



SAFETY DATA SHEET

1. Identification

Product identifier	Aprepitant
Other means of identification	
Catalog number	1041904
CAS number	170729-80-3
Chemical name	3-[[[(2R,3S)-2-[(R)-1-[3,5-Bis(trifluoromethyl)phenyl]ethoxy]-3-(4-fluorophenyl)morpholino]methyl]-1H-1,2,4-triazol-5(4H)-one
Recommended use	For analytical laboratory use only.
Recommended restrictions	Not for use as a drug. Not for administration to humans or animals.

Manufacturer/Importer/Supplier/Distributor information

Manufacturer

Company name	U. S. Pharmacopeia	
Address	12601 Twinbrook Parkway Rockville MD 20852-1790 United States	
Telephone	Customer Service	301-881-0666
Website	www.usp.org	
E-mail	RSTECH@usp.org	
Emergency phone number	CHEMTREC within US & Canada	1-800-424-9300
	CHEMTREC outside US & Canada	+1 703-527-3887

2. Hazard(s) identification

Physical hazards	Not classified.	
Health hazards	Serious eye damage/eye irritation	Category 2B
Environmental hazards	Not classified.	
OSHA defined hazards	Not classified.	
Label elements		
Hazard symbol	None.	
Signal word	Warning	
Hazard statement	Causes eye irritation.	
Precautionary statement		
Prevention	Wash thoroughly after handling.	
Response	If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.	
Storage	Not available.	
Disposal	Not available.	
Hazard(s) not otherwise classified (HNOC)	This product is supplied in a small quantity which does not constitute a combustible dust hazard. The physical properties of this material indicate that in large quantities accumulated dust may be hazardous.	
Supplemental information	Pharmacologically active material.	

3. Composition/information on ingredients

Substance

Chemical name	Common name and synonyms	CAS number	%
Aprepitant		170729-80-3	100

Information provided in the SDS is not specific to the lot provided. Refer to the label and USP Certificate/Product Information Sheet for the assigned value of a particular lot.

4. First-aid measures

Inhalation	If breathing is difficult, remove to fresh air and keep at rest in a position comfortable for breathing. Call a physician if symptoms develop or persist.
Skin contact	Rinse skin with water/shower. Get medical attention if irritation develops and persists.
Eye contact	Rinse with water. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical attention if irritation develops and persists.
Ingestion	Rinse mouth. Get medical attention if symptoms occur.
Most important symptoms/effects, acute and delayed	Pharmacologically active material. Occupational exposure may cause physiological effects.
Indication of immediate medical attention and special treatment needed	Provide general supportive measures and treat symptomatically.
General information	Remove from exposure. Remove contaminated clothing. For treatment advice, seek guidance from an occupational health physician or other licensed health-care provider familiar with workplace chemical exposures. In the United States, the national poison control center phone number is 1-800-222-1222. If person is not breathing, give artificial respiration. If breathing is difficult, give oxygen if available. Persons developing serious hypersensitivity (anaphylactic) reactions must receive immediate medical attention.

5. Fire-fighting measures

Suitable extinguishing media	Water. Foam. Dry chemical or CO2. Use fire-extinguishing media appropriate for surrounding materials.
Unsuitable extinguishing media	None known.
Specific hazards arising from the chemical	Explosion hazard: Avoid generating dust; fine dust dispersed in air in sufficient concentrations and in the presence of an ignition source is a potential dust explosion hazard.
Special protective equipment and precautions for firefighters	Wear suitable protective equipment.
Fire fighting equipment/instructions	Use water spray to cool unopened containers. As with all fires, evacuate personnel to a safe area. Firefighters should use self-contained breathing equipment and protective clothing.
Specific methods	Use standard firefighting procedures and consider the hazards of other involved materials.
General fire hazards	No unusual fire or explosion hazards noted.

6. Accidental release measures

Personal precautions, protective equipment and emergency procedures	Keep unnecessary personnel away. Keep people away from and upwind of spill/leak. Dust deposits should not be allowed to accumulate on surfaces, as these may form an explosive mixture if they are released into the atmosphere in sufficient concentration. Wear appropriate protective equipment and clothing during clean-up. Avoid inhalation of dust from the spilled material. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing. Ensure adequate ventilation. Local authorities should be advised if significant spillages cannot be contained. For personal protection, see section 8 of the SDS.
Methods and materials for containment and cleaning up	Avoid the generation of dusts during clean-up. Sweep up or vacuum up spillage and collect in suitable container for disposal. Clean surface thoroughly to remove residual contamination. For waste disposal, see section 13 of the SDS.
Environmental precautions	Avoid discharge into drains, water courses or onto the ground.

