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**1. PRODUCT AND COMPANY IDENTIFICATION****1.1 Product identifiers**

Product name : Boc-4-phenyl-Phe-OH

Product Number : 464546

Brand : Aldrich

CAS-No. : 147923-08-8

**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  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

**1.4 Emergency telephone number**

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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**2. HAZARDS IDENTIFICATION****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Reproductive toxicity (Category 2), H361

Acute aquatic toxicity (Category 3), H402

Chronic aquatic toxicity (Category 3), H412

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)

H361

Suspected of damaging fertility or the unborn child.

H412

Harmful to aquatic life with long lasting effects.

Precautionary statement(s)

P201

Obtain special instructions before use.

P202

Do not handle until all safety precautions have been read and understood.

P273

Avoid release to the environment.

P281

Use personal protective equipment as required.

P308 + P313

IF exposed or concerned: Get medical advice/ attention.

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

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### 3. COMPOSITION/INFORMATION ON INGREDIENTS

#### 3.1 Substances

Synonyms : Boc-4-phenyl-L-phenylalanine  
(S)-2-(Boc-amino)-3-(4-biphenyl)propionic acid  
Boc-Bip-OH

Formula : C<sub>20</sub>H<sub>23</sub>NO<sub>4</sub>  
Molecular weight : 341.40 g/mol  
CAS-No. : 147923-08-8

#### Hazardous components

Component	Classification	Concentration
<b>Toluene</b>		
	Flam. Liq. 2; Skin Irrit. 2; Repr. 2; STOT SE 3; STOT RE 2; Asp. Tox. 1; Aquatic Acute 2; H225, H304, H315, H336, H361, H373, H401	>= 1 - < 5 %

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

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### 4. FIRST AID MEASURES

#### 4.1 Description of first aid measures

##### General advice

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

##### 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

Flush eyes with water as a precaution.

##### 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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### 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

No data available

#### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

#### 5.4 Further information

No data available

## 6. ACCIDENTAL RELEASE MEASURES

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

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.  
For personal protection see section 8.

### 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

### 6.3 Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

### 6.4 Reference to other sections

For disposal see section 13.

## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.  
Provide appropriate exhaust ventilation at places where dust is formed.  
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.

### 7.3 Specific end use(s)

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

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Toluene	108-88-3	TWA	100 ppm 375 mg/m <sup>3</sup>	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		STEL	150 ppm 560 mg/m <sup>3</sup>	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		TWA	200 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
	Remarks	Z37.12-1967		
		CEIL	300 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		Z37.12-1967		
		Peak	500 ppm	USA. Occupational Exposure Limits (OSHA) - Table Z-2
		Z37.12-1967		
		TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Visual impairment Female reproductive Pregnancy loss 2015 Adoption Substances for which there is a Biological Exposure Index or Indices (see BEI® section) Not classifiable as a human carcinogen		

		TWA	100 ppm 375 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		ST	150 ppm 560 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits

#### Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Toluene	108-88-3	Toluene	0.0200 mg/l	In blood	ACGIH - Biological Exposure Indices (BEI)
	Remarks	Prior to last shift of workweek			
		Toluene	0.0300 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			
		o-Cresol	0.3000 mg/g	Urine	ACGIH - Biological Exposure Indices (BEI)
		End of shift (As soon as possible after exposure ceases)			

## 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

Safety glasses with side-shields conforming to EN166 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

Impervious clothing, 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 particle respirator type N100 (US) or type P3 (EN 143) 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

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |                                 |   |
|---------------------------------|---|
| a) Appearance                   | Form: solid   |
| b) Odour                        | No data available                                       |
| c) Odour Threshold              | No data available                                       |
| d) pH                           | No data available                                       |
| e) Melting point/freezing point | Melting point/range: 103 - 107 °C (217 - 225 °F) - lit. |
| f) Initial boiling point and    | No data available                                       |

	boiling range	
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)	Vapour pressure	No data available
l)	Vapour density	No data available
m)	Relative density	No data available
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	No data available
p)	Auto-ignition 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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## 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 (NOx)

Other decomposition products - No data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

Inhalation: 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 sensitisation**

No data available

**Germ cell mutagenicity**

No data available

**Carcinogenicity**

IARC: No component 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 component 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 identified as a carcinogen or potential carcinogen by OSHA.

**Reproductive toxicity**

No data available

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

RTECS: Not available

Inhalation studies on toluene have demonstrated the development of inflammatory and ulcerous lesions of the penis, prepuce, and scrotum in animals., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence (Toluene)

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**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**

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Harmful to aquatic life.

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## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

#### Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

#### Contaminated packaging

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

#### DOT (US)

Not dangerous goods

#### IMDG

Not dangerous goods

#### IATA

Not dangerous goods

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## 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

The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
Toluene	108-88-3	2007-07-01

#### SARA 311/312 Hazards

Acute Health Hazard, Chronic Health Hazard

#### Massachusetts Right To Know Components

	CAS-No.	Revision Date
Toluene	108-88-3	2007-07-01

#### Pennsylvania Right To Know Components

	CAS-No.	Revision Date
3-(4-BIPHENYLYL)-N-(TERT-BUTOXYCARBONYL)-L-ALANINE	147923-08-8	
Toluene	108-88-3	2007-07-01

#### New Jersey Right To Know Components

	CAS-No.	Revision Date
3-(4-BIPHENYLYL)-N-(TERT-BUTOXYCARBONYL)-L-ALANINE	147923-08-8	
Toluene	108-88-3	2007-07-01

#### California Prop. 65 Components

	CAS-No.	Revision Date
WARNING: This product contains a chemical known to the State of California to cause birth defects or other reproductive harm.	108-88-3	2009-02-01

Toluene

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## 16. OTHER INFORMATION

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

Aquatic Acute	Acute aquatic toxicity
Asp. Tox.	Aspiration hazard
Flam. Liq.	Flammable liquids
H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H336	May cause drowsiness or dizziness.
H361	Suspected of damaging fertility or the unborn child.
H373	May cause damage to organs through prolonged or repeated exposure.
H401	Toxic to aquatic life.
H402	Harmful to aquatic life.
H412	Harmful to aquatic life with long lasting effects.
Repr.	Reproductive toxicity
Skin Irrit.	Skin irritation
STOT RE	Specific target organ toxicity - repeated exposure
STOT SE	Specific target organ toxicity - single exposure

#### HMIS Rating

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	0
Physical Hazard	0

#### NFPA Rating

Health hazard:	2
Fire Hazard:	0
Reactivity Hazard:	0

#### Further information

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#### Preparation Information

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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