

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.7

Revision Date 02.07.2024

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

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

Product name : tert-Butanol EMPLURA®

Product Number : 8.22264
Catalogue No. : 822264
Brand : Millipore
Index-No. : 603-005-00-1
REACH No. : 01-2119444321-51-XXXX
CAS-No. : 75-65-0

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

Company : Sigma-Aldrich Chemie GmbH
Eschenstrasse 5
D-82024 TAUFKIRCHEN

Telephone : +49 (0)89 6513-1130
Fax : +49 (0)89 6513-1161
E-mail address : technischerservice@merckgroup.com

1.4 Emergency telephone

Emergency Phone # : 0800 181 7059 (CHEMTREC Deutschland)
+49 (0)696 43508409 (CHEMTREC weltweit)

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.

Eye irritation, (Category 2) H319: Causes serious eye irritation.

Specific target organ toxicity - H336: May cause drowsiness or dizziness.



single exposure, (Category 3),
Central nervous system

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.

H319

Causes serious eye irritation.

H332

Harmful if inhaled.

H335

May cause respiratory irritation.

H336

May cause drowsiness or dizziness.

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.

P304 + P340 + P312

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.

P305 + P351 + P338

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Supplemental Hazard
Statements

none

Reduced Labeling (<= 125 ml)

Pictogram



Signal Word

Danger

Hazard Statements

none

Precautionary Statements

none

Supplemental Hazard
Statements

none

2.3 Other hazards

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:

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 | : C ₄ H ₁₀ O |
| Molecular weight | : 74,12 g/mol |
| CAS-No. | : 75-65-0 |
| EC-No. | : 200-889-7 |
| Index-No. | : 603-005-00-1 |

| Component | | Classification | Concentration |
|---------------------|--------------|---|---------------|
| tert-Butanol | | | |
| CAS-No. | 75-65-0 | Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2; STOT SE 3; H225, H332, H319, H336, H335 Concentration limits: 20 %: STOT SE 3, H335; | <= 100 % |
| EC-No. | 200-889-7 | | |
| Index-No. | 603-005-00-1 | | |

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. Call in ophthalmologist. 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

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. Chemisorb®). 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.

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).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,4 mm

Break through time: 480 min



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

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: Chloroprene

Minimum layer thickness: 0,65 mm

Break through time: 240 min

Material tested: KCL 720 Camapren®

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

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.

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 | solid |
| b) Color | colorless |
| c) Odor | camphor-like |
| d) Melting point/freezing point | Melting point: 24 - 25 °C |
| e) Initial boiling point and boiling range | 81 - 83 °C at 1.013 hPa |
| f) Flammability (solid, gas) | No data available |
| g) Upper/lower flammability or explosive limits | Upper explosion limit: 8,0 %(V) Lower explosion limit: 2,3 %(V) |
| h) Flash point | 15 °C - closed cup |
| i) Autoignition temperature | 470 °C at 1.013 hPa - see user defined free text |
| j) Decomposition temperature | No data available |
| k) pH | at 20 °C |

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| | |
|---|---|
| | neutral |
| l) Viscosity | Viscosity, kinematic: 5,72 mm ² /s at 25 °C - OECD Test Guideline 114 2,3 mm ² /s at 45 °C - OECD Test Guideline 114 |
| | Viscosity, dynamic: 3,3 mPa.s at 30 °C |
| m) Water solubility | at 20 °C soluble |
| n) Partition coefficient: n-octanol/water | log Pow: 0,30 - Bioaccumulation is not expected. |
| o) Vapor pressure | 40,7 hPa at 20 °C |
| p) Density | 0,775 g/cm ³ at 20 °C |
| Relative density | No data available |
| q) Relative vapor density | No data available |
| r) Particle characteristics | No data available |
| s) Explosive properties | No data available |
| t) Oxidizing properties | none |

9.2 Other safety information

| | |
|------------------------|--|
| Surface tension | 69,8 mN/m at 1,09g/l at 21 °C - OECD Test Guideline 115 |
| Dissociation constant | 19,2 at 20 °C |
| Relative vapor density | 2,56 |

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

Violent reactions possible with:

Alkali metals
Alkaline earth metals
Strong acids
Aluminum
Strong oxidizing agents

10.4 Conditions to avoid

Warming.



10.5 Incompatible materials

No data available

10.6 Hazardous decomposition products

Peroxides

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 - 3.046 mg/kg

(US-EPA)

Acute toxicity estimate Inhalation - 4 h - 11,1 mg/l - vapor

(Expert judgment)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

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

(US-EPA)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 24 h

(Draize Test)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation.

(US-EPA)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: sister chromatid exchange assay

Test system: Chinese hamster ovary cells



Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 479

Result: negative

Test Type: Micronucleus test

Species: Mouse

Cell type: Red blood cells (erythrocytes)

Application Route: Oral

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

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Inhalation - May cause drowsiness or dizziness. - Nervous system

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

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.

drying, cracking of the skin, Skin irritation

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

Liver - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

| | |
|------------------|--|
| Toxicity to fish | flow-through test LC50 - Pimephales promelas (fathead minnow) - > 961 mg/l - 96 h (OECD Test Guideline 203) |
|------------------|--|

| | |
|---------------------------------------|--|
| Toxicity to daphnia and other aquatic | static test EC50 - Daphnia magna (Water flea) - 933 mg/l - 48 h (Directive 67/548/EEC, Annex V, C.2.) |
|---------------------------------------|--|

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invertebrates

Toxicity to algae static test ErC50 - Pseudokirchneriella subcapitata (green algae) - > 976 mg/l - 72 h
(OECD Test Guideline 201)

Toxicity to bacteria static test EC50 - Pseudomonas putida - > 10.000 mg/l - 16 h
(DIN 38 412 Part 8)

static test EC10 - Pseudomonas putida - 6.900 mg/l - 16 h
(DIN 38 412 Part 8)

Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity) semi-static test EC50 - Daphnia magna (Water flea) - > 100 mg/l - 21 d
(OECD Test Guideline 211)

semi-static test NOEC - Daphnia magna (Water flea) - 100 mg/l - 21 d
(OECD Test Guideline 211)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 56 d
Result: 66 % - Inherently biodegradable.
Remarks: (ECHA)

12.3 Bioaccumulative potential

No data available

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

No data available



SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1120

IMDG: 1120

IATA: 1120

14.2 UN proper shipping name

ADR/RID: BUTANOLS

IMDG: BUTANOLS

IATA: Butanols

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

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.

Authorisations and/or restrictions on use

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. |
| H319 | Causes serious eye irritation. |
| H332 | Harmful if inhaled. |
| H335 | May cause respiratory irritation. |
| H336 | May cause drowsiness or dizziness. |

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



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