

SAFETY DATA SHEET
4-tert-Butylbenzaldehyde

According to Regulation (EC) No 1907/2006, Annex II, as amended. Commission Regulation (EU) No 2015/830 of 28 May 2015.

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1. Product identifier**

Product name	4-tert-Butylbenzaldehyde
Product number	FB55060
CAS number	939-97-9
EC number	213-367-9

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

Identified uses Laboratory reagent. Manufacture of substances. Research and development.

1.3. Details of the supplier of the safety data sheet

Supplier	Carbosynth Ltd 8&9 Old Station Business Park Compton Berkshire RG20 6NE UK +44 1635 578444 +44 1635 579444 info@carbosynth.com
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1.4. Emergency telephone number

Emergency telephone +44 7887 998634

SECTION 2: Hazards identification**2.1. Classification of the substance or mixture****Classification (EC 1272/2008)**

Physical hazards	Not Classified
Health hazards	Acute Tox. 4 - H302 Resp. Sens. 1 - H334 Skin Sens. 1 - H317
Environmental hazards	Aquatic Acute 1 - H400 Aquatic Chronic 1 - H410

2.2. Label elements

EC number 213-367-9

Pictogram



Signal word

Danger

4-tert-Butylbenzaldehyde

Hazard statements	H302 Harmful if swallowed. H317 May cause an allergic skin reaction. H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled. H410 Very toxic to aquatic life with long lasting effects.
Precautionary statements	P273 Avoid release to the environment. P280 Wear protective gloves/ protective clothing/ eye protection/ face protection. P301+P312 IF SWALLOWED: Call a POISON CENTRE/doctor if you feel unwell. P302+P352 IF ON SKIN: Wash with plenty of water. P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing. P501 Dispose of contents/ container in accordance with national regulations.

2.3. Other hazards

No data available.

SECTION 3: Composition/information on ingredients

3.1. Substances

Product name	4-tert-Butylbenzaldehyde
CAS number	939-97-9
EC number	213-367-9
Chemical formula	C ₁₁ H ₁₄ O

SECTION 4: First aid measures

4.1. Description of first aid measures

General information	Get medical advice/attention if you feel unwell.
Inhalation	Remove person to fresh air and keep comfortable for breathing. When breathing is difficult, properly trained personnel may assist affected person by administering oxygen. If breathing stops, provide artificial respiration. Get medical attention if symptoms are severe or persist.
Ingestion	Do not induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth thoroughly with water. Give plenty of water to drink. Get medical attention if symptoms are severe or persist.
Skin contact	Remove contaminated clothing. Rinse with water. Continue to rinse for at least 15 minutes. Wash contaminated clothing before reuse. Get medical attention if symptoms are severe or persist.
Eye contact	Rinse immediately with plenty of water. Continue to rinse for at least 15 minutes. Get medical attention if symptoms are severe or persist.

4.2. Most important symptoms and effects, both acute and delayed

General information	See Section 11 for additional information on health hazards.
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4.3. Indication of any immediate medical attention and special treatment needed

Notes for the doctor	Treat symptomatically.
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SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media	Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.
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5.2. Special hazards arising from the substance or mixture

4-tert-Butylbenzaldehyde

Specific hazards	None known.
Hazardous combustion products	Thermal decomposition or combustion products may include the following substances: Harmful gases or vapours. Oxides of carbon.
5.3. Advice for firefighters	
Special protective equipment for firefighters	Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing conforming to European standard EN469 (including helmets, protective boots and gloves) will provide a basic level of protection for chemical incidents. Use protective equipment appropriate for surrounding materials.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions	Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material. Avoid inhalation of vapours. Provide adequate ventilation. Keep unnecessary and unprotected personnel away from the spillage.
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6.2. Environmental precautions

Environmental precautions	Avoid discharge into drains or watercourses or onto the ground.
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6.3. Methods and material for containment and cleaning up

Methods for cleaning up	Wear protective clothing as described in Section 8 of this safety data sheet. Absorb spillage with sand or other inert absorbent. Clear up spills immediately and dispose of waste safely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. Provide adequate ventilation. For waste disposal, see Section 13.
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6.4. Reference to other sections

Reference to other sections	For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.
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SECTION 7: Handling and storage

7.1. Precautions for safe handling

Usage precautions	Wear protective clothing as described in Section 8 of this safety data sheet. Wash hands thoroughly after handling. Provide adequate ventilation. Avoid contact with skin and eyes. Avoid inhalation of vapours.
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7.2. Conditions for safe storage, including any incompatibilities

Storage precautions	Keep container tightly closed. Store contents under inert gas. Store away from incompatible materials (see Section 10). Protect from light. Store at room temperature.
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7.3. Specific end use(s)

Specific end use(s)	The identified uses for this product are detailed in Section 1.2.
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SECTION 8: Exposure Controls/personal protection

8.1. Control parameters

Occupational exposure limits

No exposure limits known for ingredient(s).

