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 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. 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: 2319 Class: 3 Packing group: III
Proper shipping name: Terpene hydrocarbons, n.o.s.
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 2319 Class: 3 Packing group: III EMS-No: F-E, S-D
Proper shipping name: TERPENE HYDROCARBONS, N.O.S. (3,7-Dimethylocta-1,3,6-triene)
Marine pollutant : yes

IATA

UN number: 2319 Class: 3 Packing group: III
Proper shipping name: Terpene hydrocarbons, n.o.s.

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

Massachusetts Right To Know Components

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

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

Pennsylvania Right To Know Components

3,7-Dimethylocta-1,3,6-triene	CAS-No. 13877-91-3	Revision Date
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New Jersey Right To Know Components

3,7-Dimethylocta-1,3,6-triene	CAS-No. 13877-91-3	Revision Date
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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 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.

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