1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1 Product Identifier

Chemical Name 4-[2-(2-Amino-4,7-dihydro-4-oxo-3H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoic Acid

Catalogue # A604905

1.2 Relevant Identified Uses of the Substance or Mixture and Uses Advised Against

Product Uses To be used only for scientific research and development. Not for use in humans or animals.

1.3 Details of the Supplier of the Safety Data Sheet

Company Toronto Research Chemicals
2 Brisbane Road
Toronto, ON M3J 2J8
CANADA

Telephone +14166659696
FAX +14166654439
Email orders@trc-canada.com

1.4 Emergency Telephone Number

Emergency# +1(416) 665-9696 between 0800-1700 (GMT-5)

2. HAZARDS IDENTIFICATION

WHMIS Classification (Canada) GHS Hazards Classification (According to EU Regulation 1272/2008 and US OSHA 1910.1200)

D2B Toxic Material Causing Other Toxic Effects

Skin Irritation (Category 2)
Serious Eye Irritation (Category 2A)
Specific Target Organ Toxicity, Single Exposure; Respiratory Tract Irritation (Category 3)

GHS Symbols (Canada) Moderate Skin/Eye/Respiratory Tract Irritant

2.1/2.2 Classification of the Substance or Mixture and Label Elements

GHS Hazard Statements

H315 Causes skin irritation.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation.

GHS Precautionary Statements

P261 Avoid breathing dust/fume/gas/mist/vapours/spray
P280 Wear protective gloves/protective clothing/eye protection/face protection.
2.3 Unclassified Hazards/Hazards Not Otherwise Classified

No data available.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Molecular Formula: \( \text{C}_{15}\text{H}_{14}\text{N}_{4}\text{O}_{3} \)  
Molecular Weight: 298.30

CAS Registry #: 137281-39-1  
EC#: 429-790-9

Synonyms

4-[2-(2-Amino-4,7-dihydro-4-oxo-1H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoic Acid;

3.2 Mixtures

Not a mixture.

4. FIRST AID MEASURES

4.1 Description of First Aid Measures

General Advice
If medical attention is required, show this safety data sheet to the doctor.

If Inhaled
If inhaled, move person to fresh air. If not breathing, give artificial respiration and consult a physician.

In Case of Skin Contact
Wash affected area with soap and water. Consult a physician if any exposure symptoms are observed.

In Case of Eye Contact
Immediately rinse eyes with plenty of water for at least 15 minutes. Consult a physician.

If Swallowed
Never give anything by mouth to an unconscious person. Rinse mouth with water. Do NOT induce vomiting unless advised to do so by a physician or Poison Control Center. Seek medical attention.

4.2 Most Important Symptoms and Effects, Both Acute and Delayed

The most important known symptoms and effects are described in the labeling (see section 2.2) and/or section 11.

4.3 Indication of any Immediate Medical Attention and Special Treatment Needed

No data available.

5. FIREFIGHTING MEASURES

5.1 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

5.3 Advice for Firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further Information

No data available.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.
**7. HANDLING AND STORAGE**

**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.

**Conditions for safe storage**
Keep container tightly closed in a dry and well-ventilated place. Keep in a dry place.

Storage conditions: -20°C Freezer

**7.3 Specific End Uses**
For scientific research and development only. Not for use in humans or animals.

**8. EXPOSURE CONTROLS/PERSONAL PROTECTION**

**8.1 Control Parameters**
Contains no components with established occupational exposure limits.

**8.2 Exposure Controls**

**Appropriate Engineering Controls**
A laboratory fume hood or other appropriate form of local exhaust ventilation should be used to avoid exposure.

**Personal Protective Equipment**
All recommendations below are advisory in nature and a risk assessment should be performed by the employer/end user prior to use of this product. The type of protective equipment must be selected based on the amount and concentration of the dangerous material being used in the workplace.

**Eye/Face Protection**
Safety goggles or face shield. All equipment should have been tested and approved under appropriate standards, such as NIOSH (US), CSA (Canada), or EN 166 (EU).

**Skin Protection**
Gloves should be used when handling this material. Gloves are to be inspected prior to use. Contaminated gloves are to be removed using proper glove removal technique so that the outer surface of the glove does not contact bare skin. Dispose of contaminated gloves after use in compliance with good laboratory practices and local requirements.

Gloves used for incidental exposures (splash protection) should be designated as “chemical resistant” by EU standard EN 374 with the resistance codes corresponding to the anticipated use of the material. Unrated gloves are not recommended.
Suggested gloves: AnsellPro Sol-Vex nitrile gloves style 37-175, 15 mil thickness.
Penetration time has not been determined.

Gloves used for prolonged direct exposure (immersion) should be designated “chemical resistant” as per EN 734 with the resistance codes corresponding to the anticipated use of the material.
Penetration time has not been determined.

These recommendations may not apply if the material is mixed with any other chemical, or dissolved into a solution. A risk assessment must be performed to ensure the gloves will still offer acceptable protection.

