

SAFETY DATA SHEET

Version 6.7
Revision Date 09/06/2024
Print Date 09/07/2024**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**Product name : 4-*tert*-ButylbenzaldehydeProduct Number : 384038
Brand : Aldrich
CAS-No. : 939-97-9**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 sheetCompany : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATESTelephone : +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)**Acute toxicity, Oral (Category 3), H301
Skin sensitization (Category 1), H317
Reproductive toxicity (Category 2), H361
Short-term (acute) aquatic hazard (Category 1), H400

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 Statements

H301 Toxic if swallowed.
 H317 May cause an allergic skin reaction.
 H361 Suspected of damaging fertility or the unborn child.
 H400 Very toxic to aquatic life.

Precautionary Statements

P201 Obtain special instructions before use.
 P202 Do not handle until all safety precautions have been read and understood.
 P261 Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
 P264 Wash skin thoroughly after handling.
 P270 Do not eat, drink or smoke when using this product.
 P272 Contaminated work clothing must not be allowed out of the workplace.
 P273 Avoid release to the environment.
 P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
 P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
 P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
 P308 + P313 IF exposed or concerned: Get medical advice/ attention.
 P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
 P363 Wash contaminated clothing before reuse.
 P391 Collect spillage.
 P405 Store locked up.
 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 : C₁₁H₁₄O
 Molecular weight : 162.23 g/mol
 CAS-No. : 939-97-9
 EC-No. : 213-367-9

Component	Classification	Concentration
4-tert-butylbenzaldehyde	Acute Tox. 3; Skin Sens. 1; Repr. 2; Aquatic Acute	<= 100 %

	1; H301, H317, H361, H400 M-Factor - Aquatic Acute: 10	
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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. Call in physician.

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

If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂) Foam 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.

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 carefully 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.

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. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

7.3 Specific end use(s)

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

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: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: 480 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: 480 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, 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.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: clear, liquid Color: colorless
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/ range: 245 - 246 °C (473 - 475 °F)
f) Initial boiling point and boiling range	130 °C 266 °F at 33 hPa - lit.
g) Flash point	101 °C (214 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 5.6 %(V) Lower explosion limit: 1.3 %(V)
k) Vapor pressure	0.04 hPa at 20 °C (68 °F)
l) Vapor density	No data available
m) Density	0.97 g/cm ³ at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	0.12 g/l at 20 °C (68 °F) - OECD Test Guideline 105
o) Partition coefficient: n-octanol/water	log Pow: 3.1 at 25 °C (77 °F) - Bioaccumulation is not expected.
p) Autoignition temperature	400 °C (752 °F) at 1,013.25 hPa - DIN 51794
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

No data available

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

Violent reactions possible with:
Strong oxidizing agents

10.4 Conditions to avoid

Exposure to air may affect product quality. Exposure to light may affect product quality.
Strong heating.

10.5 Incompatible materials

No data available

10.6 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 - male and female - 50.6 mg/kg
(OECD Test Guideline 401)
Inhalation: No data available
LD50 Dermal - Rat - > 2,000 mg/kg
Remarks: (External MSDS)

Skin corrosion/irritation

Skin - Rabbit
Result: No skin irritation - 24 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit
Result: No eye irritation
(OECD Test Guideline 405)

Respiratory or skin sensitization

May cause an allergic skin reaction. (ECHA)

Germ cell mutagenicity

Test Type: Ames test

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Test system: S. typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative

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

Suspected of damaging fertility.
Suspected of damaging the unborn child.

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.

If inhaled

After absorption of large quantities:

narcosis

Systemic effects:

Headache
Dizziness
Drowsiness
inebriation
Unconsciousness
Convulsions
Tremors
ataxia (impaired locomotor coordination)
respiratory arrest

Further data:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	static test LC50 - Leuciscus idus (Golden orfe) - 8.0 mg/l - 96.0 h Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates	EC50 - Daphnia magna (Water flea) - 0.277 mg/l - 48 h Remarks: (ECHA)
Toxicity to algae	static test ErC50 - Desmodesmus subspicatus (green algae) - 13.6 mg/l - 72 h Remarks: (ECHA)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 90 - 100 % - Readily biodegradable. (OECD Test Guideline 301B)
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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.

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.

SECTION 14: Transport information**DOT (US)**

UN number: 2810 Class: 6.1 Packing group: III
Proper shipping name: Toxic, liquids, organic, n.o.s. (4-tert-butylbenzaldehyde) (4-tert-butylbenzaldehyde)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 2810 Class: 6.1 Packing group: III EMS-No: F-A, S-A
Proper shipping name: TOXIC LIQUID, ORGANIC, N.O.S. (4-tert-butylbenzaldehyde) (4-tert-butylbenzaldehyde)
Marine pollutant : yes

IATA

UN number: 2810 Class: 6.1 Packing group: III
Proper shipping name: Toxic liquid, organic, n.o.s. (4-tert-butylbenzaldehyde) (4-tert-butylbenzaldehyde)

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

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Maine Chemicals of High Concern

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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

4-tert-butylbenzaldehyde

939-97-9

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.

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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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