

## SAFETY DATA SHEET

Version 6.3  
Revision Date 10/12/2020  
Print Date 06/01/2022

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : *N*-Boc-hexahydro-1*H*-azepin-4-one

Product Number : 00833  
Brand : Sigma-Aldrich  
CAS-No. : 188975-88-4

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

Identified uses : Laboratory chemicals, Synthesis of substances

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

**1.4 Emergency telephone**

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-  
527-3887 CHEMTREC (International) 24  
Hours/day; 7 Days/week

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Acute toxicity, Oral (Category 4), H302  
Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319  
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335  
For the full text of the H-Statements mentioned in this Section, see Section 16.

**2.2 GHS Label elements, including precautionary statements**

Pictogram



Signal word

Warning

|                            |                                                                                                                                  |
|----------------------------|----------------------------------------------------------------------------------------------------------------------------------|
| Hazard statement(s)        |                                                                                                                                  |
| H302                       | Harmful if swallowed.                                                                                                            |
| H315                       | Causes skin irritation.                                                                                                          |
| H319                       | Causes serious eye irritation.                                                                                                   |
| H335                       | May cause respiratory irritation.                                                                                                |
| Precautionary statement(s) |                                                                                                                                  |
| P261                       | Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.                                                                            |
| P264                       | Wash skin thoroughly after handling.                                                                                             |
| P270                       | Do not eat, drink or smoke when using this product.                                                                              |
| P271                       | Use only outdoors or in a well-ventilated area.                                                                                  |
| P280                       | Wear protective gloves/ eye protection/ face protection.                                                                         |
| P301 + P312 + P330         | IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.                                                      |
| P302 + P352                | IF ON SKIN: Wash with plenty of soap and water.                                                                                  |
| P304 + P340 + P312         | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.      |
| P305 + P351 + P338         | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. |
| P332 + P313                | If skin irritation occurs: Get medical advice/ attention.                                                                        |
| P337 + P313                | If eye irritation persists: Get medical advice/ attention.                                                                       |
| P362                       | Take off contaminated clothing and wash before reuse.                                                                            |
| P403 + P233                | Store in a well-ventilated place. Keep container tightly closed.                                                                 |
| P405                       | Store locked up.                                                                                                                 |
| P501                       | Dispose of contents/ container to an approved waste disposal plant.                                                              |

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                  |                                                                                    |
|------------------|------------------------------------------------------------------------------------|
| Synonyms         | : 1-Boc-homopiperazin-4-one<br>tert-Butyl hexahydro-4-oxo-1H-azepine-1-carboxylate |
| Formula          | : C <sub>11</sub> H <sub>19</sub> NO <sub>3</sub>                                  |
| Molecular weight | : 213.27 g/mol                                                                     |
| CAS-No.          | : 188975-88-4                                                                      |

| Component                              | Classification                                                                      | Concentration |
|----------------------------------------|-------------------------------------------------------------------------------------|---------------|
| <b>N-Boc-hexahydro-1H-azepin-4-one</b> |                                                                                     |               |
|                                        | Acute Tox. 4; Skin Irrit. 2;<br>Eye Irrit. 2A; STOT SE 3;<br>H302, H315, H319, H335 | <= 100 %      |

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

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 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 2.2) and/or in section 11

### 4.3 Indication of any immediate medical attention and special treatment needed

No data available

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides, Nitrogen oxides (NO<sub>x</sub>)

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

No data available

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## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.  
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

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

## 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

For precautions see section 2.2.

### 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.

Recommended storage temperature 2 - 8 °C

Store under inert gas. Air sensitive.

Storage class (TRGS 510): 10: Combustible liquids

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### Personal protective equipment

##### Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

##### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

##### Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

## Control of environmental exposure

Do not let product enter drains.