8.2. Exposure controls

Appropriate engineering controls	Provide adequate ventilation.
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4-tert-Butylbenzaldehyde

Eye/face protection	Unless the assessment indicates a higher degree of protection is required, the following protection should be worn: Tight-fitting safety glasses. Personal protective equipment for eye and face protection should comply with European Standard EN166.
Hand protection	Wear protective gloves. To protect hands from chemicals, gloves should comply with European Standard EN374.
Other skin and body protection	Wear appropriate clothing to prevent repeated or prolonged skin contact.
Respiratory protection	Respiratory protection complying with an approved standard should be worn if a risk assessment indicates inhalation of contaminants is possible. Ensure all respiratory protective equipment is suitable for its intended use and is 'CE'-marked. Gas and combination filter cartridges should comply with European Standard EN14387. Full face mask respirators with replaceable filter cartridges should comply with European Standard EN136. Half mask and quarter mask respirators with replaceable filter cartridges should comply with European Standard EN140.
Environmental exposure controls	Keep container tightly sealed when not in use.

SECTION 9: Physical and Chemical Properties

9.1. Information on basic physical and chemical properties

Appearance	Liquid.
Colour	Colourless to pale yellow.
Odour	No data available.
Odour threshold	No data available.
pH	No data available.
Melting point	No data available.
Initial boiling point and range	No data available.
Flash point	101°C Closed cup.
Evaporation rate	No data available.
Flammability (solid, gas)	No data available.
Upper/lower flammability or explosive limits	Lower flammable/explosive limit: 1.3 g/100 g Upper flammable/explosive limit: 5.6 g/100 g
Vapour pressure	No data available.
Vapour density	No data available.
Relative density	0.97 g/cm ³ @ 25°C
Solubility(ies)	Insoluble in water. Soluble in the following materials: Methanol.
Partition coefficient	log Pow: 3.1
Auto-ignition temperature	400°C
Decomposition Temperature	No data available.
Viscosity	0.004 Pa s @ 20°C
Explosive properties	No data available.
Oxidising properties	No data available.

4-tert-Butylbenzaldehyde

9.2. Other information

Molecular weight 162.23

SECTION 10: Stability and reactivity

10.1. Reactivity

Reactivity No data available.

10.2. Chemical stability

Stability Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions

Possibility of hazardous reactions No data available.

10.4. Conditions to avoid

Conditions to avoid Avoid heat. Air. Light.

10.5. Incompatible materials

Materials to avoid Oxidising agents.

10.6. Hazardous decomposition products

Hazardous decomposition products Oxides of carbon.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - oral

Acute toxicity oral (LD₅₀ mg/kg) 500.0

Species Rat

Notes (oral LD₅₀) Acute Tox. 4 - H302 Harmful if swallowed.

ATE oral (mg/kg) 500.0

Acute toxicity - dermal

Notes (dermal LD₅₀) Based on available data the classification criteria are not met.

Acute toxicity - inhalation

Notes (inhalation LC₅₀) Based on available data the classification criteria are not met.

Skin corrosion/irritation

Animal data Based on available data the classification criteria are not met.

Serious eye damage/irritation

Serious eye damage/irritation Based on available data the classification criteria are not met.

Respiratory sensitisation

Respiratory sensitisation There is evidence that the product can cause respiratory hypersensitivity.

Skin sensitisation

Skin sensitisation May cause skin sensitisation or allergic reactions in sensitive individuals.

Germ cell mutagenicity

Genotoxicity - in vitro Based on available data the classification criteria are not met.

4-tert-Butylbenzaldehyde

Carcinogenicity

Carcinogenicity Based on available data the classification criteria are not met.

IARC carcinogenicity 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.

Reproductive toxicity

Reproductive toxicity - fertility Based on available data the classification criteria are not met.

Reproductive toxicity - development Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

STOT - single exposure Not classified as a specific target organ toxicant after a single exposure.

Specific target organ toxicity - repeated exposure

STOT - repeated exposure Not classified as a specific target organ toxicant after repeated exposure.

Aspiration hazard

Aspiration hazard Based on available data the classification criteria are not met.

General information

The severity of the symptoms described will vary dependent on the concentration and the length of exposure.

Inhalation May cause sensitisation or allergic reactions in sensitive individuals.

