

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 04.06.2019

Version 10.2

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

| | |
|---------------------------|--|
| Catalogue No. | 818282 |
| Product name | Di-tert-butyl dicarbonate for synthesis |
| REACH Registration Number | A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline. |
| CAS-No. | 24424-99-5 |

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

| | |
|-----------------|---|
| Identified uses | Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal (www.merckgroup.com). |
|-----------------|---|

1.3 Details of the supplier of the safety data sheet

| | |
|------------------------|---|
| Company | Merck KGaA * 64271 Darmstadt * Germany * Phone: +49 6151 72-0 |
| Responsible Department | LS-QHC * e-mail: prodsafe@merckgroup.com |

1.4 Emergency telephone number **Please contact the regional company representation in your country.****SECTION 2. Hazards identification****2.1 Classification of the substance or mixture****Classification (REGULATION (EC) No 1272/2008)**

Flammable liquid, Category 3, H226
Acute toxicity, Category 2, Inhalation, H330
Skin irritation, Category 2, H315
Eye irritation, Category 2, H319
Skin sensitisation, Category 1, H317

For the full text of the H-Statements mentioned in this Section, see Section 16.

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2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

Hazard statements

H226 Flammable liquid and vapour.
H315 Causes skin irritation.
H317 May cause an allergic skin reaction.
H319 Causes serious eye irritation.
H330 Fatal if inhaled.

Precautionary statements

Prevention

P210 Keep away from heat.
P280 Wear protective gloves.

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position 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.
P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/physician.

Reduced labelling (≤ 125 ml)

Hazard pictograms



Signal word

Danger

Hazard statements

H317 May cause an allergic skin reaction.
H330 Fatal if inhaled.

Precautionary statements

P280 Wear protective gloves.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/physician.

Contains: di(tert-butyl) carbonate

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CAS-No. 24424-99-5

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

| | |
|------------|---|
| Formula | C ₁₀ H ₁₈ O ₅ (Hill) |
| EC-No. | 246-240-1 |
| Molar mass | 218,25 g/mol |

Hazardous components (REGULATION (EC) No 1272/2008)

Chemical name (Concentration)

| CAS-No. | Registration number | Classification |
|---------|---------------------|----------------|
|---------|---------------------|----------------|

di(tert-butyl) carbonate (<= 100 %)

24424-99-5 *)

Flammable liquid, Category 3, H226
Acute toxicity, Category 2, H330
Skin irritation, Category 2, H315
Eye irritation, Category 2, H319
Skin sensitisation, Category 1, H317

*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

For the full text of the H-Statements mentioned in this Section, see Section 16.

3.2 Mixture

Not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

General advice

First aider needs to protect himself.

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

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

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4.2 Most important symptoms and effects, both acute and delayed

Cough, Shortness of breath
irritant effects, Allergic reactions

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water, Foam, Carbon dioxide (CO₂), 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

Combustible.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

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

5.3 Advice for firefighters

Special protective equipment for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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 vapours, aerosols. Avoid generation and inhalation of dusts in all circumstances. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

Protective equipment 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 carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area. Take up carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

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Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

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

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Protected from light.

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorised persons.

Recommended storage temperature see product label.

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

8.2 Exposure controls

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Safety glasses

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Hand protection

full contact:

Glove material: butyl-rubber
Glove thickness: 0,7 mm
Break through time: > 480 min

splash contact:

Glove material: Nitrile rubber
Glove thickness: 0,40 mm
Break through time: > 120 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 898 Butoject® (full contact), KCL 730 Camatril® -Velours (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Other protective equipment

Flame retardant antistatic protective clothing.

Respiratory protection

required when dusts/vapours/aerosols are generated.

Recommended Filter type: Filter A-(P3)

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.

Environmental exposure controls

Do not let product enter drains.

Risk of explosion.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

| | |
|-----------------|---------------------------|
| Form | solid to liquid |
| Colour | colourless |
| Odour | No strong odour known. |
| Odour Threshold | No information available. |
| pH | No information available. |

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| | |
|--|--|
| Melting point | 20 - 24 °C |
| Boiling point/boiling range | 56 - 57 °C at 0,7 hPa |
| Flash point | 37 °C Method: c.c. |
| Evaporation rate | No information available. |
| Flammability (solid, gas) | No information available. |
| Lower explosion limit | No information available. |
| Upper explosion limit | No information available. |
| Vapour pressure | No information available. |
| Relative vapour density | No information available. |
| Density | 1,02 g/cm ³ at 20 °C |
| Relative density | No information available. |
| Water solubility | at 20 °C insoluble |
| Partition coefficient: n-octanol/water | log Pow: 1,87 (calculated) (Lit.) Bioaccumulation is not expected. |
| Auto-ignition temperature | No information available. |
| Decomposition temperature | No information available. |
| Viscosity, dynamic | No information available. |
| Explosive properties | Not classified as explosive. |
| Oxidizing properties | none |

