

SAFETY DATA SHEET

Version 3.15
Revision Date 05/08/2015
Print Date 11/10/2018

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name : 2-(4-*tert*-Butylbenzyl)propionaldehyde

Product Number : 95338
Brand : Sigma-Aldrich

CAS-No. : 80-54-6

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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 4), H302
Skin irritation (Category 2), H315
Skin sensitisation (Category 1), H317
Reproductive toxicity (Category 2), H361
Acute aquatic toxicity (Category 2), H401
Chronic aquatic toxicity (Category 2), H411

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 statement(s)

H302 Harmful if swallowed.
H315 Causes skin irritation.
H317 May cause an allergic skin reaction.
H361 Suspected of damaging fertility or the unborn child.
H411 Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

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/ vapours/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P272	Contaminated work clothing should not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell. 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.
P362	Take off contaminated clothing and wash 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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : 4-tert-Butyl- α -methyl-hydrocinnamaldehyde
4-tert-Butyl- α -methyl-benzenepropanal

Formula : C₁₄H₂₀O
Molecular weight : 204.31 g/mol
CAS-No. : 80-54-6
EC-No. : 201-289-8

Hazardous components

Component	Classification	Concentration
2-(4-tert-Butylbenzyl)propionaldehyde		
	Acute Tox. 4; Skin Irrit. 2; Skin Sens. 1; Repr. 2; Aquatic Acute 2; Aquatic Chronic 2; H302, H315, H317, H361, H411	<= 100 %

No components need to be disclosed according to the applicable regulations.
For the full text of the H-Statements mentioned in this Section, see Section 16.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

5. FIREFIGHTING MEASURES

- 5.1 Extinguishing media**
Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.
- 5.2 Special hazards arising from the substance or mixture**
Carbon oxides
- 5.3 Advice for firefighters**
Wear self-contained breathing apparatus for firefighting if necessary.
- 5.4 Further information**
No data available

6. ACCIDENTAL RELEASE MEASURES

- 6.1 Personal precautions, protective equipment and emergency procedures**
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.
For personal protection see section 8.
- 6.2 Environmental precautions**
Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.
- 6.3 Methods and materials for containment and cleaning up**
Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.
- 6.4 Reference to other sections**
For disposal see section 13.

7. HANDLING AND STORAGE

- 7.1 Precautions for safe handling**
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
For precautions see section 2.2.
- 7.2 Conditions for safe storage, including any incompatibilities**
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.
Recommended storage temperature 2 - 8 °C
Store under inert gas. Air sensitive.
Storage class (TRGS 510): Combustible liquids
- 7.3 Specific end use(s)**
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

- 8.1 Control parameters**
Components with workplace control parameters
Contains no substances with occupational exposure limit values.
- 8.2 Exposure controls**
Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

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.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance	Form: clear, viscous liquid Colour: colourless
b) Odour	No data available
c) Odour Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/freezing point: < -19.99 °C (< -3.98 °F) at 1,013.250 hPa (760.000 mmHg) - OECD Test Guideline 102
f) Initial boiling point and boiling range	279.4 - 285.5 °C (534.9 - 545.9 °F) at 1,013.250 hPa (760.000 mmHg) - OECD Test Guideline 103
g) Flash point	113.75 - 114.25 °C (236.75 - 237.65 °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) Vapour pressure	No data available
l) Vapour density	No data available
m) Relative density	0.946 g/mL at 20 °C (68 °F)
n) Water solubility	ca.0.045 g/l at 20 °C (68 °F) - OECD Test Guideline 105 - slightly soluble
o) Partition coefficient: n-octanol/water	log Pow: 4.73 at 25 °C (77 °F)
p) Auto-ignition temperature	242 °C (468 °F) at 1,010 hPa (758 mmHg)
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

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

No data available

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

Other decomposition products - No data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 1,390 mg/kg
(OECD Test Guideline 401)

Inhalation: No data available

LD50 Dermal - Rat - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

Respiratory or skin sensitisation

Maximisation Test (GPMT) - Guinea pig
Result: May cause sensitisation by skin contact.
(OECD Test Guideline 406)

Germ cell mutagenicity

Ames test

Salmonella typhimurium

Result: negative

OECD Test Guideline 474

Mouse - male and female

Result: negative

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.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a

carcinogen or potential carcinogen by ACGIH.

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 identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

Reproductive toxicity - Rat - Oral

Paternal Effects: Testes, epididymis, sperm duct.

Suspected human reproductive toxicant

Developmental Toxicity - Rabbit - Oral

Specific Developmental Abnormalities: Musculoskeletal system.

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Additional Information

Repeated dose toxicity - Rat - male and female - Oral - No observed adverse effect level - 25 mg/kg

RTECS: MW4895000

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish	flow-through test LC50 - Danio rerio (zebra fish) - 2.04 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	Immobilization EC50 - Daphnia magna (Water flea) - 9.84 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	Growth inhibition EC50 - Desmodesmus subspicatus (green algae) - ca. 32.5 mg/l - 72 h (OECD Test Guideline 201)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
Result: 80.7 % - Readily biodegradable
(OECD Test Guideline 301B)

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 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Toxic to aquatic life with long lasting effects.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

Not dangerous goods

IMDG

UN number: 3082 Class: 9 Packing group: III EMS-No: F-A, S-F
Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (2-(4-tert-Butylbenzyl)propionaldehyde)
Marine pollutant: yes

IATA

UN number: 3082 Class: 9 Packing group: III
Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (2-(4-tert-Butylbenzyl)propionaldehyde)

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.

15. REGULATORY INFORMATION

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

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.

SARA 311/312 Hazards

Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

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

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
2-(4-tert-Butylbenzyl)propionaldehyde	80-54-6	

New Jersey Right To Know Components

	CAS-No.	Revision Date
2-(4-tert-Butylbenzyl)propionaldehyde	80-54-6	

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.	Acute toxicity
Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity

H302	Harmful if swallowed.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H361	Suspected of damaging fertility or the unborn child.
H401	Toxic to aquatic life.
H411	Toxic to aquatic life with long lasting effects.
Repr.	Reproductive toxicity

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	1
Physical Hazard	0

NFPA Rating

Health hazard:	2
Fire Hazard:	1
Reactivity Hazard:	0

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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