

safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



tert-Butanol ≥99 %, for synthesis

article number: **4323**
Version: **1.0 en**

date of compilation: 2015-09-29

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

1.1 Product identifier

Identification of the substance	tert-Butanol
Article number	4323
Registration number (REACH)	This information is not available.
Index No	603-005-00-1
EC number	200-889-7
CAS number	75-65-0

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

Identified uses: laboratory chemical

1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co KG
Schoemperlenstr. 3-5
D-76185 Karlsruhe
Germany

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e-mail: sicherheit@carlroth.de

Website: www.carlroth.de

Competent person responsible for the safety data sheet : Department Health, Safety and Environment

e-mail (competent person) : sicherheit@carlroth.de

1.4 Emergency telephone number

Emergency information service **Poison Centre Munich: +49/(0)89 19240**

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008 (CLP)

Classification acc. to GHS			
Section	Hazard class	Hazard class and category	Hazard statement
2.6	flammable liquids	(Flam. Liq. 2)	H225
3.1I	acute toxicity (inhal.)	(Acute Tox. 4)	H332
3.3	serious eye damage/eye irritation	(Eye Irrit. 2)	H319
3.8R	specific target organ toxicity - single exposure (respiratory tract irritation)	(STOT SE 3)	H335

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Remarks

For full text of Hazard- and EU Hazard-statements: see SECTION 16.

2.2 Label elements

Labelling according to Regulation (EC) No 1272/2008 (CLP)

Signal word

Danger

Pictograms



Hazard statements

H225	Highly flammable liquid and vapour.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.
H335	May cause respiratory irritation.

Precautionary statements

Precautionary statements - prevention

P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P280	Wear protective gloves/eye protection.

Precautionary statements - response

P304+P340	IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P305+P351+P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P312	Call a POISON CENTER/doctor if you feel unwell.

Precautionary statements - storage

P403+P233	Store in a well-ventilated place. Keep container tightly closed.
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Labelling of packages where the contents do not exceed 125 ml

Signal word: **Danger**

Symbol(s)



2.3 Other hazards

There is no additional information.

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SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	tert-Butanol
Index No	603-005-00-1
EC number	200-889-7
CAS number	75-65-0
Molecular formula	C ₄ H ₁₀ O
Molar mass	74,12 g/mol

SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

Following skin contact

Rinse skin with water/shower. In case of skin irritation, consult a physician.

Following eye contact

Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart. In case of eye irritation consult an ophthalmologist.

Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed

After eye contact: Causes tears, Conjunctival oedema (chemosis) of the eyes, Conjunctival redness of the eyes, Irritation,

Following skin contact: Localised redness,

After ingestion: Malaise, Vomiting, Deficits in perception and coordination, reaction time, or sleepiness,

Following inhalation: Cough, pain, choking, and breathing difficulties

4.3 Indication of any immediate medical attention and special treatment needed

none

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SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings
water spray, foam, alcohol resistant foam, dry extinguishing powder, carbon dioxide (CO₂)

Unsuitable extinguishing media

water jet

5.2 Special hazards arising from the substance or mixture

Combustible. Solvent vapours are heavier than air and may spread along floors. Vapours can form explosive mixtures with air.

Hazardous combustion products

In case of fire may be liberated: carbon monoxide (CO), carbon dioxide (CO₂)

5.3 Advice for firefighters

Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

Special protective equipment for firefighters

Protective clothing against liquid and gaseous chemicals, including liquid aerosols and solid particles. Self-contained breathing apparatus (SCBA). Self-contained breathing apparatus (EN 133).

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

Wearing of suitable protective equipment (including personal protective equipment referred to under Section 8 of the safety data sheet) to prevent any contamination of skin, eyes and personal clothing. Avoid contact with skin, eyes and clothes. Avoidance of ignition sources.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Explosive properties.

6.3 Methods and material for containment and cleaning up

Advices on how to contain a spill

Covering of drains.

Advices on how to clean up a spill

Absorb with liquid-binding material (e.g. sand, diatomaceous earth, acid- or universal binding agents).

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

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SECTION 7: Handling and storage

7.1 Precautions for safe handling

Provision of sufficient ventilation. Provision of sufficient ventilation.

- **Measures to prevent fire as well as aerosol and dust generation**



Keep away from sources of ignition - No smoking.

Take precautionary measures against static discharge. Due to danger of explosion, prevent leakage

of vapours into cellars, flues and ditches.

Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs. When using do not smoke.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed.

Incompatible substances or mixtures

Observe hints for combined storage.

Consideration of other advice

Ground/bond container and receiving equipment.

- **Ventilation requirements**

Use local and general ventilation.

- **Specific designs for storage rooms or vessels**

Recommended storage temperature: 15 - 25 °C.