7. Handling and storage

Precautions for safe handling	As a general rule, when handling USP materials, avoid all contact and inhalation of dust, mists, and/or vapors associated with the material. Clean equipment and work surfaces with suitable detergent or solvent after use. After removing gloves, wash hands and other exposed skin thoroughly. Avoid significant deposits of material, especially on horizontal surfaces, which may become airborne and form combustible dust clouds and may contribute to secondary explosions. Combustible dust clouds may be created where operations produce fine material (dust). Select and use containment devices and personal protective equipment based on a risk assessment of material potency and exposure potential.
Conditions for safe storage, including any incompatibilities	Store in tight container. This material should be handled and stored per label instructions to ensure product integrity.

8. Exposure controls/personal protection

Occupational exposure limits

The following constituents are the only constituents of the product which have a PEL, TLV or other recommended exposure limit. At this time, the other constituents have no known exposure limits.

Exposure limit values

Industrial Use Material	Type	Value
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Aprepitant (CAS 170729-80-3)	TWA	200 micrograms/m3
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Biological limit values

No biological exposure limits noted for the ingredient(s).

Appropriate engineering controls

For laboratory operations, use local exhaust ventilation or a ventilated enclosure for high energy operations such as particle sizing. Control exposures to below the occupational exposure level (if available). Select and use containment devices and personal protective equipment based on a risk assessment of exposure potential. Cover all containers for solutions and slurries while being transferred.

Individual protection measures, such as personal protective equipment

Eye/face protection

Wear safety glasses with side shields, chemical splash goggles, or full face shield, if necessary. Base the choice of protection on the job activity and potential for contact with eyes or face. An emergency eye wash station should be available.

Skin protection

Hand protection

Wear nitrile or other impervious gloves if skin contact is possible. When the material is dissolved or suspended in an organic solvent, wear gloves that provide protection against the solvent.

Other

Train employees in proper gowning and degowning practices. Wear lab coat. Base the choice of skin protection on the job activity, potential for skin contact and solvents and reagents in use. Do not wear protective garments in common areas (e.g., cafeterias) or out-of-doors.

Respiratory protection

Respirators are generally not required for laboratory operations. Use a tight-fitting full-face respirator with HEPA filters for spill cleanup. Choose respiratory protection appropriate to the task and the level of existing engineering controls.

Thermal hazards

Wear appropriate thermal protective clothing, when necessary.

General hygiene considerations

Handling practices in this SDS are recommendations for laboratory use of USP materials. Pharmacological effects may be seen with occupational exposure.

9. Physical and chemical properties

Appearance

Appearance descriptions are general information and not specific to any USP lot.

Physical state

Solid.

Form

Powder.

Color

White. Off-white.

Odor

Odorless.

Odor threshold

Not available.

pH

Not available.

Melting point/freezing point

471.2 - 487.4 °F (244 - 253 °C)

Initial boiling point and boiling range

Not available.

Flash point

Not available.

Evaporation rate

Not available.

Flammability (solid, gas)

Not available.

Upper/lower flammability or explosive limits

Explosive limit - lower (%)

Not available.

Explosive limit - upper (%)

Not available.

Vapor pressure

Not available.

Vapor density

Not available.

Relative density

Not available.

Solubility(ies)

Solubility (water)

Practically insoluble.

Solubility (other)

Dimethylformamide: Soluble.

	Ethanol: Sparingly soluble. Isopropyl acetate: Sparingly soluble. Dimethyl sulfoxide: Soluble.
Partition coefficient (n-octanol/water)	4.8 = Log Kow at pH7
Auto-ignition temperature	Not available.
Decomposition temperature	Not available.
Viscosity	Not available.

