

Safety Data Sheet (SDS)

Section 1: Identification

1.1 Product Identification

- Product Name: Upadacitinib
- Product Number: Sigma-1492025176
- Brand: Sigma
- CAS Number: 1310726-60-3
- Molecular Formula: C₁₇H₁₉F₃N₆O
- Molecular Weight: 380.4 g/mol
- Website: [Sigma Chemical](#)

1.2 Supplier Details

- Company Name: Sigma Chemical Co., Ltd.
- Address: Room 2-1-2301, Jiahe Xinxing, No.130, Shandong Road, Shibei District, Qingdao City, Shandong Province, China
- Phone Number: +8618661891880
- Email: chemweb3@foxmail.com
 - Business Hours:
 - Monday to Friday: 9:00 AM - 6:00 PM

- Saturday: 9:00 AM - 1:00 PM
- Sunday: Closed

1.3 Emergency Contact Number

- Emergency Contact: +8618661891880

1.4 Recommended Use and Restrictions

- Recommended Use: For research and development purposes only. Not for use as a drug, household product, or in any other application.

Restrictions: Keep out of reach of children. Use personal protective equipment as required.

Section 2: Hazard Identification

2.1 GHS Classification

- Acute Toxicity:
 - Oral: Category 4, H302 (Harmful if swallowed)
 - Inhalation: Category 4, H332 (Harmful if inhaled)
- Specific Target Organ Toxicity (Repeated Exposure):
 - Inhalation: Category 2, H373 (May cause damage to organs through prolonged or repeated exposure)

2.2 GHS Label Elements

- Pictogram: Warning

- Signal Word: Warning
- Hazard Statements:
 - H302: Harmful if swallowed
 - H332: Harmful if inhaled
- H373: May cause damage to organs through prolonged or repeated exposure
- Precautionary Statements:
 - Prevention:
 - P260: Do not breathe dust/fume/gas/mist/vapours/spray
 - P264: Wash thoroughly after handling
 - P270: Do not eat, drink, or smoke when using this product
 - Response:
 - P301+P312+P330: IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell. Rinse mouth.
 - P304+P312: IF INHALED: Call a POISON CENTER/doctor if you feel unwell.

2.3 Physical and Chemical Hazards

- Non-flammable. Ignition sources may release hazardous combustion products.

2.4 Health Hazards

- H302: Harmful if swallowed
- H332: Harmful if inhaled

H373: May cause damage to organs through prolonged or repeated exposure

2.5 Environmental Hazards

No environmental hazards identified based on current information.

Section 3: Composition/Information on Ingredients

3.1 Substance

- Synonyms:

Upadacitinib,

(3S,4R)-3-ethyl-4-(1,5,7,10-tetraazatricyclo(7.3.0.0^{2,6})dodeca-2(6),3,7,9,11-pentaen-12-yl)-N-(2,2,2-trifluoroethyl)pyrrolidine-1-carboxamide,

(3S,4R)-3-ethyl-4-(3H-imidazo(1,2-a)pyrrolo(2,3-e)pyrazin-8-yl)-N-(2,2,2-trifluoroethyl)-1-pyrrolidinecarboxamide, 4RA0KN46E0, Abt-494, DTXCID401513480, DTXSID901027919

- Molecular Formula: C₁₇H₁₉F₃N₆O
- Molecular Weight: 380.4 g/mol
- CAS Number: 1310726-60-3
- Hazardous Components:

- Component: Upadacitinib
- Classification:
- Acute Toxicity: Category 4 (Oral), H302
- Acute Toxicity: Category 4 (Inhalation), H332

Specific Target Organ Toxicity (Repeated Exposure): Category 2, H373

Section 4: First Aid Measures

4.1 First Aid Measures

- Inhalation: Remove victim to fresh air. If feeling unwell, call a POISON CENTER/doctor.
- Skin Contact: Immediately wash with plenty of water for at least 15 minutes. Remove contaminated clothing and wash before reuse. Get medical attention if irritation persists.
- Eye Contact: Rinse immediately with plenty of water for at least 15 minutes. Remove contact lenses if present and easy to do. Continue rinsing. Get medical attention if eye irritation persists.

Ingestion: Do NOT induce vomiting. Rinse mouth with water. Call a POISON CENTER/doctor if feeling unwell.

4.2 Most Important Symptoms and Effects

Symptoms: Difficulty in breathing. Symptoms of overexposure may include headache, dizziness, tiredness, nausea, and vomiting.

4.3 Immediate Medical Attention and Special Treatment

Medical Treatment: Treat symptomatically and supportively. No specific antidote available.

Section 5: Firefighting Measures

5.1 Extinguishing Media

Suitable Extinguishing Agents: Use fire extinguishing methods suitable for the surrounding environment. Solid water stream may be inefficient.

