

Inobrodib (CCS-1477) SDS | MSDS

1.PRODUCT AND COMPANY IDENTIFICATION

Product identifier

- **Product Name:** Inobrodib (CCS-1477)
- **Catalog Number:** S9667
- **CAS Number:** 2222941-37-7
- **IUPAC Name:** 2-Piperidinone, 1-(3,4-difluorophenyl)-6-[5-(3,5-dimethyl-4-isoxazolyl)-1-(trans-4-methoxycyclohexyl)-1H-benzimidazol-2-yl]-, (6S)-

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

Classification of the substance or mixture:

- Acute toxicity - oral 3 (H301): Toxic if swallowed.

Label elements:

The substance is classified and labeled according to the Globally Harmonized System (GHS).

Pictogram:



Signal word: Danger

Hazard statements:

- H301: Toxic if swallowed.

Precautionary statements:

- P264: Wash thoroughly after handling.
- P270: Do not eat, drink or smoke when using this product.
- P301+P310: If swallowed: Immediately call a poison center/doctor.
- P321: Specific treatment (see on this label).
- P330: Rinse mouth.
- P405: Store locked up.
- P501: Dispose of contents/container in accordance with local/regional/national/international regulations.

Classification system:

- NFPA ratings (scale 0 - 4): Health = 2, Fire = 0, Reactivity = 0.
- HMIS-ratings (scale 0 - 4): Health = 2, Fire = 0, Physical Hazard = 0.

Other hazards:

- Results of PBT and vPvB assessment: Not applicable.
- Hazards not otherwise classified: There are no adverse physical or health effects known that are not covered by the hazard classes of the Hazard Communications Standard.

3. Composition/information on ingredients

Chemical characterization: Substances

CAS No. Description: 2222941-37-7

Name: 2-Piperidinone, 1-(3,4-difluorophenyl)-6-[5-(3,5-dimethyl-4-isoxazolyl)-1-(trans-4-methoxycyclohexyl)-1H-benzimidazol-2-yl]-, (6S)-

4. First-aid measures

Description of first aid measures:

- **General information:** Immediately remove any clothing soiled by the product. In case of irregular breathing or respiratory arrest, provide artificial respiration.
- **After inhalation:** In case of unconsciousness, place patient stably in side position for transportation.
- **After skin contact:** Immediately wash with water and soap and rinse thoroughly.
- **After eye contact:** Rinse opened eye for several minutes under running water. Then consult a doctor.
- **After swallowing:** Do not induce vomiting; immediately call for medical help.

Most important symptoms and effects, both acute and delayed:

No further relevant information available.

Indication of any immediate medical attention and special treatment needed:

No further relevant information available.

5. Fire-fighting measures

Extinguishing media:

- **Suitable extinguishing agents:** Use fire fighting measures that suit the environment. A solid water stream may be inefficient.

Special hazards arising from the substance or mixture:

No further relevant information available.

Advice for firefighters:

- **Protective equipment:** No special measures required.

6. Accidental release measures

Personal precautions, protective equipment and emergency procedures:

Not required.

Environmental precautions:

Do not allow to enter sewers/surface or ground water.

Methods and material for containment and cleaning up:

Dispose of contaminated material as waste according to section 13.

Reference to other sections:

- See Section 7 for information on safe handling.
- See Section 8 for information on personal protection equipment.
- See Section 13 for disposal information.

Protective Action Criteria for Chemicals:

- PAC-1: Substance is not listed.
- PAC-2: Substance is not listed.
- PAC-3: Substance is not listed.

7. Handling and storage

Precautions for safe handling:

Thorough dedusting.

Information about protection against explosions and fires:

No special measures required.

Conditions for safe storage, including any incompatibilities:

- **Storage:** Store in accordance with information listed on the product insert.
- **Requirements to be met by storerooms and receptacles:** No special requirements.
- **Information about storage in one common storage facility:** Not required.
- **Further information about storage conditions:** None.

Specific end use(s):

No further relevant information available.

8. Exposure controls/personal protection

Control parameters:

- **Components with limit values that require monitoring at the workplace:** Not required.
- **Additional information:** The lists that were valid during the creation were used as a basis.

Exposure controls:

- **Appropriate engineering controls:** No further data; see section 7.

Personal protective equipment:

- **General protective and hygienic measures:** Keep away from foodstuffs, beverages and feed. Immediately remove all soiled and contaminated clothing. Wash hands before breaks and at the end of work.
- **Breathing equipment:** Not required.
- **Protection of hands:** The glove material has to be impermeable and resistant to the product/the substance/the preparation. Due to missing tests, no recommendation to the glove material can be given. Selection of the glove material should consider penetration times, rates of diffusion, and degradation.
- **Material of gloves:** The selection of suitable gloves depends not only on the material but also on further marks of quality and varies from manufacturer to manufacturer.
- **Penetration time of glove material:** The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.
- **Eye protection:** Not required.

