

## SAFETY DATA SHEET

Version 6.6  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 2,4,7,9-Tetramethyl-5-decyne-4,7-diol,  
mixture of (±) and *meso*

Product Number : 278386  
Brand : Aldrich  
CAS-No. : 126-86-3

**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 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)**

Serious eye damage (Category 1), H318  
Skin sensitization (Category 1), H317  
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**

Pictogram



Signal word

Danger

Hazard statement(s)	
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H412	Harmful to aquatic life with long lasting effects.
Precautionary statement(s)	
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P272	Contaminated work clothing must not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P363	Wash contaminated clothing before reuse.
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

Formula	: C <sub>14</sub> H <sub>26</sub> O <sub>2</sub>
Molecular weight	: 226.36 g/mol
CAS-No.	: 126-86-3
EC-No.	: 204-809-1

Component	Classification	Concentration
<b>2,4,7,9-tetramethyldec-5-yne-4,7-diol</b>		
	Eye Dam. 1; Skin Sens. 1; Aquatic Acute 3; Aquatic Chronic 3; H318, H317, H402, H412	<= 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

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. Consult a physician.

**In case of eye contact**

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

**If swallowed**

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

**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

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**SECTION 5: Firefighting measures****5.1 Extinguishing media****Suitable extinguishing media**

Water Foam Carbon dioxide (CO<sub>2</sub>) 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.

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**

Prevent fire extinguishing water from contaminating surface water or the ground water system.

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**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Avoid inhalation of vapours/aerosols or dusts.

Avoid substance contact. Ensure adequate ventilation. 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.

**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 with suitable equipment. Dispose of properly. Clean up affected area.

**6.4 Reference to other sections**

For disposal see section 13.

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## **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**

#### **Storage conditions**

Tightly closed. Dry.

Storage class (TRGS 510): 13: Non Combustible Solids

### **7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## **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). Tightly fitting safety goggles

##### **Skin protection**

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

##### **Full contact**

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

##### **Splash contact**

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

##### **Body Protection**

protective clothing

##### **Respiratory protection**

required when dusts/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.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

a) Appearance	Form: Wax like Color: white
b) Odor	odorless
c) Odor Threshold	Not applicable
d) pH	No data available
e) Melting point/freezing point	Melting point/range: 42 - 44 °C (108 - 111 °F) - lit.
f) Initial boiling point and boiling range	255 °C 491 °F - lit.
g) Flash point	No data available
h) Evaporation rate	No data available
i) Flammability (solid, gas)	The product is not flammable. - Test N.1: Test method for readily combustible solids
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	< 1 hPa at 20 °C (68 °F) - OECD Test Guideline 104
l) Vapor density	No data available
m) Relative density	0.882 g/cm <sup>3</sup> at 25 °C (77 °F) -
n) Water solubility	1.7 g/l at 20 °C (68 °F) - OECD Test Guideline 105 - soluble
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**

Surface tension	32.7 mN/m at 0.1g/l at 20 °C (68 °F)
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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 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

no information available

### 10.5 Incompatible materials

Strong oxidizing agents, Acid chlorides, Acid anhydrides, Strong bases

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - male and female - > 500 mg/kg

Remarks:

(ECHA)

LD50 Dermal - Rat - male and female - > 2,000 mg/kg

(OECD Test Guideline 402)

#### Skin corrosion/irritation

Skin - Rabbit

Result: slight irritation - 4 h

(OECD Test Guideline 404)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Corrosive

(US-EPA)

#### Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: positive

(OECD Test Guideline 429)

#### Germ cell mutagenicity

Ames test

Salmonella typhimurium

Result: negative

Chromosome aberration test in vitro

Chinese hamster ovary cells

Result: negative

In vitro mammalian cell gene mutation test

mouse lymphoma cells

Result: negative

#### Carcinogenicity

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- 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**

### **11.2 Additional Information**

Repeated dose toxicity - Rat - male and female - Oral - 30 Days - NOAEL (No observed adverse effect level) - 150 mg/kg  
Not available

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

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## **SECTION 12: Ecological information**

### **12.1 Toxicity**

Toxicity to fish	static test LC50 - Cyprinus carpio (Carp) - 42 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 91 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata - 82 mg/l - 72 h (OECD Test Guideline 201)
	static test NOEC - Pseudokirchneriella subcapitata - 1 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC50 - activated sludge - ca. 630 mg/l - 0.5 h (OECD Test Guideline 209)

### **12.2 Persistence and degradability**

Biodegradability	aerobic - Exposure time 60 d Result: 8 - 12 % - Not readily biodegradable. Remarks: (ECHA)
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### **12.3 Bioaccumulative potential**

Bioaccumulation	Cyprinus carpio (Carp) - 28 d
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at 24 °C(2,4,7,9-tetramethyldec-5-yne-4,7-diol)

Bioconcentration factor (BCF): < 24

#### **12.4 Mobility in soil**

#### **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**

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### **SECTION 13: Disposal considerations**

#### **13.1 Waste treatment methods**

##### **Product**

Waste material must be disposed of in accordance with the national and local No mixing with other waste. Handle uncleaned containers like the product. See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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### **SECTION 14: Transport information**

#### **DOT (US)**

Not dangerous goods

#### **IMDG**

Not dangerous goods

#### **IATA**

Not dangerous goods

#### **Further information**

Not classified as dangerous in the meaning of transport regulations.

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### **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**

Acute Health Hazard

#### **Massachusetts Right To Know Components**

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



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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](http://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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