

Alisertib (MLN8237) SDS | MSDS

1. PRODUCT AND COMPANY IDENTIFICATION

Product identifier

- **Product Name:** Alisertib (MLN8237)
- **Catalog Number:** S1133
- **CAS Number:** 1028486-01-2
- **IUPAC Name:** Benzoic acid, 4-[[9-chloro-7-(2-fluoro-6-methoxyphenyl)-5H-pyrimido[5,4-d][2]benzazepin-2-yl]amino]-2-methoxy-

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. Hazard(s) identification

The substance is not classified as hazardous according to the Globally Harmonized System (GHS).

- **GHS Label Elements:** None
- **Hazard Pictograms:** None
- **Signal Word:** None
- **Hazard Statements:** None
- **NFPA Ratings (Scale 0-4):** Health = 0, Fire = 0, Reactivity = 0.
- **HMIS Ratings (Scale 0-4):** Health = 0, Fire = 0, Physical Hazard = 0.
- **Other Hazards:** The results of PBT and vPvB assessment indicate these are not applicable. There are no known adverse physical or health effects under the Hazard Communications Standard.

3. Composition/information on ingredients

- **Chemical Characterization:** Substances
- **CAS No. Description:** 1028486-01-2
- **Name:** Benzoic acid, 4-[[9-chloro-7-(2-fluoro-6-methoxyphenyl)-5H-pyrimido[5,4-d][2]benzazepin-2-yl]amino]-2-methoxy-

4. First-aid measures

- **General Information:** No special measures required.
- **After Inhalation:** Supply fresh air; consult a doctor in case of complaints.
- **After Skin Contact:** Generally, the product does not irritate the skin.
- **After Eye Contact:** Rinse the opened eye for several minutes under running water.
- **After Swallowing:** If symptoms persist, consult a doctor.
- **Most Important Symptoms and Effects:** No further relevant information available.
- **Indication of Immediate Medical Attention:** No further relevant information available.

5. Fire-fighting measures

- **Extinguishing Media:** Use fire-extinguishing measures that suit the environment. A solid water stream may be inefficient.
- **Special Hazards:** No further relevant information available.
- **Advice for Firefighters:** No special protective equipment measures required.

6. Accidental release measures

- **Personal Precautions:** Not required.
- **Environmental Precautions:** Do not allow to enter sewers, surface water, or ground water.
- **Methods for Containment and Cleaning Up:** Pick up mechanically.
- **Reference to Other Sections:** See Section 7 for safe handling, Section 8 for personal protection equipment, and Section 13 for disposal information.
- **Protective Action Criteria (PAC):** The substance is not listed for PAC-1, PAC-2, or PAC-3.

7. Handling and storage

- **Precautions for Safe Handling:** No special measures required.
- **Information About Protection Against Explosions and Fires:** No special measures required.
- **Conditions for Safe Storage:** Store in accordance with the information listed on the product insert.
- **Requirements for Storerooms and Receptacles:** No special requirements.
- **Information About Storage in One Common Storage Facility:** Not required.
- **Further Information:** None.

8. Exposure controls/personal protection

- **Control Parameters:** No components with limit values require monitoring at the workplace.
- **Engineering Controls:** No further data; see Section 7.
- **Personal Protective Equipment:**
 - **General Hygiene:** Follow usual precautionary measures for handling chemicals.
 - **Breathing Equipment:** Not required.
 - **Protection of Hands:** Use impermeable and resistant gloves. Due to missing tests, no specific glove material recommendation can be provided. Selection should consider penetration times, rates of diffusion, and degradation.
 - **Eye Protection:** Not required.

