

Chemical Safety Data Sheet MSDS / SDS

4-N-Boc-aminocyclohexanone

Revision Date:2026-05-31 Revision Number:1

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

Product identifier

Product name : 4-N-Boc-aminocyclohexanone
CBnumber : CB2149316
CAS : 179321-49-4
EINECS Number : 672-405-6
Synonyms : 4-N-Boc-aminocyclohexanone,tert-butyl 4-oxocyclohexylcarbamate

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Warning

Precautionary statements

P273 Avoid release to the environment.

Hazard statements

H400 Very toxic to aquatic life

SECTION 3: Composition/information on ingredients

Substance

Product name : 4-N-Boc-aminocyclohexanone
Synonyms : 4-N-Boc-aminocyclohexanone,tert-butyl 4-oxocyclohexylcarbamate

CAS : 179321-49-4
EC number : 672-405-6
MF : C11H19NO3
MW : 213.27

SECTION 4: First aid measures

4.1 Description of first aid measures

If inhaled

After inhalation: fresh air.

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. Remove contact lenses.

If swallowed

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

The most important known symptoms and effects are described in the labelling (see section 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

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

Nitrogen oxides (NO_x)

5.3 Advice for firefighters

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

5.4 Further information

Suppress (knock down) gases/vapours/mists with a water spray jet. 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: Avoid inhalation of dusts. Ensure adequate ventilation. 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.

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

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Dry.

Storage stability Recommended storage temperature

2 - 8 °C

Storage class

Storage class (TRGS 510): 11: Combustible Solids

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
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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: 0,11 mm

Break through time: 480 min

Material tested:KCL 741 L

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm

Break through time: 480 min

Material tested:KCL 741 L

Respiratory protection

required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: Filter type P1

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.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

a) Physical state	solid
b) Color	White to Almost white
c) Odor	No data available
d) Melting point/freezing point	Melting point/ range: 114 - 118 °C
e) Initial boiling point and boiling range	335.9±31.0 °C(Predicted)
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	No data available
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	No data available

n) Partition coefficient n-octanol/water	log Pow: 1,396
o) Vapor pressure	No data available
p) Density	1.06±0.1 g/cm ³ (Predicted)
Relative density	1.06±0.1 g/cm ³ (Predicted)
q) Relative vapour density	No data available
r) Particle characteristics	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available
Solubility	soluble in Methanol

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - 2.500 mg/kg

Oral: No data available

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Classified based on available data. For more details, see section 2

Serious eye damage/eye irritation

Classified based on available data. For more details, see section 2

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

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.

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

SECTION 12: Ecological information

12.1 Toxicity

No data available

12.2 Persistence and degradability

No data available

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: 3077

IMDG: 3077

IATA: 3077

14.2 UN proper shipping name

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (4-(Boc- amino)cyclohexanone)

IMDG: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (4-(Boc- amino)cyclohexanone)

IATA: Environmentally hazardous substance, solid, n.o.s. (4-(Boc- amino)cyclohexanone)

14.3 Transport hazard class(es)

ADR/RID: 9

IMDG: 9

IATA: 9

14.4 Packaging group

ADR/RID: III

IMDG: III

IATA: III

14.5 Environmental hazards

ADR/RID: yes

IMDG Marine pollutant: yes

IATA: yes

14.6 Special precautions for user

Tunnel restriction code : (-)

Further information: EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids. Packages smaller than or equal to 5 kg / L , not dangerous goods of

Class 9

14.7 Maritime transport in bulk according to IMO instruments

Not applicable for product as supplied.

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.

International Chemical Weapons Convention : (CWC) Schedules of Toxic Chemicals and Precursors

REACH - Restrictions on the manufacture, : placing on the market and use of certain dangerous substances, preparations and articles (Annex XVII)

Regulation (EU) No 649/2012 of the European : Parliament and the Council concerning the export and import of dangerous chemicals

REACH - Candidate List of Substances of Very : High Concern for Authorisation (Article 59).

This product contains a substance listed on Annex XIV of the REACH Regulation (EC) Nr.

1907/2006.

Listed substance / Sunset Date : After the sunset date the use of this substance requires either an authorization or can only be used for exempted uses, e.g. use in scientific research and development which includes routine analytics or use as intermediate.

Regulation (EU) No 2024/590 on substances that : deplete the ozone layer National legislation

Seveso III: Directive 2012/18/EU of the E1 ENVIRONMENTAL HAZARDS

European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

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

AIIIC - 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 Harmonised 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 Organisation
ISHL - Industrial Safety and Health Law (Japan)
ISO - International Organisation for Standardisation
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 - Organisation 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

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability

of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.