7.3 Specific end use(s)

No information available.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

National limit values

Occupational exposure limit values (Workplace Exposure Limits)

Country	Name of agent	CAS No	Notation	Identifier	TWA [mg/m ³]	STEL [mg/m ³]	Source
UK	2-methylpropan-2-ol	75-65-0		WEL	308	462	EH40/2005

Notation

STEL Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute period unless otherwise specified

TWA Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours time-weighted average

Relevant DNELs/DMELs/PNECs and other threshold levels

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• human health values

Endpoint	Threshold level	Protection goal, route of exposure	Used in	Exposure time
DNEL	214 mg/m ³	human, inhalatory	worker (industry)	acute - systemic effects
DNEL	5,5 mg/kg	human, dermal	worker (industry)	chronic - systemic effects
DNEL	2,7 mg/m ³	human, inhalatory	worker (industry)	chronic - systemic effects

• environmental values

Endpoint	Threshold level	Environmental compartment	Exposure time
PNEC	6,64 mg/l	freshwater	short-term (single instance)
PNEC	0,664 mg/l	marine water	short-term (single instance)
PNEC	690 mg/l	sewage treatment plant (STP)	short-term (single instance)
PNEC	5,8 mg/kg	freshwater sediment	short-term (single instance)
PNEC	0,58 mg/kg	marine sediment	short-term (single instance)
PNEC	1 mg/kg	soil	short-term (single instance)
PNEC	9,33 mg/l	water	continuous

8.2 Exposure controls

Individual protection measures (personal protective equipment)



Eye/face protection

Use safety goggle with side protection.

Skin protection

• hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves.

• type of material

FKM: fluoro-elastomer

• material thickness

0,4 mm.

• breakthrough times of the glove material

>480 minutes (permeation: level 6)

• other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

Flame-retardant protective clothing.

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Respiratory protection

Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of $> 65\text{ }^{\circ}\text{C}$, colour code: Brown).

Observe the wear time limits according GefStoffV in combination with the rules for using respiratory protection apparatus (BGR 190).

Environmental exposure controls

Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Appearance

Physical state	liquid (fluid)
Colour	colourless
Odour	like camphor
Odour threshold	71 ppm

Other physical and chemical parameters

pH (value)	7 (20 °C)
Melting point/freezing point	25,7 °C at 101,3 kPa
Initial boiling point and boiling range	82,41 °C at 101,3 kPa
Flash point	$< 23\text{ }^{\circ}\text{C}$
Evaporation rate	no data available
Flammability (solid, gas)	not relevant (fluid)

Explosive limits

- lower explosion limit (LEL) 2,3 vol% (70 g/m³)
- upper explosion limit (UEL) 8 vol% (250 g/m³)

Explosion limits of dust clouds not relevant

- lower explosion limit (LEL) 70 g/m³
- upper explosion limit (UEL) 250 g/m³

Vapour pressure 5.413 Pa at 25 °C

Density 0,78 g/cm³

Vapour density 2,56 air = 1

Bulk density Not applicable

Relative density Information on this property is not available.

Solubility(ies)

Water solubility 1.000 g/l at 25 °C

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Partition coefficient

n-octanol/water (log KOW) 0,317 (pH value: 6,8, 22,5 °C) (ECHA)

Auto-ignition temperature 470 °C - ECHA

Decomposition temperature no data available

Viscosity

• dynamic viscosity 3,3 mPa s at 30 °C

Explosive properties none

Oxidising properties none

9.2 Other information

There is no additional information.

Surface tension 69,8 mN/m (21 °C)

Refractive index 1,384

SECTION 10: Stability and reactivity

10.1 Reactivity

risk of ignition, Vapours can form explosive mixtures with air

10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

10.3 Possibility of hazardous reactions

Violent reaction with: Alkaline earth metal, Strong oxidiser

10.4 Conditions to avoid

There are no specific conditions known which have to be avoided.

10.5 Incompatible materials

aluminium

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Shall not be classified as acutely toxic.

Exposure route	Endpoint	Value	Species	Source
oral	LD50	3384 mg/kg	rat	ECHA
dermal	LD50	>2000 mg/kg	rabbit	ECHA

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Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Causes serious eye irritation.

Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor as a reproductive toxicant

• Specific target organ toxicity - single exposure

May cause respiratory irritation.

• Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

Symptoms related to the physical, chemical and toxicological characteristics

• If swallowed

nausea, vomiting, deficits in perception and coordination, reaction time, or sleepiness

• If in eyes

conjunctival suffusion, conjunctivitis (pink eye), causes tears

• If inhaled

cough, pain, choking, and breathing difficulties

• If on skin

localised redness

Other information

None.

