

Safety Data Sheet

#90022664 · Full 16-section SDS

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

PRODUCT	CAS NUMBER	FORMULA	VERSION	REVISION DATE
Sodium tert-butoxide	865-48-5	C4H9NaO	11	13 Oct 2026

SECTION 1

Identification

1.1 Product identifier

Product name Sodium tert-butoxide

CAS number 865-48-5

EC / EINECS number 212-741-9

Chemical formula C4H9NaO

Molecular weight 96.10

SMILES [Na].OC(C)(C)C

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

Laboratory use, industrial use, professional use (industrial). For research use only. Not for human or animal use.

1.3 Details of the supplier of the safety data sheet

Molekula Limited
1 Millennium Way, Newton Aycliffe
Durham, DL5 6JW, United Kingdom
info@molekula.com · +44 (0) 3302 000333

1.4 Emergency telephone number

0344 892 0111 — National Poisons Information Service (NPIS) (United Kingdom — for healthcare professionals (via TOXBASE))

SECTION 2

Hazard identification

2.1 Classification of the substance or mixture

Flam. Sol. 1 or Flam. Sol. 2; H228

Self-heat. 1; H251

Skin Corr. 1B; H314

2.2 Label elements



DANGER

CODE	HAZARD STATEMENT
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EUH014	Reacts violently with water
H228	Flammable solid
H251	Self-heating; may catch fire
H314 (sub cat. 1B)	Causes severe skin burns and eye damage

CODE	PRECAUTIONARY STATEMENT
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P210	Keep away from heat/sparks/open flames/hot surfaces - No smoking
P260	Do not breathe dust/fume/gas/mist/vapours/spray
P280	Wear protective gloves/protective clothing/eye protection/face protection
P301+P330+P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting
P302+P352	IF ON SKIN: Wash with soap and water
P305+P351+P338	IF IN EYES: Rinse continuously with water for several minutes. Remove contact lenses if present and easy to do, continue rinsing

2.3 Other hazards

Reacts violently with water; not PBT/vPvB under REACH

SECTION 3

Composition / information on ingredients

3.1 Substances

Name	Sodium tert-butoxide
CAS number	865-48-5
EC number	212-741-9
Concentration / purity	c. 100%
Classification according to Regulation (EC) No 1272/2008	Flam. Sol. 1 or Flam. Sol. 2; H228 Self-heat. 1; H251 Skin Corr. 1B; H314
Hazard statements	EUH014, H228, H251, H314 (sub cat. 1B)
Acute toxicity estimate (ATE)	<i>No data available</i>
Impurities / stabilising additives	None

SECTION 4

First-aid measures

4.1 Description of first aid measures

Inhalation	Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/doctor.
Skin contact	Take off immediately all contaminated clothing. Rinse skin with water/shower. Wash contaminated clothing before reuse.
Eye contact	Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER or doctor/physician.
Ingestion	Rinse mouth. Do NOT induce vomiting. Immediately call a POISON CENTER or doctor/physician.

Get medical attention if any discomfort continues. Show this Safety Data Sheet (SDS) to medical personnel. First aiders/ medical personnel need to protect themselves.

4.2 Most important symptoms and effects, both acute and delayed

Immediately call a POISON CENTER or doctor/physician.

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5

Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media Dry powder, sand

Unsuitable extinguishing media Water jet. Foam

5.2 Special hazards arising from the substance or mixture

Flammable solid; self-heating risk; may form flammable/explosive vapor-air mixtures; hazardous decomposition products: carbon oxides (CO, CO₂), sodium oxides

5.3 Advice for firefighters

Keep container tightly closed; use water spray for cooling exposed containers; avoid fire-fighting water entering environment; do not enter fire area without proper protective equipment

SECTION 6

Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Do not breathe dust or mist. Wear protective gloves/protective clothing/eye protection/face protection.

6.2 Environmental precautions

Prevent entry to sewers/public waters; notify authorities if contamination occurs; avoid water/moist air contact

6.3 Methods and material for containment and cleaning up

Dispose of contents/container to an approved waste disposal plant.

6.4 Reference to other sections

For specific precautions, see Section 8 and Section 13.

SECTION 7

Handling & storage

7.1 Precautions for safe handling

Keep away from heat/sparks/open flames/hot surfaces. No smoking. Do not breathe dust or mist. Wear protective gloves/protective clothing/eye protection/face protection. Ground/bond container and receiving equipment. Use explosion-proof electrical/ventilating/lighting/equipment.

7.2 Conditions for safe storage, including any incompatibilities

Storage temperature Ambient

Conditions for safe storage (incompatibilities) Keep cool. Protect from sunlight. Store away from other materials. Hygroscopic. Store under inert gas. Reacts violently with water.

7.3 Specific end use(s)

See Section 1.2.

