

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.8 Revision Date 02.07.2024 Print Date 07.07.2024

GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

SECTION 1: Identification of the substance/mixture and of the company/undertaking

Product identifiers 1.1

Product name tert-Butyl acetate for synthesis

Product Number : 8.02189 802189 Catalogue No. Brand : Millipore Index-No.

: 607-026-00-7

REACH No. : A registration number is not available for this substance as the

substance or its uses are exempted from registration or the

annual tonnage does not require a registration.

CAS-No. : 540-88-5

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

Identified uses : Chemical for synthesis

1.3 Details of the supplier of the safety data sheet

: Merck KGaA Company

> Frankfurter Str. 250 D-64271 DARMSTADT

Telephone : +49 (0)6151 72-0 +49 6151 727780 Fax

E-mail address TechnicalService@merckgroup.com

1.4 Emergency telephone

Emergency Phone # : +(44)-870-8200418 (CHEMTREC (GB))

> +(353)-19014670 (CHEMTREC Ireland) 001-803-017-9114 (CHEMTREC India)

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Flammable liquids, (Category 2) H225: Highly flammable liquid and vapor.

Acute toxicity, (Category 4) H332: Harmful if inhaled.

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Specific target organ toxicity single exposure, (Category 3), Central nervous system

H336: May cause drowsiness or dizziness.

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

H335: May cause respiratory irritation.

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal Word Danger

Hazard Statements

H225 Highly flammable liquid and vapor.

Harmful if inhaled. H332

May cause respiratory irritation. H335 May cause drowsiness or dizziness. H336

Precautionary Statements

P210 Keep away from heat, hot surfaces, sparks, open flames and

other ignition sources. No smoking.

P233 Keep container tightly closed.

P240 Ground and bond container and receiving equipment.

P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.

P242 Use non-sparking tools.

P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable

for breathing. Call a POISON CENTER/ doctor if you feel unwell.

Supplemental Hazard information (EU)

EUH066 Repeated exposure may cause skin dryness or cracking.

Reduced Labeling (<= 125 ml)

Pictogram



Signal Word Danger Hazard Statements none **Precautionary Statements** none Supplemental Hazard information (EU)

EUH066 Repeated exposure may cause skin dryness or cracking.

Other hazards 2.3

Canada

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological information:

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The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher. Toxicological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.1 Substances

Formula : C6H12O2

Molecular weight : 116,16 g/mol

CAS-No. : 540-88-5

EC-No. : 208-760-7

Index-No. : 607-026-00-7

Component		Classification	Concentration
tertbutyl acetate			
CAS-No. EC-No. Index-No.	540-88-5 208-760-7 607-026-00-7	Flam. Liq. 2; Acute Tox. 4; STOT SE 3; H225, H332, H336, H335	<= 100 %

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. 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. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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

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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.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

5.4 Further information

Remove container from danger zone and cool with water. 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. Keep away from heat and sources of ignition. 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. Risk of explosion.

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 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

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

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Hygiene measures

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

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Recommended storage temperature see product label.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

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

8.2 Exposure controls

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

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).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0,4 mm

Break through time: 30 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter A-(P2)

The entrepeneur 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.

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Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Physical state liquidb) Color colorless

c) Odor camphor-like

d) Melting point/ range: < -58 °C - (ECHA)

point/freezing point

explosive limits

gas)

e) Initial boiling point 98 °C at 1.013 hPa and boiling range

f) Flammability (solid, No data available

g) Upper/lower Lower explosion limit: 1,5 - 1,7 %(V) flammability or

h) Flash point 4 °C - closed cup

i) Autoignition 589 °C

temperature at 1.015 hPa - ASTM E-659

j) Decomposition No data available temperature

k) pH No data available

I) Viscosity Viscosity, kinematic: < 1 mm2/s at 25 °C - ASTM D 445

Viscosity, dynamic: No data available

m) Water solubility ca.6,7 g/l at 23 °C - OECD Test Guideline 105- soluble
 n) Partition coefficient: log Pow: 1,64 at 21,7 °C - OECD Test Guideline 107 - Bioaccumulation is not expected.

o) Vapor pressure 56 hPa at 20 °C - ASTM D 2879-86

p) Density 0,866 g/cm3 at 20 °C

Relative density

No data available

q) Relative vapor
density

No data available

r) Particle No data available characteristics

s) Explosive properties No data available

t) Oxidizing properties none

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9.2 Other safety information

Surface tension 64 mN/m at 1g/l at 20 °C

- OECD Test Guideline 115

Relative vapor

density

4,65

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapors may form explosive mixture with air.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Risk of explosion with:

Strong oxidizing agents

can decompose violently in contact with:

alkali hydroxides

Violent reactions possible with:

strong alkalis Strong acids

nitrates

10.4 Conditions to avoid

Warming.

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 - 4.100 mg/kg

(US-EPA)

LC50 Inhalation - Rat - male and female - 22,98 mg/l - vapor

Remarks: (ECHA)

Symptoms: Possible damages:, mucosal irritations

LD50 Dermal - Rabbit - male and female - > 2.000 mg/kg

(US-EPA)

Skin corrosion/irritation

Remarks: (ECHA) Skin - Rabbit

Result: No skin irritation - 4 h

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(US-EPA)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation - 72 h

(US-EPA)

Respiratory or skin sensitization

Buehler Test - Guinea pig

Result: negative

(US-EPA)

Germ cell mutagenicity

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Human lymphocytes

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: In vivo micronucleus test

Species: Rat

Application Route: inhalation (vapor) Method: OECD Test Guideline 474

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation. - Respiratory system Oral, Inhalation - May cause drowsiness or dizziness. - Central nervous system

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

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11.2 Additional Information

Endocrine disrupting properties

Product:

The substance/mixture does not contain Assessment

> components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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

Systemic effects:

After absorption:

Headache Dizziness Nausea Vomiting

After absorption of large quantities:

narcosis

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish semi-static test LC50 - Oncorhynchus mykiss (rainbow trout) - 240

mg/I - 96 h

(OECD Test Guideline 203)

Toxicity to daphnia and other aquatic

invertebrates

static test EC50 - Daphnia magna (Water flea) - 350 mg/l - 48 h

(OECD Test Guideline 202)

Toxicity to algae static test ErC50 - Pseudokirchneriella subcapitata - 16 mg/l - 72 h

(OECD Test Guideline 201)

12.2 Persistence and degradability

aerobic - Exposure time 28 d Biodegradability

Result: 50 % - Inherently biodegradable.

(OECD Test Guideline 301D)

12.3 Bioaccumulative potential

No data available

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12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Endocrine disrupting properties

Product:

Assessment : The substance/mixture does not contain components

considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

12.7 Other adverse effects

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1123 IMDG: 1123 IATA: 1123

14.2 UN proper shipping name

ADR/RID: BUTYL ACETATES IMDG: BUTYL ACETATES IATA: Butyl acetates

14.3 Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA: 3

14.4 Packaging group

ADR/RID: II IMDG: II IATA: II

14.5 Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

14.6 Special precautions for user

Tunnel restriction code : (D/E)

Further information : No data available

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SECTION 15: Regulatory information

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

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

National legislation

Seveso III: Directive 2012/18/EU of the P5c FLAMMABLE LIQUIDS European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.

Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of H-Statements

H225	Highly flammable liquid and vapor.
H332	Harmful if inhaled.
H335	May cause respiratory irritation.
H336	May cause drowsiness or dizziness.
EUH066	Repeated exposure may cause skin dryness or cracking.

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Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM -American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; 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; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; 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 Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; 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; n.o.s. Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization 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; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; 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

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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