SECTION 12: Ecological information

12.1 Toxicity

acc. to 1272/2008/EC: Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)

Endpoint	Value	Species	Source	Exposure time
LC50	>961 mg/l	fish	ECHA	96 hours
EC50	933 mg/l	aquatic invertebrates	ECHA	48 hours

Aquatic toxicity (chronic)

Endpoint	Value	Species	Source	Exposure time
EC50	>976 mg/l	algae	ECHA	24 h
NOEC	332 mg/l	fish	ECHA	120 h
growth (EbCx) 10%	6,9 g/l	microorganisms	ECHA	16 h

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12.2 Process of degradability

The substance is readily biodegradable.
Theoretical Oxygen Demand: 2,59 mg/mg
Theoretical Carbon Dioxide: 2,375 mg/mg

Process	Degradation rate	Time
biotic/abiotic	>99,9 %	19 d
carbon dioxide generation	2,6 - 5,1 %	29 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)

0,317 (pH value: 6,8, 22,5 °C)

12.4 Mobility in soil

Data are not available.

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Other adverse effects

Slightly hazardous to water.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

Sewage disposal-relevant information

Do not empty into drains.

Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used.

13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions.

SECTION 14: Transport information

14.1	UN number	1120
14.2	UN proper shipping name	BUTANOLS
	Hazardous ingredients	Tert-Butanol
14.3	Transport hazard class(es)	
	Class	3 (flammable liquids)
14.4	Packing group	II (substance presenting medium danger)
14.5	Environmental hazards	NONE (non-environmentally hazardous acc. to the dangerous goods regulations)

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14.6 Special precautions for user

Provisions for dangerous goods (ADR) should be complied within the premises.

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

The cargo is not intended to be carried in bulk.

14.8 Information for each of the UN Model Regulations

• Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN)

UN number	1120
Proper shipping name	BUTANOLS
Particulars in the transport document	UN1120, BUTANOLS, 3, II, (D/E)
Class	3
Classification code	F1
Packing group	II
Danger label(s)	3



Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
Transport category (TC)	2
Tunnel restriction code (TRC)	D/E
Hazard identification No	33

• International Maritime Dangerous Goods Code (IMDG)

UN number	1120
Proper shipping name	BUTANOLS
Particulars in the shipper's declaration	UN1120, BUTANOLS, 3, II, 23°C c.c.
Class	3
Packing group	II
Danger label(s)	3



Special provisions (SP)	-
Excepted quantities (EQ)	E2
Limited quantities (LQ)	1 L
EmS	F-E, S-D
Stowage category	B

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SECTION 15: Regulatory information

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

Relevant provisions of the European Union (EU)

- **Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)**

Not listed.

- **Regulation 1005/2009/EC on substances that deplete the ozone layer (ODS)**

Not listed.

- **Regulation 850/2004/EC on persistent organic pollutants (POP)**

Not listed.

- **Restrictions according to REACH, Annex XVII**

not listed

- **List of substances subject to authorisation (REACH, Annex XIV)**

not listed

- **Seveso Directive**

96/82/EC (Seveso II)				
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes)		Notes
7b	highly flammable	5.000	50.000	24)

Notation

24) Highly flammable liquids: substances and preparations having a flash point lower than 21 °C and which are not extremely flammable (risk phrase R 11, second indent)

2012/18/EU (Seveso III)				
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements		Notes
P5c	flammable liquids (cat. 2, 3)	5.000	50.000	51)

Notation

51) Flammable liquids, categories 2 or 3 not covered by P5a and P5b

- **Limitation of emissions of volatile organic compounds due to the use of organic solvents in certain paints and varnishes and vehicle refinishing products (2004/42/EC, Deco-Paint Directive)**

VOC content 100 %

- **Directive on industrial emissions (VOCs, 2010/75/EU)**

VOC content 100 %

- **Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS) - Annex II**

not listed

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Regulation 166/2006/EC concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

Directive 2000/60/EC establishing a framework for Community action in the field of water policy (WFD)

not listed

National inventories

Substance is listed in the following national inventories:

- EINECS/ELINCS/NLP (Europe)
- REACH (Europe)

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
DMEL	Derived Minimal Effect Level
DNEL	Derived No-Effect Level
EH40/2005	EH40/2005 Workplace exposure limits, Table 1: List of approved workplace exposure limits (http://www.nationalarchives.gov.uk/doc/open-government-licence/)
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IMDG	International Maritime Dangerous Goods Code
index No	the Index number is the identification code given to the substance in Part 3 of Annex VI to Regulation (EC) No 1272/2008
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
VOC	Volatile Organic Compounds

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Abbr.	Descriptions of used abbreviations
vPvB	very Persistent and very Bioaccumulative

Key literature references and sources for data

- Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU
- Regulation (EC) No. 1272/2008 (CLP, EU GHS)

List of relevant phrases (code and full text as stated in chapter 2 and 3)

Code	Text
H225	highly flammable liquid and vapour
H319	causes serious eye irritation
H332	harmful if inhaled
H335	may cause respiratory irritation

Disclaimer

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.