SECTION 8

Exposure controls / personal protection

8.1 Control parameters

Occupational exposure limits (OEL / WEL) Not applicable

DNEC/PNEC data

DNEC

Acute effects local (Inhalation): 1 mg/m³

Acute effects systemic (Inhalation): 1 mg/m³

Chronic effects local (Inhalation): 1 mg/m³

Chronic effects systemic (Inhalation): 1 mg/m³

PNEC

Fresh water: 0.11 mg/L

Fresh water sediment: 0.419 mg/kg sediment dw

Water Intermittent: 1.1 mg/L

Microorganisms in sewage treatment: 10 mg/L

Soil (Agriculture): 0.0192 mg/kg soil dw

Marine water: 0.011 mg/L

Marine water sediment: 0.0419 mg/kg sediment dw

8.2 Exposure controls

Eye / face protection	Safety glasses Wear eye/face protection as recommended. All eye/face protection should comply with EN ISO 16321-1:2022.
Skin / hand protection	Nitrile gloves Thickness: 0.11mm. Breakthrough time: 480mins.
Respiratory protection	Keep self-contained breathing apparatus readily available for emergency use. Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided. Respiratory equipment: Reusable Air-Purifying Respirator (APR). Filter type: ABEK. Standard: EN 14387.
Other protection	<i>No data available</i>
Environmental exposure controls	<i>No data available</i>

SECTION 9

Physical & chemical properties

9.1 Information on basic physical and chemical properties

Appearance / physical state	<i>Not applicable</i>
Colour	<i>Not applicable</i>
Odour	<i>Not applicable</i>
Melting / freezing point	<i>Not applicable</i>
Boiling point	<i>Not applicable</i>
Flammability	<i>No data available</i>
Lower and upper explosion limit	2.3-8.0% DERIVED FROM: LITERATURE
Flash point	12 °C DERIVED FROM: LITERATURE
Auto-ignition temperature	<i>Not applicable</i>
Decomposition temperature	<i>No data available</i>
pH	<i>Not applicable</i>
Acidity	Base DERIVED FROM: LITERATURE
Kinematic viscosity	<i>No data available</i>
Solubility	<i>Not applicable</i>
Partition coefficient n-octanol/water (log value)	<i>Not applicable</i>
Vapour pressure	<i>Not applicable</i>
Density (g/mL)	1.025 g/mL DERIVED FROM: LITERATURE
Relative vapour density	<i>No data available</i>
Particle characteristics	<i>No data available</i>

9.2 Other information

No data available

SECTION 10

Stability & reactivity

10.1 Reactivity

Self-heating: may catch fire.

Reacts violently with water.

10.2 Chemical stability

Reacts violently with water. Stable under the prescribed storage conditions

10.3 Possibility of hazardous reactions

Risk of explosion with Water

Possible formation of Hydrogen

Violent reactions possible with: Alkali metals, Halogenated hydrocarbon acids

The generally known reaction partners of water

10.4 Conditions to avoid

Heat/sparks/open flames/hot surfaces. Water. Air sensitive

10.5 Incompatible materials

Risk of explosion with Water

Possible formation of Hydrogen

Violent reactions possible with: Alkali metals, Halogenated hydrocarbon, acids

The generally known reaction partners of water.

10.6 Hazardous decomposition products

See section 5

SECTION 11

Toxicological information

11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008

Acute toxicity (LD50 / LC50)	Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract
Skin corrosion / irritation	Causes severe skin burns.
Eye corrosion / irritation	Causes severe eye damage.
Respiratory / skin sensitisation	<i>Not applicable</i>
Carcinogenicity	<i>Not applicable</i>
Mutagenicity	<i>Not applicable</i>
Reproductive toxicity	<i>Not applicable</i>
STOT (single / repeated exposure)	<i>Not applicable</i>

Aspiration hazard

Not applicable

11.2 Information on other hazards

Not applicable

SECTION 12

Ecological information

12.1 Toxicity

Not applicable

12.2 Persistence and degradability

Not applicable

12.3 Bioaccumulative potential

Not applicable

12.4 Mobility in soil

Not applicable

12.5 Results of PBT and vPvB assessment

Not applicable

12.6 Endocrine disrupting properties

See Section 11.2.

12.7 Other adverse effects

No data available

SECTION 13

Disposal considerations

13.1 Waste treatment methods

Dispose of contents/container to an approved waste disposal plant.

SECTION 14

Transport information

14.1 UN number or ID number

UN3206

14.2 UN proper shipping name

ALKALI METAL ALCOHOLATES, SELF- HEATING, CORROSIVE, N.O.S

14.3 Transport hazard class(es)

4.2 (8)



14.4 Packing group

II

14.5 Environmental hazards

Not a marine pollutant

14.6 Special precautions for user

Special precautions for user Various special provisions (e.g., 182, 274) and packing instructions (e.g., P410) apply across transport modes. Limited quantities are forbidden for air transport. For sea transport, it is a free-flowing hygroscopic powder that causes burns.

Transport category	2
Tunnel code	(D/E)
Packing instruction (ADR)	P410
Packing instruction (IMDG)	P410

14.7 Maritime transport in bulk according to IMO instruments

No data available

SECTION 15

Regulatory information

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

Substance-specific regulations (e.g. licences) National Regulations:
-Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances
Other regulations, limitations and legal regulations:
-Directive 94/33/EC- The protection of young people at work.

REACH code Y110

ECHA notification *Not applicable*

15.2 Chemical safety assessment

Not applicable

SECTION 16

Other information

Revision notes / other information

Full statement of H-Phrases:
EUH014 Reacts violently with water
H228 Flammable solid
H251 Self-heating; may catch fire
H314b Causes severe skin burns and eye damage

This Safety Data Sheet was generated automatically from the data Molekula holds against this product, in the 16-section GHS/CLP format. Fields shown as "No data available" carry no recorded value; fields shown as "Not applicable" were assessed as not relevant to this substance. For queries, contact Molekula at info@molekula.com.