9. Physical and chemical properties

- **Physical State:** powder
- **Appearance (Form):** powder
- **Color:** Not determined.
- **Odor:** Characteristic.
- **Structural Formula:** C₂₇H₂₀CIFN₄O₄
- **Molecular Weight:** 518.9 g/mol
- **Melting Point/Melting Range:** Undetermined.
- **Boiling Point/Boiling Range:** Undetermined.
- **Flammability:** Product is not flammable.
- **Explosion Limits:** Lower and Upper not determined.
- **Flash Point:** Not applicable.
- **Decomposition Temperature:** Not determined.
- **pH-value:** Not applicable.
- **Viscosity (Kinematic/Dynamic):** Not applicable.
- **Solubility:** DMF: 2 mg/mL; DMF:PBS(pH 7.2)(1:1): 0.5 mg/mL; DMSO: 1 mg/mL.
- **Water Solubility:** Not determined.
- **Partition Coefficient (n-octanol/water):** Not determined.
- **Vapor Pressure:** Not applicable.
- **Density/Relative Density:** Not determined.
- **Vapor Density:** Not applicable.
- **Particle Characteristics:** Not determined.
- **Ignition Temperature:** Not determined.
- **Danger of Explosion:** Product does not present an explosion hazard.

10. Stability and reactivity

- **Reactivity:** No further relevant information available.
- **Chemical Stability:** Stable under recommended storage conditions. No decomposition if used according to specifications.
- **Possibility of Hazardous Reactions:** No dangerous reactions known.
- **Conditions to Avoid:** No further relevant information available.
- **Incompatible Materials:** No further relevant information available.
- **Hazardous Decomposition Products:** Carbon oxides, hydrogen chloride, hydrogen fluoride, nitrogen oxides.

11. Toxicological information

- **Acute Toxicity:** No specific data provided.
- **Primary Irritant Effect:**
 - **Skin:** No irritant effect.
 - **Eye:** No irritating effect.
- **Sensitization:** No sensitizing effects known.
- **Additional Toxicological Information:** When used and handled according to specifications, the product does not have any harmful effects according to experience and provided information. The substance is not subject to classification.
- **Carcinogenic Categories:**
 - **IARC:** Substance is not listed.
 - **NTP:** Substance is not listed.
 - **OSHA-Ca:** Substance is not listed.

12. Ecological information

- **Toxicity:** No further relevant information available regarding aquatic toxicity.
- **Persistence and Degradability:** No further relevant information available.
- **Bioaccumulative Potential:** No further relevant information available.
- **Mobility in Soil:** No further relevant information available.
- **PBT and vPvB Assessment:** Not applicable.
- **General Notes:** Water hazard class 1 (Self-assessment): slightly hazardous for water. Do not allow undiluted product or large quantities to reach ground water, water courses, or sewage systems.

13. Disposal considerations

- **Waste Treatment Methods:** Smaller quantities can be disposed of with household waste.
- **Uncleaned Packagings:** Disposal must be made according to official regulations.

14. Transport information

- **UN-Number (DOT, IMDG, IATA):** Not regulated.
- **UN Proper Shipping Name (DOT, IMDG, IATA):** Not regulated.
- **Transport Hazard Class(es) (DOT, ADN, IMDG, IATA):** Not regulated.
- **Packing Group (DOT, IMDG, IATA):** Not regulated.
- **Environmental Hazards:** Not applicable.
- **Special Precautions for User:** Not applicable.
- **Transport in Bulk (MARPOL73/78 and IBC Code):** Not applicable.
- **UN "Model Regulation":** Not regulated.

15. Regulatory information

· Safety, health and environmental regulations/legislation specific for the substance or mixture

No further relevant information available.

· Sara

· Section 355 (extremely hazardous substances): Substance is not listed.

· Section 313 (Specific toxic chemical listings): Substance is not listed.

· TSCA (Toxic Substances Control Act): Substance is not listed.

· Hazardous Air Pollutants Substance is not listed.

· Chemicals known to cause cancer: Substance is not listed.

· Chemicals known to cause reproductive toxicity for females: Substance is not listed.

· Chemicals known to cause reproductive toxicity for males: Substance is not listed.

· Chemicals known to cause developmental toxicity: Substance is not listed.

· Carcinogenic categories

· EPA (Environmental Protection Agency) Substance is not listed.

· TLV (Threshold Limit Value) Substance is not listed.

· NIOSH-Ca (National Institute for Occupational Safety and Health) Substance is not listed.

· Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16. OTHER INFORMATION

Revision Date: 2026/06/30

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.