

**Section 1. IDENTIFICATION OF THE SUBSTANCE / MIXTURE AND OF THE COMPANY / UNDERTAKING****1.1 Product identifiers**

Product Name: PD 123319 ditrifluoroacetate

Catalogue Number: P-245

Synonyms: ChEMBL157946

IUPAC Name: (6S)-1-[[[4-(dimethylamino)-3-methylphenyl]methyl]-5-(2,2-diphenylacetyl)-6,7-dihydro-4H-imidazo[4,5-c]pyridine-6-carboxylic acid;2,2,2-trifluoroacetic acid

**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Laboratory chemicals, synthesis of substances. For research purposes only. Not for human or veterinary use.

**1.3 Details of the supplier of the safety data sheet**

Company: Alomone Labs  
Jerusalem BioPark (JBP)  
PO Box 4287  
Jerusalem 9104201  
Israel

Telephone: +972-2-587-2202  
Fax: +972-2-587-1101  
Internet: [www.alomone.com](http://www.alomone.com)  
E-mail: [info@alomone.com](mailto:info@alomone.com)

**1.4 Emergency telephone number**

Telephone: +972-2-587-2202 (Sun-Thu 08.00-18.00 IST)

**Section 2. HAZARDS IDENTIFICATION****2.1 Classification of the substance or mixture**

Not a hazardous substance or mixture according to Regulation (EC) No. 1272/2008.

**2.2 Label elements**

The product does not need to be labeled in accordance with EC directives or respective national laws.

**2.3 Other hazards**

None.

**Section 3. COMPOSITION / INFORMATION ON INGREDIENTS****3.1 Substances**

Product name: PD 123319 ditrifluoroacetate

CAS Number: 136676-91-0

Molecular Formula:  $C_{35}H_{34}F_6N_4O_7$

Molecular Weight: 736.66

**Section 4. FIRST AID MEASURES****4.1 Description of first aid measures**

In all cases of exposure, obtain medical advice.

**Inhalation:** Move to fresh air and monitor breathing. If breathing becomes difficult give oxygen. If breathing stops give artificial respiration. Obtain medical attention.

**Skin Contact:** Wash off immediately with plenty of water while removing all contaminated clothing. Wash before reuse.

**Eye Contact:** Hold eyelids apart and flush eyes with plenty of water.

**Ingestion:** Rinse mouth with plenty of water. Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person.

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

No information available.

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

Show this safety data sheet to the professional medical staff. Immediate medical attention is required.

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

#### **5.1 Suitable extinguishing media**

Use dry chemical or carbon dioxide.

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

Thermal decomposition can lead to release of toxic and corrosive gases/vapors.

#### **5.3 Precautions for fire-fighters**

Wear self-contained breathing apparatus for firefighting and protective clothing to prevent contact with skin and eyes.

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

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

Do not take action without suitable protective clothing. Evacuate personnel to safe areas. Ensure adequate ventilation. Avoid dust formation. Avoid breathing vapors, mist or gas.

#### **6.2 Environmental precautions**

Do not let product enter drains.

#### **6.3 Containment and clean-up methods and materials**

Cover liquid spill with sand, earth or other non-combustible absorbent material. Cover powder spill with plastic sheet or tarp to minimize spreading. Sweep up and shovel. Keep in suitable, closed containers for disposal.

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### **Section 7. HANDLING AND STORAGE**

#### **7.1 Precautions for safe handling**

Keep away from heat. Keep away from source of ignition. Empty containers pose a fire risk, evaporate the residue under a fume hood. Avoid contact with skin. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. Avoid the formation and inhalation of dust/fumes. If ingested, seek medical advice immediately and show the container or the label.

#### **7.2 Conditions for safe storage**

Keep container tightly closed. Keep container in a cool, well-ventilated area. Keep away from direct sunlight. Shipped at room temperature. Product as supplied can be stored intact at room temperature for several weeks. For longer periods, it should be stored at -20°C

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

#### **8.1 Exposure guidelines**

Contains no substances with occupational exposure limit values.