9. Physical and chemical properties

Information on basic physical and chemical properties:

- **Physical state:** powder
- **Color:** Not determined.
- **Odor:** Characteristic
- **Structural Formula:** C₃₀H₃₂F₂N₄O₃
- **Molecular Weight:** 534.6 g/mol
- **Odor threshold:** Not determined.
- **Melting point/Melting range:** Undetermined.
- **Boiling point/Boiling range:** Undetermined.
- **Flammability:** Product is not flammable.
- **Explosion limits:** Lower: Not determined; Upper: Not determined.
- **Flash point:** Not applicable.
- **Decomposition temperature:** Not determined.
- **pH-value:** Not applicable.

- **Viscosity (Kinematic/Dynamic):** Not applicable.
- **Solubility:** DMF: 30 mg/ml; DMSO: 30 mg/ml; DMSO:PBS (pH 7.2) (1:3): 0.25 mg/ml; Ethanol: 10 mg/ml.
- **Solubility in / Miscibility with Water:** Not determined.
- **Partition coefficient (n-octanol/water):** Not determined.
- **Vapor pressure:** Not applicable.
- **Density:** Not determined.
- **Relative density:** Not determined.
- **Vapor density:** Not applicable.
- **Particle characteristics:** Not determined.
- **Appearance (Form):** powder
- **Ignition temperature:** Not determined.
- **Danger of explosion:** Product does not present an explosion hazard.
- **Evaporation rate:** Not applicable.

10. Stability and reactivity

Reactivity:

No further relevant information available.

Chemical stability:

- **Thermal decomposition / conditions to be avoided:** 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:

Strong acids, strong bases, strong oxidizing agents, strong reducing agents.

Hazardous decomposition products:

No dangerous decomposition products known.

11. Toxicological information

Information on toxicological effects:

- **Acute toxicity:** Toxic if swallowed.
- **Primary irritant effect (Skin):** No irritant effect.
- **Primary irritant effect (Eye):** No irritating effect.
- **Sensitization:** No sensitizing effects known.

Additional toxicological information:

- **Interactive effects:** No interactive effects between components are known.

Carcinogenic categories:

- **IARC (International Agency for Research on Cancer):** Substance is not listed.
- **NTP (National Toxicology Program):** Substance is not listed.
- **OSHA-Ca (Occupational Safety & Health Administration):** Substance is not listed.

Alternative sources for toxicological information:

No non-standard sources for toxicological information were used.

12. Ecological information

Toxicity:

- **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.

Results of PBT and vPvB assessment:

Not applicable.

Other adverse effects:

- **General notes:** Water hazard class 1 (Self-assessment): slightly hazardous for water. Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

13. Disposal considerations

Waste treatment methods:

- **Recommendation:** Must not be disposed of together with household garbage. Do not allow product to reach sewage system.

Uncleaned packagings:

- **Recommendation:** Disposal must be made according to official regulations.

14. Transport information

UN-Number:

- DOT, IMDG, IATA: UN3288

UN proper shipping name:

- DOT, IATA: Toxic powder, inorganic, n.o.s. (CCS-1477)
- IMDG: TOXIC POWDER, INORGANIC, N.O.S. (CCS-1477)

Transport hazard class(es):

- DOT, IMDG, IATA Class: 6.1 Toxic substances
- Label: 6.1

Packing group:

- DOT, IMDG, IATA: III

Environmental hazards:

Not applicable.

Special precautions for user:

Warning: Toxic substances

- Hazard identification number (Kemler code): 60
- EMS Number: F-A, S-A
- Stowage Category: A

Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code:

Not applicable.

Transport/Additional information:

- **DOT Quantity limitations:** On passenger aircraft/rail: 100 kg; On cargo aircraft only: 200 kg.
- **IMDG Limited quantities (LQ):** 5 kg.
- **IMDG Excepted quantities (EQ):** Code: E1 (Maximum net quantity per inner packaging: 30 g; Maximum net quantity per outer packaging: 1000 g).
- **IATA Remarks:** When sold in quantities of less than or equal to 1 mL, or 1 g, with an Excepted Quantity Code of E1, E2, E4, or E5, this item meets the De Minimis Quantities exemption, per IATA 2.6.10. Therefore packaging does not have to be labeled as Dangerous Goods/Excepted Quantity.

UN "Model Regulation":

UN 3288 TOXIC POWDER, INORGANIC, N.O.S. (CCS-1477), 6.1, III

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: 2026/07/07

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.