

# SAFETY DATA SHEET

Version 6.5  
Revision Date 09/07/2024  
Print Date 09/08/2024

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : *trans*-Nerolidol

Product Number : 18143  
Brand : Sigma-Aldrich  
CAS-No. : 40716-66-3

### 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)

Eye irritation (Category 2A), H319  
Skin sensitization (Sub-category 1B), H317  
Short-term (acute) aquatic hazard (Category 1), H400  
Long-term (chronic) aquatic hazard (Category 1), H410

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

Warning

Hazard Statements

H317

May cause an allergic skin reaction.

H319

Causes serious eye irritation.

H410

Very toxic to aquatic life with long lasting effects.

Precautionary Statements

P261

Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.

P264

Wash skin thoroughly after handling.

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

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P333 + P313

If skin irritation or rash occurs: Get medical advice/ attention.

P337 + P313

If eye irritation persists: Get medical advice/ attention.

P363

Wash contaminated clothing before reuse.

P391

Collect spillage.

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 : (E)-3,7,11-Trimethyl-1,6,10-dodecatrien-3-ol  
trans-3,7,11-Trimethyl-1,6,10-dodecatrien-3-ol

Formula : C<sub>15</sub>H<sub>26</sub>O

Molecular weight : 222.37 g/mol

CAS-No. : 40716-66-3

EC-No. : 255-053-4

Component	Classification	Concentration
<b>(E)-3,7,11-trimethyldodeca-1,6,10-trien-3-ol</b>		
	Eye Irrit. 2A; Skin Sens. 1B; Aquatic Acute 1; Aquatic Chronic 1; H319, H317, H400, H410	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

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## 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. 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

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.

Vapors 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.

### 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: Do not breathe vapors, aerosols. 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 liquid-absorbent material (e.g. Chemizorb® ). 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.

Store under inert gas. Air sensitive.

#### **Storage class**

Storage class (TRGS 510): 10: Combustible liquids

### **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). Safety glasses

### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 480 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 30 min

Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

### Body Protection

protective clothing

### Respiratory protection

Recommended Filter type: Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

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.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

a) Appearance                      Form: liquid

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b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	No data available
f) Initial boiling point and boiling range	145 - 146 °C 293 - 295 °F at 16 hPa - lit.
g) Flash point	113 °C (235 °F) - closed cup
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	No data available
l) Vapor density	No data available
m) Density	0.876 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	No data available
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	none

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 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.

### 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

Strong heating.

### 10.5 Incompatible materials

Strong oxidizing agents

### 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 - > 2,610 mg/kg  
(OECD Test Guideline 401)

Remarks: The value is given in analogy to the following substances: 3,7,11-Trimethyldodeca-1,6,10-trien-3-ol,mixed isomers

Inhalation: No data available

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

Remarks: (ECHA)

The value is given in analogy to the following substances: 3,7,11-Trimethyldodeca-1,6,10-trien-3-ol,mixed isomers

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h  
(OECD Test Guideline 404)

Remarks: The value is given in analogy to the following substances: 3,7,11-Trimethyldodeca-1,6,10-trien-3-ol,mixed isomers

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irritating to eyes. - 8 d  
(OECD Test Guideline 405)

Remarks: The value is given in analogy to the following substances: 3,7,11-Trimethyldodeca-1,6,10-trien-3-ol,mixed isomers

#### Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: Causes sensitization.  
(OECD Test Guideline 429)

Remarks: The value is given in analogy to the following substances: 3,7,11-Trimethyldodeca-1,6,10-trien-3-ol,mixed isomers

#### Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Remarks: The value is given in analogy to the following substances: 3,7,11-Trimethyldodeca-1,6,10-trien-3-ol,mixed isomers

**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**

No data available

**11.2 Additional Information**

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                      flow-through test LC50 - Pimephales promelas (fathead minnow) - 1.43 mg/l - 96 h  
Remarks: (ECHA)  
The value is given in analogy to the following substances: 3,7,11-Trimethyldodeca-1,6,10-trien-3-ol,mixed isomers

Toxicity to daphnia and other aquatic invertebrates                      static test EC50 - Daphnia magna (Water flea) - 0.51 mg/l - 48 h (Regulation (EC) No. 440/2008, Annex, C.2)  
Remarks: The value is given in analogy to the following substances: 3,7,11-Trimethyldodeca-1,6,10-trien-3-ol,mixed isomers

Toxicity to algae                      static test ErC50 - Desmodesmus subspicatus (green algae) - 2 mg/l - 72 h (OECD Test Guideline 201)  
Remarks: The value is given in analogy to the following substances: 3,7,11-Trimethyldodeca-1,6,10-trien-3-ol,mixed isomers  
  
static test NOEC - Desmodesmus subspicatus (green algae) - 0.44 mg/l - 72 h (OECD Test Guideline 201)



Remarks: The value is given in analogy to the following substances:  
3,7,11-Trimethyldodeca-1,6,10-trien-3-ol,mixed isomers

Toxicity to bacteria      static test EC50 - activated sludge - > 1,000 mg/l - 0.5 h  
(OECD Test Guideline 209)  
Remarks: The value is given in analogy to the following substances:  
3,7,11-Trimethyldodeca-1,6,10-trien-3-ol,mixed isomers

## 12.2 Persistence and degradability

Biodegradability      aerobic - Exposure time 28 d  
Result: 70 - 80 % - Readily biodegradable.  
(OECD Test Guideline 301)  
Remarks: The value is given in analogy to the following substances:  
3,7,11-Trimethyldodeca-1,6,10-trien-3-ol,mixed isomers

## 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

Discharge into the environment must be avoided.

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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 regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## SECTION 14: Transport information

### DOT (US)

Not dangerous goods

### IMDG

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UN number: 3082 Class: 9 Packing group: III EMS-No: F-A, S-F  
Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. ((E)-3,7,11-trimethyldodeca-1,6,10-trien-3-ol)  
Marine pollutant : yes  
Marine pollutant : no

**IATA**

UN number: 3082 Class: 9 Packing group: III  
Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. ((E)-3,7,11-trimethyldodeca-1,6,10-trien-3-ol)

**Further information**

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

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**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** : 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**

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

**Massachusetts Right To Know**

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

**Pennsylvania Right To Know**

(E)-3,7,11-trimethyldodeca-1,6,10-trien-3-ol 40716-66-3

**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

**New Jersey Right To Know**

(E)-3,7,11-trimethyldodeca-1,6,10-trien-3-ol

40716-66-3

**The ingredients of this product are reported in the following inventories:**

TSCA : Product contains substance(s) not listed on 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.

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**SECTION 16: Other information**

**Further information**

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](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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