

## SAFETY DATA SHEET

Version 6.10  
Revision Date 04/28/2025  
Print Date 04/29/2025

## SECTION 1. IDENTIFICATION

## 1.1 Product identifiers

Product name : (–)-*trans*-Caryophyllene

Product Number : 22075  
Brand : Sigma  
CAS-No. : 87-44-5

## 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

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


Skin sensitization : Sub-category 1B

Aspiration hazard : Category 1

## Other hazards

None known.

## GHS label elements

Hazard pictograms : 

Signal Word : Danger

Hazard Statements : H304 May be fatal if swallowed and enters airways.  
H317 May cause an allergic skin reaction.

Precautionary Statements : **Prevention:**  
P261 Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.  
P272 Contaminated work clothing must not be allowed out of the workplace.  
P280 Wear protective gloves.  
**Response:**  
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor.  
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.  
P331 Do NOT induce vomiting.  
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.  
P363 Wash contaminated clothing before reuse.  
**Storage:**  
P405 Store locked up.  
**Disposal:**  
P501 Dispose of contents/ container to an approved waste disposal plant.

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## SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

### Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
beta-Caryophyllene	87-44-5*	>= 90 - <= 100	-

\* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

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## SECTION 4. 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. 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.
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

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## SECTION 5. FIRE-FIGHTING MEASURES

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.
Specific hazards during fire fighting	: 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.

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	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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## SECTION 6. ACCIDENTAL RELEASE MEASURES

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

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## 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	: 36 - 46 °F / 2 - 8 °C

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## 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 : 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.

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.

Hand protection

Remarks : 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

Skin and body protection : protective clothing

Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : liquid, clear

Color : No data available

Odor : No data available

Odor Threshold	: No data available
pH	: No data available
Melting point/freezing point	: < 77 °F / < 25 °C
Boiling point/boiling range	: 504 - 507 °F / 262 - 264 °C
Flash point	: 221.9 °F / 105.5 °C (1,010.4 - 1,010.8 hPa) Method: Regulation (EC) No. 440/2008, Annex, A.9, closed cup
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Self-ignition	: 419 °F / 215 °C 1,021.1 - 1,022.1 hPa Method: DIN 51794
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapor pressure	: No data available
Relative vapor density	: No data available
Relative density	: No data available
Density	: 0.902 g/mL (68 °F / 20 °C)
Solubility(ies)	
Water solubility	: 0.088 g/l (68 °F / 20 °C) Method: OECD Test Guideline 105 GLP: yes
Partition coefficient: n-octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition	: No data available

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temperature

Viscosity, dynamic : No data available

Viscosity, kinematic : No data available

Flow time : No data available

Explosive properties : No data available

Oxidizing properties : none

Molecular weight : 204.35 g/mol

Particle characteristics

Particle size : No data available

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## 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 reactions : No data available

Conditions to avoid : Strong heating.

Incompatible materials : Strong oxidizing agents

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 - Mouse - male - > 5,000 mg/kg

Remarks: (ECHA)

Inhalation: No data available

Dermal: No data available

#### Skin corrosion/irritation

Skin - in vitro test

Result: No skin irritation

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**MILLIPORE**  
**SIGMA**

(OECD Test Guideline 439)

**Serious eye damage/eye irritation**

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

**Respiratory or skin sensitization**

Local lymph node assay (LLNA) - Guinea pig

Result: positive

(OECD Test Guideline 429)

**Germ cell mutagenicity**

Test Type: Micronucleus test

Test system: Human lymphocytes

Metabolic activation: without metabolic activation

Method: OECD Test Guideline 487

Result: negative

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: gene mutation test

Test system: mouse lymphoma cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: Equivocal evidence.

**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**

RTECS: DT8400000

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

### Ecotoxicity

#### Components:

##### **beta-Caryophyllene:**

Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna Straus (Water flea)): > 0.17 mg/l  
End point: Immobilization  
Exposure time: 48 h  
Test Type: static test  
Analytical monitoring: yes  
Method: OECD Test Guideline 202  
GLP: yes

Toxicity to algae/aquatic plants : ErC50 (Pseudokirchneriella subcapitata (green algae)): > 0.033 mg/l  
Exposure time: 72 h  
Test Type: static test  
Analytical monitoring: yes  
Method: OECD Test Guideline 201  
GLP: yes

### Ecotoxicology Assessment

Acute aquatic toxicity : This product has no known ecotoxicological effects.

Chronic aquatic toxicity : This product has no known ecotoxicological effects.

### Persistence and degradability

#### Components:

##### **beta-Caryophyllene:**

Biodegradability : aerobic  
Inoculum: activated sludge, non-adapted  
Result: Readily biodegradable.  
Biodegradation: 56 %  
Exposure time: 28 d  
Method: OECD Test Guideline 310  
GLP: yes

### Bioaccumulative potential

No data available

### Mobility in soil

No data available

### Other adverse effects

No data available

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## 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.

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## SECTION 14. TRANSPORT INFORMATION

### International Regulations

#### IATA-DGR

Not regulated as a dangerous good

#### IMDG-Code

Not regulated as a dangerous good

#### Transport in bulk according to IMO instruments

Not applicable for product as supplied.

### National regulation

#### 49 CFR Road

Not regulated as a dangerous good

Poison Inhalation Hazard : No

### Special precautions for user

Remarks : Not classified as dangerous in the meaning of transport regulations.

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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** : 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 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.

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**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 Harmonized 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 Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; 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

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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 - Organization 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

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Revision Date : 04/28/2025

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