Other information

Dust explosion properties

Kst	298 bar.m/s
Minimum ignition energy (MIE) - dust layer	10 - 30 mJ (without inductance)

Molecular formula C23H21F7N4O3

Molecular weight 534.43

10. Stability and reactivity

Reactivity	The product is stable and non-reactive under normal conditions of use, storage and transport.
Chemical stability	Material is stable under normal conditions.
Possibility of hazardous reactions	No dangerous reaction known under conditions of normal use.
Conditions to avoid	Contact with incompatible materials.
Incompatible materials	Strong oxidizing agents.
Hazardous decomposition products	Irritating and/or toxic fumes or gases. Emits toxic fumes under fire conditions. NOx, F-.

11. Toxicological information

Information on likely routes of exposure

Inhalation	Knowledge about health hazard is incomplete.
Skin contact	Knowledge about health hazard is incomplete.
Eye contact	Causes eye irritation.
Ingestion	Based on information from therapeutic use, this material may cause: Gastrointestinal disturbances.

Symptoms related to the physical, chemical and toxicological characteristics Headache. Dizziness. Fatigue. Gastrointestinal disturbances.

Information on toxicological effects

Acute toxicity

Product	Species	Test Results
Aprepitant (CAS 170729-80-3)		
Acute		
Oral		
LD50	Mouse	> 2000 mg/kg
	Rat	> 2000 mg/kg

Skin corrosion/irritation Based on available data, the classification criteria are not met.

Serious eye damage/eye irritation Causes eye irritation.

Local effects

500 mg Skin irritation
Result: Negative.
Species: Rabbit
Test Duration: 24 hours

Local effects

Eye irritation
 Result: Mild.
 Species: Rabbit
 Eye irritation: Bovine corneal opacity and permeability assay
 Result: Severe irritation.

Respiratory or skin sensitization

Respiratory sensitization Knowledge about health hazard is incomplete.

Skin sensitization Knowledge about health hazard is incomplete.

Germ cell mutagenicity Knowledge about mutagenicity is incomplete.

Mutagenicity

Ames test
 Result: Negative.
 Chinese hamster ovary cell chromosome aberration test
 Result: Negative.
 Human lymphoblastoid cell mutagenesis test
 Result: Negative.
 Micronucleus test
 Result: Negative.
 Species: Mouse
 Rat hepatocyte DNA strand break test
 Result: Negative.

Carcinogenicity Knowledge about carcinogenicity is incomplete.

IARC Monographs. Overall Evaluation of Carcinogenicity

Not listed.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1053)

Not listed.

US. National Toxicology Program (NTP) Report on Carcinogens

Not listed.

Reproductive toxicity Based on available data, the classification criteria are not met.

Reproductivity

0 - 2000 mg/kg/day Reproductivity / developmental, administered orally during organogenesis.
 Result: No treatment-related effects on fertility or reproductive performance; no fetal lethality or teratogenicity noted.
 Species: Rat
 0 - 25 mg/kg/day Reproductivity / developmental, administered orally during organogenesis.
 Result: Not teratogenic.
 Species: Rabbit

Specific target organ toxicity - single exposure Knowledge about health hazard is incomplete.

Specific target organ toxicity - repeated exposure Knowledge about health hazard is incomplete.

Aspiration hazard Based on available data, the classification criteria are not met.

Further information Pharmacologically active material. Occupational exposure may cause physiological effects.

12. Ecological information**Ecotoxicity**

Product	Species	Test Results
Aprepitant (CAS 170729-80-3)		
Aquatic		
<i>Chronic</i>		
Crustacea	NOEC Daphnia magna	0.018 mg/l, 21 days
Fish	NOEC Pimephales promelas	0.195 mg/l, 32 days

Persistence and degradability No data is available on the degradability of this substance.

Bioaccumulative potential

Octanol/water partition coefficient log Kow

4.8, = Log Kow

Mobility in soil

No data available.

Other adverse effects

No other adverse environmental effects (e.g. ozone depletion, photochemical ozone creation potential, endocrine disruption, global warming potential) are expected from this component.

13. Disposal considerations**Disposal instructions**

Dispose in accordance with all applicable regulations. Under RCRA, it is the responsibility of the user of the product to determine, at the time of disposal, whether the product meets RCRA criteria for hazardous waste.

Local disposal regulations

Dispose in accordance with all applicable regulations.

