

SAFETY DATA SHEET

according to the OSHA
Hazard Communication Standard

Version 8.0
Revision Date 06/15/2026
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : 4-*tert*-Butyltoluene

Product Number : B102628
Brand : Aldrich
CAS-No. : 98-51-1

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 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

Flammable liquids : Category 4

Acute toxicity (Oral) : Category 4

Acute toxicity
(Inhalation) : Category 2

Eye irritation : Category 2A

Specific target organ toxicity - single exposure : Category 3 (Respiratory system)

Short-term (acute) aquatic hazard : Category 2

Long-term (chronic) aquatic hazard : Category 2

Other hazards

None known.

GHS label elements

Hazard pictograms : 

Signal word : Danger

Hazard statements : H227 Combustible liquid.
H302 Harmful if swallowed.
H319 Causes serious eye irritation.
H330 Fatal if inhaled.
H335 May cause respiratory irritation.
H411 Toxic to aquatic life with long lasting effects.

Precautionary statements : **Prevention:**
P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P260 Do not breathe mist or vapours.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P271 Use only outdoors or in a well-ventilated area.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P284 Wear respiratory protection.

Response:
P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P337 + P313 If eye irritation persists: Get medical advice/ attention.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P391 Collect spillage.

Storage:

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.
P405 Store locked up.

Disposal:

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

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 98-51-1

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
4-tert.-butyltoluene	98-51-1*	>= 80 - <= 100	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 : First aiders need to protect themselves. Show this safety data sheet to the doctor in attendance.

If inhaled : After inhalation: fresh air. Immediately call in physician.
If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

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. Call in ophthalmologist. 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 : Carbon dioxide (CO₂)
Foam
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 : Remove container from danger zone and cool with water.
Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire- : Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe

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. Keep away from heat and sources of ignition. 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.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion	: Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.
Advice on safe handling	: Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.
Further information on storage conditions	: Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorised persons.
Storage class	: 6.1A, Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials
Recommended storage temperature	: Recommended storage temperature see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
4-tert.-butyltoluene	98-51-1	TWA	1 ppm	ACGIH
		ST	20 ppm 120 mg/m ³	NIOSH REL
		TWA	10 ppm 60 mg/m ³	NIOSH REL
		TWA	10 ppm 60 mg/m ³	OSHA Z-1

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 A (acc. to DIN 3181) for vapours of organic compounds

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

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.4 mm
Protective index : Full contact
Manufacturer : Camatril® (KCL 730 / Aldrich Z677442, Size M)

Material : butyl-rubber
Break through time : 10 min
Glove thickness : 0.7 mm
Protective index : Splash contact
Manufacturer : Butoject® (KCL 898)

Remarks : 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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

- 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 : Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

- Appearance : liquid
- Colour : colourless
- Odour : No data available
- Odour Threshold : No data available
pH : No data available
- Melting point/ range : -62 °F / -52 °C
(ECHA) (Lit.)
- Boiling point/boiling range : 376 °F / 191 °C
Method: lit.
- Flash point : 142.7 °F / 61.5 °C
(1,013 hPa)
Method: ISO 13736, 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 / : No data available

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Upper flammability limit

Lower explosion limit /
Lower flammability limit : No data available

Vapor pressure : 1.3 hPa (86 °F / 30 °C)

Relative vapour density : No data available

Relative density : No data available

Density : 0.858 g/cm³ (77 °F / 25 °C)
Method: lit.

Solubility(ies)
Water solubility : 4 g/l slightly soluble (77 °F / 25 °C)
Method: OECD Test Guideline 105

Partition coefficient: n-
octanol/water : log Pow: 4.4
(Lit.) (ECHA)

Autoignition temperature : 950 °F / 510 °C

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 : No data available

Molecular weight : 148.24 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) .

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Possibility of hazardous reactions : Violent reactions possible with:
Strong oxidizing agents

Conditions to avoid : Strong heating.

Incompatible materials : No data available

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

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 1,555 mg/kg

Remarks: Behavioral:Somnolence (general depressed activity).

Behavioral:Ataxia.

Lungs, Thorax, or Respiration:Dyspnea.

LC50 Inhalation - 4 h - 1.5 mg/l - vapour

Remarks: (ECHA)

LD50 Dermal - Rabbit - 16,934 mg/kg

Remarks: Behavioral:Tremor.

Behavioral:Convulsions or effect on seizure threshold.

Nutritional and Gross Metabolic:Changes in:Body temperature decrease.

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

(Draize Test)

Remarks: (ECHA)

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

No data available

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

No data available

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

RTECS: XS8400000

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

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

4-tert.-butyltoluene:

Toxicity to fish	: LC50 (Cyprinus carpio (Carp)): 2 mg/l Exposure time: 96 h Test Type: mortality Analytical monitoring: yes Method: Regulation (EC) No. 440/2008, Annex, C.1 GLP: yes Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates	: EC50 (Daphnia magna (Water flea)): 3.2 mg/l Exposure time: 48 h Test Type: static test Analytical monitoring: yes Method: Tested according to Directive 92/69/EEC. GLP: yes Remarks: (ECHA)
Toxicity to algae/aquatic plants	: EC50 (Algae): 4.4 mg/l Exposure time: 72 h Test Type: Growth inhibition NOEC (Algae): 0.78 mg/l Exposure time: 72 h Test Type: Growth inhibition
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)	: EC50 (Daphnia (water flea)): 0.42 mg/l Exposure time: 21 d

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NOEC (Daphnia (water flea)): 0.29 mg/l
Exposure time: 21 d

Persistence and degradability

Components:

4-tert.-butyltoluene:

Biodegradability : aerobic
Result: Not readily biodegradable.
Biodegradation: 30 - 65 %
Exposure time: 28 d
Method: OECD Test Guideline 301C
Remarks: (ECHA)

Bioaccumulative potential

Components:

4-tert.-butyltoluene:

Bioaccumulation : Species: Cyprinus carpio (Carp)
Bioconcentration factor (BCF): 0.2
Exposure time: 42 d
Concentration: 0.1 mg/l

Partition coefficient: n-octanol/water : log Pow: 4.4
Remarks: (Lit.)
(ECHA)

Mobility in soil

Components:

4-tert.-butyltoluene:

Stability in soil : Remarks: 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:

4-tert.-butyltoluene:

Additional ecological information : No data available

Endocrine disrupting properties

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 2667
Proper shipping name : Butyltoluenes
Class : 6.1
Packing group : III
Labels : Division 6.1 - Toxic substances
Packing instruction (cargo : 663
aircraft)
Packing instruction : 655
(passenger aircraft)

IMDG-Code

UN number : UN 2667
Proper shipping name : BUTYLTOLUENES

Class : 6.1
Packing group : III
Labels : 6.1
EmS Code : F-A, S-A
Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR

UN/ID/NA number : UN 2667
Proper shipping name : Butyltoluenes

Class : 6.1

Packing group : III
Labels : Division 6.1 - Toxic substances
ERG Code : 152

Marine pollutant : no
Poison Inhalation Hazard : No

Special precautions for user

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 : Fire Hazard
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 SOCM 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

4-tert.-butyltoluene

98-51-1

Pennsylvania Right To Know

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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**Relevant changes since previous version**

2. Hazards identification

Full text of other abbreviations

ACGIH	: USA. ACGIH Threshold Limit Values (TLV)
NIOSH REL	: USA. NIOSH Recommended Exposure Limits
OSHA Z-1	: USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
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
NIOSH REL / ST	: STEL - 15-minute TWA exposure that should not be exceeded at any time during a workday
OSHA Z-1 / TWA	: 8-hour time weighted average

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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