5.2 Specific Hazards Arising from the Chemical

Hazardous Combustion Products: Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x)

5.3 Firefighting Precautions

Protective Equipment: Wear self-contained breathing apparatus (pressure-demand, MSHA/NIOSH approved or equivalent) and full protective gear.

Section 6: Accidental Release Measures

6.1 Personal Precautions, Protective Equipment, and Emergency Procedures

- Personal Precautions: Ensure adequate ventilation. Use personal protective equipment as required. Ground all equipment used when handling the product. Avoid contact with skin, eyes, or clothing. Remove all sources of ignition. Take precautionary measures against static discharge.
- Environmental Precautions: Prevent seepage into sewage systems, workpits, and surface or ground water.

6.2 Methods and Materials for Containment and Clean-Up

- Containment: For small leaks, absorb with inert absorbent material (e.g., sand, diatomite, acid binders, universal binders) or collect in a tightly sealable container.
- For large leaks, enclose with banks to prevent outflow and lead the leakage to a safe place for subsequent disposal.

Clean-Up: Dispose of contents/container in accordance with local/regional/national/international regulations.

6.3 Reference to Other Sections

See Section 8 for personal protection equipment and Section 13 for disposal information.

Section 7: Handling and Storage

7.1 Handling Precautions

Handling: Ensure adequate ventilation. Wear personal protective equipment/face protection. Use spark-proof tools and explosion-proof equipment. Keep away from open flames, hot surfaces, and sources of ignition. Avoid contact with skin, eyes, or clothing. Avoid breathing dust/fume/gas/mist/vapors/spray. Avoid ingestion and inhalation. Take precautionary measures against static discharge.

7.2 Storage Conditions

Storage: Store in a dry, cool, and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks, and flame. Store in a flammable area. Keep container tightly closed in a dry and well-ventilated place. Incompatible materials include strong oxidizing agents, strong acids, strong bases, strong reducing agents, and water.

Section 8: Exposure Controls/Personal Protection

8.1 Control Parameters

Exposure Limits: No occupational exposure limits established by regional regulatory authorities.

8.2 Exposure Controls

Engineering Measures: Ensure adequate ventilation, especially in confined areas.

8.3 Personal Protective Equipment

- Respiratory Protection: Use a particulate respirator approved by NIOSH if dust particles are present.
- Eye Protection: Safety goggles or face shield.
- Skin Protection: Wear chemical-resistant gloves and protective clothing.
- Hand Protection: Chemical-resistant gloves (e.g., nitrile rubber).

Other Protective Equipment: Safety shower and eye wash station should be available.

Section 9: Physical and Chemical Properties

- Appearance: Solid
- Color: Not determined
- Odor: Characteristic
- Melting Point: Not determined
- Boiling Point: Not determined
- Flash Point: Not applicable

- Flammability: Non-flammable
- Decomposition Temperature: Not determined
- Ignition Temperature: Not determined
- Vapor Pressure: Not applicable
- Density: Not determined
- Relative Density: Not determined
- Solubility in Water: Not determined
- Partition Coefficient (n-octanol/water): Not determined
- Viscosity: Not applicable

Evaporation Rate: Not applicable

Section 10: Stability and Reactivity

- Stability: Stable under normal conditions.
- Reactivity: No hazardous reactions known.
- Conditions to Avoid: High temperatures, strong oxidizing agents.

Hazardous Decomposition Products: Carbon dioxide, carbon monoxide, nitrogen oxides.

Section 11: Toxicological Information

- Acute Toxicity: Category 4 (Oral and Inhalation)
 - Primary Irritant Effect: None
 - Sensitization: None known
 - Carcinogenic Categories:
 - IARC: Not listed
 - NTP: Not listed
 - OSHA-Ca: Not listed
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Section 12: Ecological Information

- Aquatic Toxicity: No further relevant information available.
- Persistence and Degradability: No further relevant information available.
- Bioaccumulative Potential: No further relevant information available.
- Mobility in Soil: No further relevant information available.

Water Hazard Class: 1 (Slightly hazardous for water)

Section 13: Disposal Considerations

- Waste Treatment Methods: Dispose of contents/container in accordance with local/regional/national/international regulations.

Uncleaned Packagings: Dispose of in accordance with official regulations.

Section 14: Transport Information

- UN Number: Not regulated
- UN Proper Shipping Name: Not regulated
- Transport Hazard Class: Not regulated

Packing Group: Not regulated

Section 15: Regulatory Information

- Safety, Health, and Environmental Regulations/Legislation: No further relevant information available.
 - TSCA (Toxic Substances Control Act): Not listed
 - Hazardous Air Pollutants: Not listed
 - Proposition 65: Not listed
 - EPA (Environmental Protection Agency): Not listed
 - TLV (Threshold Limit Value): Not listed
- NIOSH-Ca (National Institute for Occupational Safety and Health): Not listed