Hazardous waste code

The waste code should be assigned in discussion between the user, the producer and the waste disposal company.

Waste from residues / unused products

Empty containers or liners may retain some product residues. This material and its container must be disposed of in a safe manner (see: Disposal instructions).

Contaminated packaging

Since emptied containers may retain product residue, follow label warnings even after container is emptied.

14. Transport information**DOT****UN number**

UN3077

UN proper shipping name

Environmentally hazardous substance, solid, n.o.s. (Aprepitant)

Transport hazard class(es)**Class**

9

Subsidiary risk

-

Packing group

III

Environmental hazards**Marine pollutant**

No.

IATA**UN number**

UN3077

UN proper shipping name

Environmentally hazardous substance, solid, n.o.s. (Aprepitant)

Transport hazard class(es)**Class**

9

Subsidiary risk

-

Packing group

III

Other information**Passenger and cargo aircraft**

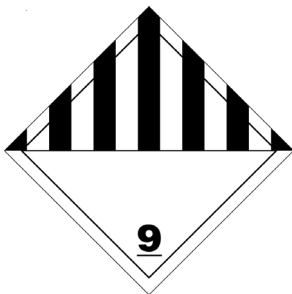
Allowed with restrictions.

Cargo aircraft only

Allowed with restrictions.

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

Not applicable.

DOT; IATA**General information**

It is the shipper's responsibility to determine the correct transport classification at the time of shipment.

15. Regulatory information**US federal regulations**

This product is a "Hazardous Chemical" as defined by the OSHA Hazard Communication Standard, 29 CFR 1910.1200.

Toxic Substances Control Act (TSCA)

TSCA Section 12(b) Export Notification (40 CFR 707, Subpt. D)

Not regulated.

CERCLA Hazardous Substance List (40 CFR 302.4)

Not listed.

SARA 304 Emergency release notification

Not regulated.

OSHA Specifically Regulated Substances (29 CFR 1910.1001-1053)

Not listed.

Superfund Amendments and Reauthorization Act of 1986 (SARA)**SARA 302 Extremely hazardous substance**

Not listed.

SARA 311/312 Hazardous chemical Yes**Classified hazard categories** Serious eye damage or eye irritation**SARA 313 (TRI reporting)**

Not regulated.

Other federal regulations**Clean Air Act (CAA) Section 112 Hazardous Air Pollutants (HAPs) List**

Not regulated.

Clean Air Act (CAA) Section 112(r) Accidental Release Prevention (40 CFR 68.130)

Not regulated.

Safe Drinking Water Act (SDWA) Not regulated.**US state regulations****California Proposition 65**California Safe Drinking Water and Toxic Enforcement Act of 1986 (Proposition 65): This material is not known to contain any chemicals currently listed as carcinogens or reproductive toxins. For more information go to www.P65Warnings.ca.gov.**International Inventories**

Country(s) or region	Inventory name	On inventory (yes/no)*
Australia	Australian Inventory of Industrial Chemicals (AICIS)	No
Canada	Domestic Substances List (DSL)	No
Canada	Non-Domestic Substances List (NDSL)	No
China	Inventory of Existing Chemical Substances in China (IECSC)	No
Europe	European Inventory of Existing Commercial Chemical Substances (EINECS)	No
Europe	European List of Notified Chemical Substances (ELINCS)	No
Japan	Inventory of Existing and New Chemical Substances (ENCS)	No
Korea	Existing Chemicals List (ECL)	No
New Zealand	New Zealand Inventory	No
Philippines	Philippine Inventory of Chemicals and Chemical Substances (PICCS)	No
Taiwan	Taiwan Chemical Substance Inventory (TCSI)	Yes
United States & Puerto Rico	Toxic Substances Control Act (TSCA) Inventory	No

*A "Yes" indicates that all components of this product comply with the inventory requirements administered by the governing country(s)

A "No" indicates that one or more components of the product are not listed or exempt from listing on the inventory administered by the governing country(s).

16. Other information, including date of preparation or last revision**Issue date** 08-29-2011**Revision date** 08-26-2024**Version #** 05**Further information** Refer to NFPA 654, Standard for the Prevention of Fire and Dust Explosions from the Manufacturing, Processing, and Handling of Combustible Particulate Solids, for safe handling.

Disclaimer

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