Ingestion May cause sensitisation or allergic reactions in sensitive individuals. May cause discomfort if swallowed. Stomach pain. Nausea, vomiting.

Skin contact May cause skin sensitisation or allergic reactions in sensitive individuals.

Eye contact No specific symptoms known.

Route of exposure Ingestion Inhalation Skin and/or eye contact

Target organs No specific target organs known.

Medical considerations Skin disorders and allergies.

SECTION 12: Ecological Information

Ecotoxicity Very toxic to aquatic life with long lasting effects.

12.1. Toxicity

Acute aquatic toxicity

LE(C)₅₀ $0.1 < L(E)C_{50} \leq 1$

M factor (Acute) 1

Acute toxicity - fish LC₅₀, 96 hour: 8 mg/l, *Leuciscus idus* (Golden orfe)

Acute toxicity - aquatic invertebrates EC₅₀, 48 hour: 0.7 mg/l, *Daphnia magna*

Acute toxicity - aquatic plants EC₅₀, 72 hour: 42.5 mg/l, *Desmodium subspicatus*

Chronic aquatic toxicity

NOEC $0.01 < NOEC \leq 0.1$

Degradability Non-rapidly degradable

M factor (Chronic) 1

4-tert-Butylbenzaldehyde

12.2. Persistence and degradability

Persistence and degradability The degradability of the product is not known.

12.3. Bioaccumulative potential

Bioaccumulative potential No data available on bioaccumulation.

Partition coefficient log Pow: 3.1

12.4. Mobility in soil

Mobility No data available.

12.5. Results of PBT and vPvB assessment

Results of PBT and vPvB assessment No data available.

12.6. Other adverse effects

Other adverse effects None known.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

General information Dispose of waste to licensed waste disposal site in accordance with the requirements of the local Waste Disposal Authority. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered.

SECTION 14: Transport information

14.1. UN number

UN No. (ADR/RID) 3082

UN No. (IMDG) 3082

UN No. (ICAO) 3082

UN No. (ADN) 3082

14.2. UN proper shipping name

Proper shipping name (ADR/RID) ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (4-tert-Butylbenzaldehyde)

Proper shipping name (IMDG) ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (4-tert-Butylbenzaldehyde)

Proper shipping name (ICAO) ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (4-tert-Butylbenzaldehyde)

Proper shipping name (ADN) ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (4-tert-Butylbenzaldehyde)

14.3. Transport hazard class(es)

ADR/RID class 9

ADR/RID classification code M6

ADR/RID label 9

IMDG class 9

ICAO class/division 9

4-tert-Butylbenzaldehyde

ADN class 9

Transport labels



14.4. Packing group

ADR/RID packing group	III
IMDG packing group	III
ADN packing group	III
ICAO packing group	III

14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant



14.6. Special precautions for user

EmS	F-A, S-F
ADR transport category	3
Emergency Action Code	•3Z
Hazard Identification Number (ADR/RID)	90

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

National regulations	Health and Safety at Work etc. Act 1974 (as amended). The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"]. EH40/2005 Workplace exposure limits.
EU legislation	Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) (as amended). Commission Regulation (EU) No 2015/830 of 28 May 2015. Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures (as amended).

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

Inventories

US - TSCA

Present.

SECTION 16: Other information

4-tert-Butylbenzaldehyde

Abbreviations and acronyms used in the safety data sheet	<p>ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road.</p> <p>ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways.</p> <p>RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail.</p> <p>IATA: International Air Transport Association.</p> <p>ICAO: Technical Instructions for the Safe Transport of Dangerous Goods by Air.</p> <p>IMDG: International Maritime Dangerous Goods.</p> <p>CAS: Chemical Abstracts Service.</p> <p>ATE: Acute Toxicity Estimate.</p> <p>LC₅₀: Lethal Concentration to 50 % of a test population.</p> <p>LD₅₀: Lethal Dose to 50% of a test population (Median Lethal Dose).</p> <p>EC₅₀: 50% of maximal Effective Concentration.</p> <p>PBT: Persistent, Bioaccumulative and Toxic substance.</p> <p>vPvB: Very Persistent and Very Bioaccumulative.</p>
Training advice	Only trained personnel should use this material.
Revision date	15/11/2017
Revision	1
SDS number	144929
Hazard statements in full	<p>H302 Harmful if swallowed.</p> <p>H317 May cause an allergic skin reaction.</p> <p>H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.</p> <p>H400 Very toxic to aquatic life.</p> <p>H410 Very toxic to aquatic life with long lasting effects.</p>

This information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.