9.2 Other data

| | |
|----------------------|--------|
| Ignition temperature | 460 °C |
|----------------------|--------|

SECTION 10. Stability and reactivity

10.1 Reactivity

Vapour/air-mixtures are explosive at intense warming.

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The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

10.2 Chemical stability

heat-sensitive

sensitive to moisture

Sensitivity to light

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong acids, Bases, Oxidizing agents, Reducing agents

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

no information available

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: > 5.000 mg/kg

(External MSDS)

Acute inhalation toxicity

LC50 Rat: 0,1 mg/l; 4 h ; dust/mist

(RTECS)

Symptoms: Cough, Shortness of breath, Possible damages:, mucosal irritations

Acute dermal toxicity

LD50 Rabbit: > 2.000 mg/kg

(External MSDS)

Skin irritation

Causes skin irritation.

Eye irritation

Causes serious eye irritation.

Sensitisation

May cause an allergic skin reaction.

Germ cell mutagenicity

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Genotoxicity in vitro

Ames test

Salmonella typhimurium

Result: negative

(National Toxicology Program)

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

11.2 Further information

After absorption:

change in weight

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

SECTION 12. Ecological information

12.1 Toxicity

No information available.

12.2 Persistence and degradability

No information available.

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 1,87

(calculated)

(Lit.) Bioaccumulation is not expected.

12.4 Mobility in soil

No information 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

Discharge into the environment must be avoided.

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SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

| | |
|--|---|
| 14.1 UN number | UN 2929 |
| 14.2 Proper shipping name | TOXIC LIQUID, FLAMMABLE, ORGANIC, N.O.S. (DI-TERT-BUTYLDICARBONATE) |
| 14.3 Class | 6.1 (3) |
| 14.4 Packing group | II |
| 14.5 Environmentally hazardous | -- |
| 14.6 Special precautions for user | yes |
| Tunnel restriction code | D/E |

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

| | |
|--|---|
| 14.1 UN number | UN 2929 |
| 14.2 Proper shipping name | TOXIC LIQUID, FLAMMABLE, ORGANIC, N.O.S. (DI-TERT-BUTYLDICARBONATE) |
| 14.3 Class | 6.1 (3) |
| 14.4 Packing group | II |
| 14.5 Environmentally hazardous | -- |
| 14.6 Special precautions for user | no |

Sea transport (IMDG)

| | |
|--|---|
| 14.1 UN number | UN 2929 |
| 14.2 Proper shipping name | TOXIC LIQUID, FLAMMABLE, ORGANIC, N.O.S. (DI-TERT-BUTYLDICARBONATE) |
| 14.3 Class | 6.1 (3) |
| 14.4 Packing group | II |
| 14.5 Environmentally hazardous | -- |
| 14.6 Special precautions for user | yes |
| EmS | F-E S-D |

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14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

SECTION 15. Regulatory information

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

EU regulations

Major Accident Hazard

SEVESO III

Legislation

ACUTE TOXIC

H2

Quantity 1: 50 t

Quantity 2: 200 t

SEVESO III

FLAMMABLE LIQUIDS

P5c

Quantity 1: 5.000 t

Quantity 2: 50.000 t

Occupational restrictions

Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC not regulated

Substances of very high concern (SVHC)

This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of $\geq 0.1\%$ (w/w).

National legislation

Storage class

3

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out.

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SECTION 16. Other information

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

| | |
|------|--------------------------------------|
| H226 | Flammable liquid and vapour. |
| H315 | Causes skin irritation. |
| H317 | May cause an allergic skin reaction. |
| H319 | Causes serious eye irritation. |
| H330 | Fatal if inhaled. |

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

Danger

Hazard statements

H226 Flammable liquid and vapour.
H315 Causes skin irritation.
H317 May cause an allergic skin reaction.
H319 Causes serious eye irritation.
H330 Fatal if inhaled.

Precautionary statements

Prevention

P210 Keep away from heat.
P280 Wear protective gloves.

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position 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.
P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/physician.

Contains: di(tert-butyl) carbonate

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

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Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.