

• SAFETY DATA SHEET

Version 6.8
Revision Date 02/12/2026
Print Date 02/13/2026

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : α -Hexylcinnamaldehyde

Product Number : 09178
Brand : Sigma-Aldrich
CAS-No. : 101-86-0

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

Skin sensitisation : Sub-category 1B

Short-term (acute) : Category 1

Sigma-Aldrich - 09178

Page 1 of 14


aquatic hazard

Long-term (chronic) aquatic hazard : Category 2

Other hazards

None known.

GHS label elements

Hazard pictograms : 

Signal word : Warning

Hazard statements : H317 May cause an allergic skin reaction.
H400 Very toxic to aquatic life.
H411 Toxic to aquatic life with long lasting effects.

Precautionary statements : **Prevention:**
P261 Avoid breathing mist or vapours.
P272 Contaminated work clothing must not be allowed out of the workplace.
P273 Avoid release to the environment.
P280 Wear protective gloves.
Response:
P302 + P352 IF ON SKIN: Wash with plenty of water.
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
P362 + P364 Take off contaminated clothing and wash it before reuse.
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. : 101-86-0

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
α -Hexylcinnamaldehyde	101-86-0*	$\geq 80 - \leq 100$	TSC

Sigma-Aldrich - 09178

Page 2 of 14

butyl hydroxytoluene (BHT)	128-37-0*	>= 0.1 - <= 1	TSC
-------------------------------	-----------	---------------	-----

* Indicates that the identifier is a CAS No.

TSC- the actual concentration or concentration range is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

- General advice : Show this 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: immediately make victim drink water (two glasses at most). Consult a physician.
- 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 : Water
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	:	Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	:	Advice for non-emergency personnel: Do not breathe vapours, 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 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 : 36 - 46 °F / 2 - 8 °C

Further information on storage stability : Store under inert gas.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
butyl hydroxytoluene (BHT)	128-37-0	TWA (Inhalable fraction and vapor)	2 mg/m ³	ACGIH
		TWA	10 mg/m ³	NIOSH REL

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.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

- Appearance : liquid
- Color : yellow
- Odor : No data available
- Odor Threshold : No data available
pH : No data available
- Melting point : No data available
- Boiling point/boiling range : 345 - 349 °F / 174 - 176 °C (20 hPa)
Method: lit.
- Flash point : 235 °F / 113 °C
Method: closed cup
- 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 : No data available
- Relative vapour density : No data available

Relative density	: No data available
Density	: 1.550 g/cm ³ (68 °F / 20 °C)
Solubility(ies)	
Water solubility	: 0.005 g/l negligible (77 °F / 25 °C)
Partition coefficient: n-octanol/water	: No data available
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	: Not classified as explosive.
Oxidizing properties	: none
Molecular weight	: 216.32 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) .
Contains the following stabiliser(s):	: butyl hydroxytoluene (BHT) (>=0.075 - <=0.15 %)
Possibility of hazardous reactions	: Violent reactions possible with: Strong oxidizing agents Strong bases
Conditions to avoid	: Strong heating.
Incompatible materials	: No data available

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

Acute toxicity estimate Oral - 3,102 mg/kg
(Calculation method)

LD50 Oral - Rat - 3,100 mg/kg

Remarks: (RTECS)

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Moderate skin irritation - 24 h

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

May cause sensitisation by skin contact.

Germ cell mutagenicity

No data available

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

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

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

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

α -Hexylcinnamaldehyde:

Toxicity to fish : LC50 (Fish): 2.36 mg/l
Exposure time: 96 h
Remarks: (ECOTOX Database)

Toxicity to algae/aquatic plants : EC50 (algae): 0.34 mg/l
Exposure time: 96 h
Remarks: (ECOTOX Database)

M-Factor (Acute aquatic toxicity) : 1

Ecotoxicology Assessment

Chronic aquatic toxicity : Toxic to aquatic life with long lasting effects.

butyl hydroxytoluene (BHT):

Toxicity to fish : LC50 (Danio rerio (zebra fish)): > 0.57 mg/l
End point: mortality
Exposure time: 96 h
Test Type: semi-static test
Analytical monitoring: yes
Method: Directive 67/548/EEC, Annex V, C.1.
GLP: yes

Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): 0.48 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 (Desmodesmus subspicatus (green algae)): > 0.4 mg/l
Exposure time: 72 h
Test Type: static test
Analytical monitoring: yes
Method: Regulation (EC) No. 440/2008, Annex, C.3
GLP: yes

Toxicity to fish (Chronic toxicity) : NOEC (Oryzias latipes): 0.053 mg/l
Exposure time: 30 d
Method: OECD Test Guideline 210
GLP: yes

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity) : EC50 (Daphnia magna (Water flea)): 0.096 mg/l
End point: reproduction rate
Exposure time: 21 d
Method: OECD Test Guideline 211
GLP: yes

Toxicity to microorganisms : EC50 (activated sludge): > 10,000 mg/l
Exposure time: 3 h
Test Type: static test
Method: OECD Test Guideline 209
GLP: yes

Ecotoxicology Assessment

Acute aquatic toxicity : no acute aquatic toxicity

Chronic aquatic toxicity : Very toxic to aquatic life with long lasting effects.

Persistence and degradability

Components:

α -Hexylcinnamaldehyde:

Biodegradability : Result: Readily biodegradable.

Bioaccumulative potential

Components:

butyl hydroxytoluene (BHT):

Partition coefficient: n-octanol/water : log Pow: 5.1
GLP: yes
Remarks: Potential bioaccumulation (ECHA)

Mobility in soil

No data available

Other adverse effects

Product:

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances
Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

Components:

α -Hexylcinnamaldehyde:

Additional ecological information : Discharge into the environment must be avoided.

butyl hydroxytoluene (BHT):

Results of PBT and vPvB assessment : Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

Additional ecological information : Discharge into the environment must be avoided.

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. (α-Hexylcinnamaldehyde)
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. (α-Hexylcinnamaldehyde)
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 : 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.

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCOMI Intermediate or Final VOC's (40 CFR 60.489).

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

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:

US 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

ACGIH : USA. ACGIH Threshold Limit Values (TLV)
NIOSH REL : USA. NIOSH Recommended Exposure Limits
ACGIH / TWA : 8-hour, time-weighted average
NIOSH REL / TWA : Time-weighted average concentration for up to a 10-hour workday during a 40-hour workweek

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 -

Sigma-Aldrich - 09178

Page 13 of 14

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.

Copyright 2025 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

Revision Date : 02/12/2026

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

US / EN