

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 18.02.2011

Version 1.2

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

1.1 Product identifier

Catalogue No.	841179
Product name	N-tert-Butyl- α -phenylnitron 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.

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.merck-chemicals.com).
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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.
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SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

This substance is not classified as dangerous according to European Union legislation.

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)
Not a dangerous substance according to GHS.

CAS-No. 3376-24-7

Labelling (67/548/EEC or 1999/45/EC)

The product does not need to be labelled in accordance with EC directives or respective national laws.

EC-No. 222-168-6

2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

Formula	$C_{11}H_{15}NO$ (Hill)
CAS-No.	3376-24-7
EC-No.	222-168-6
Molar mass	177,24 g/mol

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SECTION 4. First aid measures

4.1 Description of first aid measures

After inhalation: fresh air.

After skin contact: wash off with plenty of water. Remove contaminated clothing.

After eye contact: rinse out with plenty of water.

After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

4.2 Most important symptoms and effects, both acute and delayed

We have no description of any toxic symptoms.

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water, 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

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

Fire may cause evolution of:
nitrogen oxides

5.3 Advice for firefighters

Special protective equipment for fire-fighters

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

Further information

Prevent fire extinguishing water from contaminating surface water or the ground water system.
Suppress (knock down) gases/vapours/mists with a water spray jet.

SECTION 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Ensure adequate ventilation.
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 empty into drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7.2 and 10.5).

Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

Indications about waste treatment see section 13.

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SECTION 7. Handling and storage

7.1 Precautions for safe handling

Observe label precautions.

7.2 Conditions for safe storage, including any incompatibilities

Tightly closed. Dry.

Store below +15°C.

7.3 Specific end uses

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.

Hygiene measures

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

Eye/face protection

Safety glasses

Hand protection

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 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 741 Dermatril® L (full contact), KCL 741 Dermatril® L (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).

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Respiratory protection

required when dusts are generated.

Recommended Filter type: Filter P 1 (acc. to DIN 3181) for solid particles of inert substances

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 empty into drains.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	powder, finecrystalline
Colour	white
Odour	No strong odour known.
Odour Threshold	No information available.
pH	No information available.
Melting point	71 - 73 °C
Boiling point	No information available.
Flash point	No information available.
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.
Relative density	No information available.
Water solubility	at 20 °C insoluble
Partition coefficient: n-octanol/water	log Pow: 1,26 (experimental) Bioaccumulation is not expected.
Autoignition temperature	No information available.
Decomposition temperature	No information available.

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Viscosity, dynamic	No information available.
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Explosive properties	No information available.
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Oxidizing properties	No information available.
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9.2 Other data

none

SECTION 10. Stability and reactivity

10.1 Reactivity

See section 10.3.

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:

Strong oxidizing agents

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

in the event of fire: See chapter 5.

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Specific target organ toxicity - single exposure

The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

Based on available data the classification criteria are not met.

11.2 Further information

Quantitative data on the toxicity of this product are not available.

Further toxicological data:

Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.

Further data:

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

No information available.

12.2 Persistence and degradability

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No information available.

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 1,26

(experimental)

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

Additional ecological information

Do not allow to run into surface waters, wastewater, or soil.

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

Not classified as dangerous in the meaning of transport regulations.

SECTION 15. Regulatory information

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

EU regulations

Major Accident Hazard 96/82/EC

Legislation Directive 96/82/EC does not apply

Storage class 10 - 13

15.2 Chemical Safety Assessment

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

SECTION 16. Other information

Training advice

Provide adequate information, instruction and training for operators.

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.

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.