

# Capadenoson SDS/MSDS (Safety Data Sheet)

## 1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

\* Product Name: Capadenoson

\* Catalog Number: E2985

\* CAS Number: 544417-40-5

\* IUPAC Name: 3,5-Pyridinedicarbonitrile, 2-amino-6-[[[2-(4-chlorophenyl)-4-thiazolyl]methyl]thio]-4-[4-(2-hydroxyethoxy)phenyl]

Relevant identified uses and uses advised against

\* Identified uses: For research and development use only; laboratory chemicals; manufacture of substances.

\* Uses advised against: Not for pharmaceutical, household, or other unapproved uses.

Details of the supplier

\* Company: Selleck Chemicals

\* TollFree: +1 877 796-6397

\* Tel: +1 832 582-8158

\* Fax: +1 832 582-8590

Emergency telephone number

\* Emergency phone #: +1 832 582-8158

## 2. HAZARDS IDENTIFICATION

### 2.1 GHS classification in accordance with 29 CFR 1910 (OSHA HCS):

Reproductive toxicity: Category 2. H361

Specific target organ toxicity (single exposure): Category 1. H370

### 2.2 GHS Label elements, including precautionary statements

Hazard Pictogram(s)



Signal Word

Warning

Hazard statement(s)

H361: Suspected of damaging fertility or the unborn child

H370: Causes damage to organs

Precautionary statement(s)

None.

Prevention

P203: Obtain, read and follow all safety instructions before use.

P260: Do not breathe dust/fume/gas/mist/vapors/spray.

P264: Wash hands thoroughly after handling.

P270: Do not eat, drink or smoke when using this product.

P280: Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.

|                 |                                                                                                                                                                                                                      |
|-----------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Response</b> | P308+P316: IF exposed or concerned: Get emergency medical help immediately.<br>P318: if exposed or concerned, get medical advice.<br>P321: Specific treatment (see information on this label and safety datasheet)). |
| <b>Storage</b>  | P405: Store locked up.                                                                                                                                                                                               |
| <b>Disposal</b> | P501: P501 Dispose of contents/ container to an approved waste disposal plant.                                                                                                                                       |

### 2.3 Other hazards

None.

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Product name: Capadenoson

CAS Number: 544417-40-5

PubChem CID: 9936489

Molecular formula: C<sub>25</sub>H<sub>18</sub>ClN<sub>5</sub>O<sub>2</sub>S<sub>2</sub>

Molecular weight: 520.0 g/mol

IUPAC name: 2-amino-6-[[2-(4-chlorophenyl)-1,3-thiazol-4-yl]methylsulfanyl]-4-[4-(2-hydroxyethoxy)phenyl]pyridine-3,5-dicarbonitrile

### 3.2 Mixtures

Not applicable (pure substance).

## 4. FIRST-AID MEASURES

### 4.1 Description of first aid measures

Inhalation: Move to fresh air. Keep at rest in a position comfortable for breathing. Seek medical attention if symptoms persist.

Skin contact: Wash with plenty of soap and water. Remove contaminated clothing. Seek medical attention if irritation develops.

Eye contact: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing. Seek medical attention.

Ingestion: Rinse mouth. Do NOT induce vomiting unless directed by medical personnel. Seek medical attention.

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

See Section 11 (Toxicological Information).

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

Treat symptomatically. Contact a poison control center or physician for severe exposure.

## 5. FIRE-FIGHTING MEASURES

### 5.1 Extinguishing media

Suitable: Water spray, dry chemical, carbon dioxide (CO<sub>2</sub>), alcohol-resistant foam.

Unsuitable: None known.

## **5.2 Specific hazards arising from the substance or mixture**

Combustible. Heating may produce toxic fumes.

## **5.3 Advice for firefighters**

Wear self-contained breathing apparatus (SCBA) and full protective clothing.

Fight fire from upwind. Cool containers with water spray until fire is extinguished.

# **6. ACCIDENTAL RELEASE MEASURES**

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

Wear appropriate personal protective equipment (see Section 8).

Avoid breathing dust/vapor. Ensure adequate ventilation.

Evacuate personnel to safe areas. Keep people away from and upwind of spill.

## **6.2 Environmental precautions**

Prevent product from entering drains, waterways, or soil.

Contain spill with inert absorbent material.

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

Sweep up or absorb with inert material (e.g., sand, vermiculite).

Place in sealed, labeled container for disposal.

Wash spill area with water.

# **7. HANDLING AND STORAGE**

## **7.1 Precautions for safe handling**

Handle in accordance with good industrial hygiene and safety practices.

Wear appropriate PPE (see Section 8). Avoid contact with skin, eyes, and clothing.

Wash hands thoroughly after handling. Do not eat, drink, or smoke in work area.

Avoid dust formation. Use only in a chemical fume hood or well-ventilated area.

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

Store in a cool, dry, well-ventilated area. Keep container tightly closed.

Store away from incompatible materials (see Section 10).

Protect from light and moisture.

Recommended storage (industry convention for research compounds): -20°C for long-term storage; 2-8°C for short-term use and transport.

