

## SAFETY DATA SHEET

### 1. PRODUCT AND COMPANY IDENTIFICATION

#### 1.1 Product identifiers

Chemical name: 2-S-(4-Isothiocyanatobenzyl)-1,4,7-triazacyclononane-1,4,7-triacetic acid  
Synonym: *p*-SCN-Bn-NOTA  
Product Number: B-605  
Brand: Macrocyclics  
CAS-No.: 147597-66-8

#### 1.2 Relevant identified uses of the substance

Identified uses : Laboratory and research chemicals

#### 1.3 Details of the supplier providing the safety data sheet

Company: Macrocyclics  
700 Klein Rd.  
Plano, TX 75074  
USA  
Telephone: 469-786-6079  
Fax: 469-814-9116

#### 1.4 Emergency telephone number

Emergency Phone #: 469-786-6079

### 2. HAZARDOUS IDENTIFICATION

#### 2.1 Classification of the compound

##### GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

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

Hazardous statement(s)

H315: May causes skin irritation

H335: May cause respiratory irritation

Precautionary statement(s)

P261: Avoid breathing dust.

P264:	Wash skin thoroughly after handling.
P280:	Wear protective gloves/eye protection/face protection.
P302 + P352:	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340:	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P305 + 351 + P338:	If IN EYES: Rinse with water for several minutes. Remove contacts if present and continue rinsing.
P312:	Contact a physician
P332 + P313:	If skin irritation persists seek medical attention
P337 + P313:	If eye irritation persists seek medical attention
P362:	Remove contaminated clothing and wash before reuse
P403 + P233:	Store in well-ventilated area. Keep container tightly sealed.
P405:	Store in secure location.
P501:	Dispose of contents by approved waste management procedures

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS – None

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## 3. COMPOSITION INFORMATION OF INGREDIENTS

### 3.1 Substances

Synonym:	<i>p</i> -SCN-Bn-NOTA
Formula:	C <sub>20</sub> H <sub>26</sub> N <sub>4</sub> O <sub>6</sub> S·3HCl
Molecular Weight:	559.9 g/mol
CAS-No:	147597-66-8

#### Hazardous components

Component	Classification
2-S-(4-Isothiocyanatobenzyl)-1,4,7-triazacyclononane-1,4,7-triacetic acid	Skin irrit. 2; Eye Irrit. 2A STOT SE 3; H315, H319, H335

For full text of the H-Statements see Section 16

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## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult physician. Present this safety data sheet to the physician in attendance.

#### If inhaled

Move person into fresh air. Consult physician.

#### In case of skin contact

Wash contacted area with soap and water.

#### In case of eye contact

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

#### If swallowed

Rinse mouth with water and consult a physician.

### 4.2 Most important symptoms and effects, acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2,2) and/or section 11.

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

No data available

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### **5. FIRE FIGHTING MEASURES**

#### **5.1 Extinguishing media**

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

#### **5.2 Special hazards arising from the substance**

Carbon dioxide, nitrogen oxides

#### **5.3 Advice for firefighters**

Wear self-contained breathing apparatus for fighting fire if necessary.

#### **5.4 Further information**

No data available

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### **6. ACCIDENTAL RELEASE MEASURES**

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

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

#### **6.2 Environmental precautions**

Do not allow product to enter water drains.

#### **6.3 Methods and materials for containment and clean up**

Manage disposal without creating dust. Seep up and deposit in suitable, close container for disposal.

#### **6.4 Reference to other sections**

For disposal see section 13.

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### **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 might be formed. For precautions see section 2.2.

#### **7.2 Conditions for safe storage, including possible incompatibilities**

Keep container tightly closed in a dry and well-ventilated environment.  
Storage temperature: 25°C or below.

#### **7.3 Specific end use(s)**

Research and development

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### **8. EXPOSURE CONTROL/PERSONAL PROTECTION**

- 8.1 Control parameters**  
Components 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**

Safety glasses with side-shields conforming to 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.

**Body protection**

Impervious clothing. The type of lab coat or other protective equipment must be selected according the amount of product being handled and the specific laboratory conditions.

**Respiratory protection**

It is recommended to handle this material in an appropriate chemical fume hood if possible. For small exposures use dust mask or type P95 (US) or P1 (EU EN 143) particle respirator.

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**9. PHYSICAL AND CHEMICAL PROPERTIES**

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

a)	Appearance	solid
b)	Odor	no data available
c)	Odor threshold	no data available
d)	pH	no data available
e)	Melting/freezing point	no data available
f)	Boiling point	no data available
g)	Flash point	no data available
h)	Evaporation rate	no data available
i)	Flammability	no data available
j)	Explosive limits	no data available
k)	Vapor pressure	no data available
l)	Vapor density	no data available
m)	Relative density	no data available
o)	Partition coefficient	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

## 10. STABILITY DATA

### 10.1 Reactivity

No data availability

### 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 availability

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

No data availability

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

No data availability

#### Skin corrosion/irritation

No data availability

#### Eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

No data availability

#### Carcinogenicity

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

ACGIH: No components of this product present at levels greater than or equal to 0.1% is Identified as probable, possible or confirmed human carcinogen.

OSHA: No components of this product present at levels greater than or equal to 0.1% is Identified as probable, possible or confirmed human carcinogen.

#### Reproductive toxicity

No data availability

**Specific target organ toxicity – single exposure**

Inhalation – May cause respiratory irritation.

**Specific target organ toxicity – repeated exposure**

No data available

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**12. ECOLOGICAL INFORMATION**

**12.1 Toxicity**

No data available

**12.2 Persistence and degradability**

No data availability

**12.3 Bioaccumulative potential**

No data availability

**12.4 Mobility in soil**

No data availability

**12.5 Results of PBT and vPvB assessment**

No data availability

**12.6 Other adverse effects**

No data availability

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**13. DISPOSAL CONSIDERATIONS**

**13.1. Waste treatment methods**

**Product**

Contact a licensed professional disposal service to dispose of non-recyclable material

**Contaminated packaging and containers**

Dispose of as unused product

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**14. TRANSPORTATION INFORMATION**

**DOT (US)**

Not dangerous goods

**IMDG**

Not dangerous goods

**IATA**

Not dangerous goods

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**15. REGULATORY INFORMATION**

**SARA 302 Components**

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

**SARA 313 Components**

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

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**16. OTHER INFORMATION****Full text of H-Statements referred to under sections 2 and 3.**

Eye Irrit.	Eye irritation
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
Skin Irrit.	Skin irritation
STOT SE	Specific target organ toxicity - single exposure

**HMIS Rating**

Health hazard:	1
Flammability:	0
Physical hazard:	0

**NFPA Rating**

Health hazard:	1
Fire hazard:	0
Reactivity hazard	0

**Further information**

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Macrocyclics shall not be held liable for any damage resulting from handling or from contact with the above product.

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