## 8.2 Exposure controls

Ensure adequate ventilation, especially in confined areas. Use in a fume hood where applicable. Ensure laboratory is equipped with a safety shower and eye wash station. General industrial hygiene practice.

### Personal protective equipment

**Eye/face:** Safety goggles.

**Skin:** Chemical resistant gloves. Gloves should be inspected before use. Wash and dry hands thoroughly after handling.

**Body:** Wear appropriate protective clothing. Remove and wash contaminated clothing before re-use.

**Respiratory protection:** Use a suitable respirator as conditions warrant.

## Section 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Basic physical and chemical properties

Physical state: Powder form

Odor: Not available

Odor threshold: Not available

pH: Not available

Boiling point/range: Not available

Flash point: Not available

Evaporation rate: Not available

Flammability (solid, gas): Not available

Upper/lower flammability or explosive limits: Not available

Melting/freezing point: Not available

Vapor pressure: Not available

Vapor density: Not available

Relative Density: Not available

Explosive properties: Not available

Flash point: Not available

Viscosity: Not available

Solubility: 100 mM in H<sub>2</sub>O. Centrifuge all product preparations before use (10000 x g 5 min)

Partition coefficient: Not available

Auto-ignition temperature: Not available

Decomposition temperature: Not available

Explosive properties: Not available

Oxidizing properties: Not available

### 9.2 Other information

No data available.

## Section 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

Stable under recommended transport or storage conditions.

### 10.2 Chemical stability

Stable under recommended conditions.

### 10.3 Possibility of hazardous reactions

Hazardous reactions will not occur under normal transport or storage conditions. Decomposition may occur on exposure to conditions or materials listed below.

### 10.4 Conditions to avoid

Heat.

### 10.5 Incompatible materials

Strong oxidizing agents, strong acids/bases.

### 10.6 Hazardous combustion or decomposition products

May emit toxic gases upon thermal decomposition.

## Section 11. TOXICOLOGICAL INFORMATION

## 11.1 Toxicological effects

### Acute toxicity

Does not present acute toxicity hazard based on supplied information.

### Skin corrosion/irritation

No information available.

### Eye damage/irritation

No information available.

### Respiratory/skin sensitization

No information available.

### Mutagenicity

No information available.

### Carcinogenicity

No information available.

### Reproductive toxicity

No information available.

### Aspiration/inhalation exposure

No information available.

### Routes of exposure/symptoms

Inhalation: There may be irritation of the throat with a feeling of tightness in the chest.

Ingestion: There may be irritation of the throat.

Skin: There may be mild irritation at the site of contact.

Eyes: There may be irritation and redness.

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## Section 12. ECOLOGICAL INFORMATION

### 12.1 Toxicity

No data available.

### 12.2 Persistence and degradability

No data available.

### 12.3 Bio-accumulative 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.

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## Section 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste methods

#### Product

Transfer to a suitable container and arrange for collection by specialized disposal company in accordance with federal, state and local environmental control regulations.

#### Contaminated packaging

Dispose in a regulated landfill site or other method for hazardous or toxic waste in accordance with federal, state and local

environmental control regulations.

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#### **Section 14. TRANSPORT INFORMATION**

**ADR** Not dangerous goods.

**IATA** Not dangerous goods.

**DOT** Not dangerous goods.

**TGD** Not dangerous goods.

**IMDG/IMO** Not dangerous goods.

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#### **Section 15. REGULATORY INFORMATION**

This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.

##### **15.1 Chemical safety assessment**

None has been made for this product.

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#### **Section 16. OTHER INFORMATION**

The above information is believed to be correct but does not purport to be all inclusive and should be used as a guide only for experienced personnel. Always consult your safety advisor and follow local and national safety legislation. The absence of warning may not, under any circumstances, be taken to mean that no hazard exists. Alomone Labs disclaims all liability for any damage resulting from use of this material.

**Last modified: January 8, 2025**

**Document creation date: January 8, 2025**