

SAFETY DATA SHEET

1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Chemical name: 3,6,9,15-Tetraazabicyclo[9.3.1] pentadeca-1(15),11,13-triene-4-S-(4-isothiocyanatobenzyl)-3,6,9-triacetic acid
 Synonym: *p*-SCN-Bn-PCTA
 Product Number: B-405
 Brand: Macrocytics
 CAS-No.: 949147-44-8

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: Macrocytics
 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

3. COMPOSITION INFORMATION OF INGREDIENTS

3.1 Substances

Synonym:	<i>p</i> -SCN-Bn-PCTA
Formula:	C ₂₅ H ₂₉ N ₅ O ₆ S·3HCl
Molecular Weight:	637.0 g/mol
CAS-No:	949147-44-8

Hazardous components

Component	Classification
3,6,9,15-Tetraazabicyclo[9.3.1] pentadeca-1(15),11,13-triene-4-S-(4-isothiocyanatobenzyl)-3,6,9-triacetic	Skin irrit. 2; Eye Irrit. 2A STOT SE 3; H315, H319, H335

For full text of the H-Statements see Section 16

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

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

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. Sweep up and deposit in suitable, close container 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 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: -20 °C or below.

7.3 Specific end use(s)

Research and development

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.

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

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

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

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

14. TRANSPORTATION INFORMATION

DOT (US)

Not dangerous goods

IMDG

Not dangerous goods

IATA

Not dangerous goods

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.

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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