[Note: This is a general industry recommendation. Always verify exact storage conditions with the supplier Certificate of Analysis (COA).]

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

## **8.1 Exposure controls**

8.1.1 Occupational exposure limits (OEL)

OSHA PEL: Not established.

ACGIH TLV: Not established.

NIOSH REL: Not established.

No occupational exposure limit values are established for this substance.

Use the lowest feasible exposure level (ALARA principle).

#### 8.1.2 Appropriate engineering controls

Use in a well-ventilated area. Chemical fume hood recommended for powder handling.

### 8.2 Individual protection measures

#### 8.2.1 Eye/face protection

Wear safety glasses with side shields.

#### 8.2.2 Skin protection

Wear protective gloves. Recommended material: Nitrile rubber.

Wear suitable protective clothing (lab coat).

#### 8.2.3 Respiratory protection

Respiratory protection usually not required under normal use with adequate ventilation.

Use N95 respirator for large-scale powder handling.

#### 8.2.4 Thermal hazards

Not applicable.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- a) Appearance: Solid powder (typical for research compounds)
- 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: No data available
- n) Water solubility: Soluble in DMSO; slightly soluble in water
- o) Partition coefficient: n-octanol/water: Log P (n-octanol/water): 5.1
- 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 information

Topological Polar Surface Area (TPSA): 182 Å<sup>2</sup>

Complexity: 774

## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No specific reactivity hazards identified under normal handling conditions.

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No hazardous reactions under normal conditions.

### 10.4 Conditions to avoid

Avoid heat, sparks, open flames, direct sunlight, and moisture.

Avoid strong oxidizing agents, strong acids, and strong bases.

### 10.5 Incompatible materials

Strong oxidizing agents, strong acids, strong bases.

### 10.6 Hazardous decomposition products

Thermal decomposition may produce: Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>), Nitrogen oxides (NO<sub>x</sub>), Sulfur oxides (SO<sub>x</sub>), Hydrogen chloride (HCl).

See also Section 5 (Fire-fighting measures) for combustion products.

## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity:

No acute toxicity 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:

No data available.

#### Reproductive toxicity:

Suspected of damaging fertility or the unborn child (H361).

#### Specific target organ toxicity (single exposure):

H370

#### Specific target organ toxicity (repeated exposure):

No data available.

**Aspiration hazard:**

No data available.

**11.2 Additional information**

No additional toxicological information available.

**12. ECOLOGICAL INFORMATION**

**12.1 Toxicity**

No ecotoxicity data available.

**12.2 Persistence and degradability**

No data available.

**12.3 Bioaccumulative potential**

Log P (n-octanol/water): 5.1

Potential for bioaccumulation exists (Log P > 3).

**12.4 Mobility in soil**

No data available.

**12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available.

**12.6 Other adverse effects**

No other adverse ecological effects identified.

**13. DISPOSAL CONSIDERATIONS**

**13.1 Waste treatment methods**

Waste Treatment Methods: Waste material must be disposed of in accordance with national and local regulations. Leave chemicals in original containers and do not mix with other waste. Handle uncleaned containers in the same manner as the product itself.

**14. TRANSPORT INFORMATION**

**14.1 UN number**

Not regulated as dangerous goods (research quantities typically exempt).

**14.2 UN proper shipping name**

Not subject to transport regulations (small quantities for research use).

**14.3 Transport hazard class(es)**

Not classified as dangerous goods for transport (research quantities).

**14.4 Packing group**

Not applicable (not regulated as dangerous goods in typical research quantities).

**14.5 Environmental hazards**

Marine pollutant: No (not classified as environmentally hazardous per GHS).

**14.6 Special precautions for user**

Transport in original packaging. Ensure containers are tightly sealed.

For bulk or commercial quantities, consult applicable transport regulations (DOT, IATA, IMDG).

**14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code**

Not applicable.

**15. REGULATORY INFORMATION****15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

US EPA / TSCA: Not available in public databases.

EU ECHA / REACH: Not available in public databases.

**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.

**SARA 311/312 Hazards:**

Acute (short-term) health hazard

Chronic (long-term) health hazard

**Massachusetts Right To Know Components:**

This material contains components subject to the Massachusetts Right to Know Act. See Section 2 for hazard classification.

**Pennsylvania Right To Know Components:**

This material contains components subject to the Pennsylvania Right to Know Act. See Section 2 for hazard classification.

**New Jersey Right To Know Components:**

This material contains components subject to the New Jersey Right to Know Act. See Section 2 for hazard classification.

**California Prop. 65 Components:**

This product does not contain any chemicals known to the State of California to cause cancer, birth defects, or any other reproductive harm.

**15.2 Chemical safety assessment**

A chemical safety assessment has not been carried out for this substance.

For research-use-only compounds, no CSA is required under REACH Annex I.

**16. OTHER INFORMATION**

Revision Date: 2026/09/08

Further Information: The information provided is believed to be correct but is not exhaustive and should be used only as a guideline based on current knowledge. It does not represent a guarantee of the properties of the product.

Selleck Chemicals Corporation and its Affiliates shall not be held liable for any damage resulting from handling or

contact with the product.