

• SAFETY DATA SHEET

Version 6.6
Revision Date 11/17/2025
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : 3-Methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)-4-penten-2-ol

Product Number : 44064
Brand : Sigma-Aldrich
CAS-No. : 67801-20-1

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 number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Short-term (acute) : Category 2

aquatic hazard

Long-term (chronic) aquatic hazard : Category 2

Other hazards

None known.

GHS label elements

Hazard pictograms :



Hazard statements : H411 Toxic to aquatic life with long lasting effects.

Precautionary statements : **Prevention:**
P273 Avoid release to the environment.

Response:
P391 Collect spillage.

Disposal:
P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 67801-20-1

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
3-Methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)-4-penten-2-ol	67801-20-1*	>= 90 - <= 100	-

* Indicates that the identifier is a CAS No.
Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

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: make victim drink water (two glasses at most). Consult doctor if feeling unwell.
- 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
- Protection of first-aiders : For personal protection see section 8.
- Notes to physician : No data available

SECTION 5. FIREFIGHTING MEASURES

- Suitable extinguishing media : Foam
Carbon dioxide (CO₂)
Dry powder
- Unsuitable extinguishing media : For this substance/mixture no limitations of extinguishing agents are given.
- Specific hazards during fire fighting : Combustible.
- Vapours are heavier than air and may spread along floors.
- Forms explosive mixtures with air on intense heating.
- Development of hazardous combustion gases or vapours possible in the event of fire.
- Hazardous combustion products : Carbon oxides
- Specific extinguishing methods : No data available
- Further information : Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters : In the event of fire, wear self-contained breathing apparatus.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:
Do not breathe vapours, aerosols.
Evacuate the danger area, observe emergency procedures, consult an expert.
Advice for emergency responders:
For personal protection see section 8.

Environmental precautions : Do not let product enter drains.

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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Further information on storage conditions : Tightly closed.

Storage class : 10, Combustible liquids

Recommended storage temperature : Recommended storage temperature see product label.

Further information on storage stability : Store under inert gas.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures : No data available

Personal protective equipment

Respiratory protection : Not required; except in case of aerosol formation.

Hand protection

Remarks : not required

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Safety glasses

Hygiene measures : Change contaminated clothing. Wash hands after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : viscous liquid

Color : colourless

Odor : No data available

Odor Threshold : No data available
pH : No data available

Melting point/ range : < -58 °F / < -50 °C
Method: OECD Test Guideline 102

Boiling point/boiling range : 541 °F / 283 °C
Method: OECD Test Guideline 103

Flash point : 226 °F / 108 °C
Method: ISO 2719

Evaporation rate : No data available

Flammability (solid, gas) : No data available

Flammability (liquids) : No data available

Burning rate : No data available

Upper explosion limit /
Upper flammability limit : No data available

Lower explosion limit /
Lower flammability limit : No data available

Vapor pressure	: 0.0089 hPa (77 °F / 25 °C) Method: OECD Test Guideline 104
Relative vapour density	: No data available
Relative density	: No data available
Density	: 0.901 g/cm ³ (68 °F / 20 °C) Method: OECD Test Guideline 109
Solubility(ies)	
Water solubility	: 0.034 g/l slightly soluble (68 °F / 20 °C) Method: OECD Test Guideline 105
Partition coefficient: n-octanol/water	: log Pow: 4.2 (95 °F / 35 °C) Method: OECD Test Guideline 117
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: none
Surface tension	: 62.1 mN/m, 68 °F / 20 °C
Molecular weight	: 208.34 g/mol
Particle characteristics	
Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Forms explosive mixtures with air on intense heating. A range from approx. 15 Kelvin below the flash point is to be rated as critical.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous	: No data available

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



reactions

Conditions to avoid : Strong heating.

Incompatible materials : Strong oxidizing agents

Hazardous decomposition : In the event of fire: see section 5 products

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - > 5,000 mg/kg

Inhalation: No data available

LD50 Dermal - Rat - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: Mild skin irritation - 4 h

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Mild eye irritation - 1 h

Respiratory or skin sensitization

in vivo assay - Mouse

Result: Did not cause sensitisation on laboratory animals.
(OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Mouse

Test system: lymphocyte

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Carcinogenicity

IARC: No component 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 component 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

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

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - No observed adverse effect level - 1,000 mg/kg

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

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

3-Methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)-4-penten-2-ol:

- Toxicity to fish : LC50 (Pimephales promelas (fathead minnow)): 2.3 mg/l
Exposure time: 96 h
Test Type: semi-static test
Method: OECD Test Guideline 203
- Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): 1.9 mg/l
Exposure time: 48 h
Test Type: static test
Method: OECD Test Guideline 202
- Toxicity to algae/aquatic plants : EC50 (Pseudokirchneriella subcapitata (green algae)): 13 mg/l
Exposure time: 96 h
Test Type: static test
Method: OECD Test Guideline 201
- Toxicity to microorganisms : EC50 (Sludge Treatment): 52.5 mg/l
Exposure time: 3 h
Test Type: Respiration inhibition
Method: OECD Test Guideline 209

Persistence and degradability

Components:

3-Methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)-4-penten-2-ol:

- Biodegradability : aerobic
Inoculum: activated sludge
Concentration: 100 mg/l
Result: Not readily biodegradable.

Biodegradation: 66 %
Exposure time: 28 d
Method: OECD Test Guideline 301F
Remarks: The 10 day time window criterion is not fulfilled.

Bioaccumulative potential

Components:

3-Methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)-4-penten-2-ol:

Partition coefficient: n- : log Pow: 4.2 (95 °F / 35 °C)
octanol/water pH: 7
Method: OECD Test Guideline 117

Mobility in soil

No data available

Other adverse effects

No data available

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : 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

International Regulations

IATA-DGR

UN/ID No. : UN 3082
Proper shipping name : Environmentally hazardous substance, liquid, n.o.s. (3-Methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)-4-penten-2-ol)
Class : 9
Packing group : III
Labels : Class 9 - Miscellaneous dangerous substances and articles
Packing instruction (cargo aircraft) : 964
Packing instruction (passenger aircraft) : 964

IMDG-Code

UN number : UN 3082
Proper shipping name : ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S.

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(3-Methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)-4-penten-2-ol)

Class : 9
Packing group : III
Labels : 9
EmS Code : F-A, S-F
Marine pollutant : yes

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

Not regulated as a dangerous good

Poison Inhalation Hazard : No

Special precautions for user

Remarks : EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids. Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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 : No SARA Hazards

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 components 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

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent,

Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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.

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