**Body Protection**
Fire resistant (Nomex) lab coat or coveralls.

**Respiratory Protection**
Recommended respirators are NIOSH-approved N100 or CEN-approved FFP3 particulate respirators. These are to be only used as a backup to local exhaust ventilation or other engineering controls. If the respirator is the only means of protection, a full-face supplied air respirator must be used.

**9. PHYSICAL AND CHEMICAL PROPERTIES**

**9.1 Information on Basic Physical and Chemical Properties**

<table>
<thead>
<tr>
<th>A) Appearance</th>
<th>B) Odour</th>
</tr>
</thead>
<tbody>
<tr>
<td>-20˚C Freezer</td>
<td></td>
</tr>
</tbody>
</table>
C) Odour Threshold
No data available

D) pH
No data available

E) Melting Point/Freezing Point
>270°C (dec.)

F) Initial Boiling Point/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/Explosive Limits
No data available

K) Vapour Pressure
No data available

L) Vapour Density
No data available

M) Relative Density
No data available

N) Solubility
DMSO (Slightly), Methanol (Slightly, Heated)

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

9.2 Other Information
no data available

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
In the event of fire: See section 5. Other decomposition products: No data available.

11. TOXICOLOGICAL INFORMATION

11.1 Information on Toxicological Effects

A) Acute Toxicity
Oral LD50: No data available.
Dermal LD50: No data available.

B) Skin Corrosion/Irritation
Moderate skin irritant.

C) Serious Eye Damage/Irritation
Moderate eye irritant.

D) Respiratory or Skin Sensitization
No data available

E) Germ Cell Mutagenicity
No data available

F) Carcinogenicity
No data available

G) Reproductive Toxicity/Teratogenicity
No data available

H) Single Target Organ Toxicity - Single Exposure
No data available

White to Pale Pink Solid

No data available.
J) Aspiration Hazard
No data available

K) Potential Health Effects and Routes of Exposure
Inhalation
May be harmful if inhaled. Causes respiratory tract irritation.
Ingestion
May be harmful if swallowed.
Skin
May be harmful if absorbed through skin. Causes skin irritation.
Eyes
Causes eye irritation.

L) Signs and Symptoms of Exposure
The most important known symptoms and effects are described in the labeling (see section 2.2) and/or section 11.

To the best of our knowledge, the chemical, physical, and toxicological properties of this material have not been thoroughly investigated.

M) Additional Information
RTECS: Not available.

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
No data available.

12.6 Other Adverse Effects
No data available.

13. DISPOSAL CONSIDERATIONS

13.1 Waste Treatment Methods

A) Product
Product may be burned in an incinerator equipped with afterburner and scrubber. Excess and expired materials are to be offered to a licensed hazardous material disposal company. Ensure that all Federal and Local regulations regarding the disposal and destruction of this material are followed.

B) Contaminated Packaging
Dispose of as above.

C) Other Considerations
Product is not to be disposed of in sanitary sewers, storm sewers, or landfills.

14. TRANSPORT INFORMATION

14.1 UN Number
DOT (US): N/A  IATA: N/A  IMDG: N/A  ADR/RID: N/A

14.2 UN Proper Shipping Name
DOT (US)/IATA:
Not dangerous goods
IMDG/ARD/RID:
Not dangerous goods

14.3 Transport Hazard Class(es)
DOT (US): N/A  IATA: N/A  IMDG: N/A  ADR/RID: N/A

14.4 Packing Group

This Safety Data Sheet contains 16 sections. All 16 sections must be present for this document to be valid.
14.5 Environmental Hazards
DOT (US): None  IATA: None  IMDG: None  ADR/RID: None

14.6 Special Precautions for User
None

15. REGULATORY INFORMATION
This safety data sheet complies with the requirements of WHMIS (Canada), OSHA 1910.1200 (US), and EU Regulation EC No. 1907/2006 (European Union).

15.1 Safety, Health and Environmental Regulations/Legislation Specific for the Substance or Mixture
A) Canada
   DSL/NDSL Status: This product is not listed on the Canadian DSL/NDSL.
B) United States
   TSCA Status: This product is not listed on the US EPA TSCA.
C) European Union
   ECHA Status: This product is not registered with the EU ECHA.

15.2 Chemical Safety Assessment
No data available

16. OTHER INFORMATION
16.1 Revision History
Original Publication Date: 4/11/2017

16.2 List of Abbreviations
LD50  Median lethal dose of a substance required to kill 50% of a test population.
LC50  Medial lethal concentration of a substance required to kill 50% of a test population.
LDLo  Lowest known lethal dose
TDLo  Lowest known toxic dose
IARC  International Agency for Research on Cancer
NTP   National Toxicology Program
RTECS Registry of Toxic Effects of Chemical Substances

16.3 Further Information
Copyright 2015. Toronto Research Chemicals Inc. Copies may be made for internal use only. The above information is believed to be correct to the best of our knowledge, but is to be only used as a guide. To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. Please take all due care when handling this product.