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### SECTION 9: Physical and chemical properties

#### 9.1 Information on basic physical and chemical properties

|                                                 |                                              |
|-------------------------------------------------|----------------------------------------------|
| a) Appearance                                   | Form: liquid<br>Color: light yellow          |
| b) Odor                                         | No data available                            |
| c) Odor Threshold                               | No data available                            |
| d) pH                                           | No data available                            |
| e) Melting point/freezing point                 | No data available                            |
| f) Initial boiling point and boiling range      | No data available                            |
| g) Flash point                                  | ( )No data available                         |
| h) Evaporation rate                             | No data available                            |
| i) Flammability (solid, gas)                    | No data available                            |
| j) Upper/lower flammability or explosive limits | No data available                            |
| k) Vapor pressure                               | No data available                            |
| l) Vapor density                                | No data available                            |
| m) Relative density                             | 1,054.000 g/cm <sup>3</sup> at 20 °C (68 °F) |
| n) Water solubility                             | No data available                            |
| o) Partition coefficient: n-octanol/water       | log Pow: 0.9                                 |
| p) Autoignition temperature                     | No data available                            |
| q) Decomposition temperature                    | No data available                            |
| r) Viscosity                                    | No data available                            |
| s) Explosive properties                         | No data available                            |
| t) Oxidizing properties                         | No data available                            |

#### 9.2 Other safety information

No data available

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### SECTION 10: Stability and reactivity

#### 10.1 Reactivity

No data available

## **10.2 Chemical stability**

Stable under recommended storage conditions.

## **10.3 Possibility of hazardous reactions**

No data available

## **10.4 Conditions to avoid**

No data available

## **10.5 Incompatible materials**

Strong oxidizing agents

## **10.6 Hazardous decomposition products**

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>)

Other decomposition products - No data available

In the event of fire: see section 5

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## **SECTION 11: Toxicological information**

### **11.1 Information on toxicological effects**

#### **Acute toxicity**

No data available

Dermal: No data available

No data available

#### **Skin corrosion/irritation**

No data available

#### **Serious eye damage/eye irritation**

No data available

#### **Respiratory or skin sensitization**

No data available

#### **Germ cell mutagenicity**

No data available

#### **Carcinogenicity**

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

#### **Reproductive toxicity**

No data available

No data available

#### **Specific target organ toxicity - single exposure**

Inhalation - May cause respiratory irritation.

#### **Specific target organ toxicity - repeated exposure**

No data available

#### **Aspiration hazard**

No data available

## **Additional Information**

RTECS: Not available

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### **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**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

#### **12.6 Other adverse effects**

No data available

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### **SECTION 13: Disposal considerations**

#### **13.1 Waste treatment methods**

##### **Product**

Offer surplus and non-recyclable solutions to a licensed disposal company.

##### **Contaminated packaging**

Dispose of as unused product.

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### **SECTION 14: Transport information**

#### **DOT (US)**

Not dangerous goods

#### **IMDG**

Not dangerous goods

#### **IATA**

Not dangerous goods

#### **Further information**

Not classified as dangerous in the meaning of transport regulations.

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### **SECTION 15: Regulatory information**

### **SARA 302 Components**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

### **SARA 313 Components**

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

### **Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

No components are subject to the Massachusetts Right to Know Act.

### **Pennsylvania Right To Know Components**

|                                 |                        |               |
|---------------------------------|------------------------|---------------|
| N-Boc-hexahydro-1H-azepin-4-one | CAS-No.<br>188975-88-4 | Revision Date |
|---------------------------------|------------------------|---------------|

|                                 |                        |               |
|---------------------------------|------------------------|---------------|
| N-Boc-hexahydro-1H-azepin-4-one | CAS-No.<br>188975-88-4 | Revision Date |
|---------------------------------|------------------------|---------------|

### **New Jersey Right To Know Components**

|                                 |                        |               |
|---------------------------------|------------------------|---------------|
| N-Boc-hexahydro-1H-azepin-4-one | CAS-No.<br>188975-88-4 | Revision Date |
|---------------------------------|------------------------|---------------|

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## **SECTION 16: Other information**

### **Further information**

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