

CP-690550 (Tofacitinib) Citrate SDS | MSDS

1.PRODUCT AND COMPANY IDENTIFICATION

Product identifier

- **Product Name:** CP-690550 (Tofacitinib) Citrate
- **Catalog Number:** S5001
- **CAS Number:** 540737-29-9
- **IUPAC Name:**
3-((3R,4R)-4-methyl-3-(methyl(7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino)piperidin-1-yl)-3-oxopropanenitrile citrate

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. HAZARDS IDENTIFICATION

GHS Classification

- Acute toxicity (Oral): Category 4
- Reproductive toxicity: Category 2

GHS Label Elements

Pictogram:



Signal word: Warning

Hazard statements:

- H302: Harmful if swallowed.
- H361: Suspected of damaging fertility or the unborn child.

Precautionary statements:

• **Prevention:**

- P201: Obtain special instructions before use.
- P202: Do not handle until all safety precautions have been read and understood.
- P264: Wash skin thoroughly after handling.
- P270: Do not eat, drink or smoke when using this product.
- P280: Wear protective gloves/ protective clothing/ eye protection/ face protection.

• **Response:**

- P301 + P312 + P330: IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
- P308 + P313: IF exposed or concerned: Get medical advice/ attention.

• **Storage:**

- P405: Store locked up.

• **Disposal:**

- P501: Dispose of contents/ container to an approved waste disposal plant.

Other hazards:

Limited test data available for hazard assessment; handle with caution.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture: Substance

CAS-No.: 540737-29-9

Components:

• **Chemical Name:**

3-((3R,4R)-4-methyl-3-(methyl(7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino)piperidin-1-yl)-3-oxopropanenitrile citrate

• **CAS-No.:** 540737-29-9

• **Concentration (% w/w):** >= 90 - <= 100%

• **Note:** Actual concentration is withheld as a trade secret.

4. FIRST AID MEASURES

• **General advice:** Show this safety data sheet to the doctor in attendance.

• **If inhaled:** After inhalation, move to fresh air. Call a physician.

• **In case of skin contact:** Take off immediately all contaminated clothing. Rinse skin with water/shower. Consult a physician.

• **In case of eye contact:** After eye contact, rinse out with plenty of water. Remove contact lenses. Call an ophthalmologist.

• **If swallowed:** After swallowing, immediately make victim drink water (two glasses at most). Consult a physician.

- **Most important symptoms and effects, both acute and delayed:** The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11.
- **Protection of first-aiders:** For personal protection see section 8.
- **Notes to physician:** N/A.

5. FIREFIGHTING MEASURES

- **Suitable extinguishing media:** Water, Foam, Carbon dioxide (CO₂), Dry powder.
- **Unsuitable extinguishing media:** For this substance/mixture no limitations of extinguishing agents are given.
- **Specific hazards during firefighting:** Combustible. Development of hazardous combustion gases or vapours possible in the event of fire.
- **Hazardous combustion products:** Carbon oxides, Nitrogen oxides (NO_x).
- **Specific extinguishing methods:** N/A.
- **Further information:** Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.
- **Special protective equipment for fire-fighters:** Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

6. ACCIDENTAL RELEASE MEASURES

- **Personal precautions, protective equipment and emergency procedures:**
 - **Advice for non-emergency personnel:** Avoid inhalation of powder. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, and consult an expert.
 - **Advice for emergency responders:** For personal protection see section 8.
- **Environmental precautions:** Do not let product enter drains.
- **Methods and materials for containment and cleaning up:** Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of powder.

7. HANDLING AND STORAGE

- **Precautions for safe handling:** For precautions see section 2.
- **Conditions for safe storage:** Tightly closed. Dry. Keep locked up or in an area accessible only to qualified or authorised persons.
- **Storage class:** 11, Combustible powder.
- **Recommended storage temperature:** See product label.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

- **Control parameters:** Contains no substances with occupational exposure limit values.
- **Engineering measures:** N/A.

• **Personal protective equipment:**

• **Respiratory protection:** Required when powder is generated. Recommended Filter type: Filter type P3 (based on DIN EN 143, DIN 14387).

• **Hand protection:** Handle with impervious gloves. Full and splash contact: Nitrile rubber, 0.11 mm thickness, breakthrough time 480 min (e.g., KCL 741 Dermatril L).

• **Eye protection:** Safety glasses tested and approved under government standards such as NIOSH (US) or EN 166 (EU).

• **Skin and body protection:** Protective clothing.

• **Hygiene measures:** Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

9. PHYSICAL AND CHEMICAL PROPERTIES

• **Appearance:** powder

• **Color:** N/A

• **Odor:** N/A

• **Odor Threshold:** N/A

• **pH:** N/A

• **Melting point:** N/A

• **Boiling point/boiling range:** N/A

• **Flash point:** Not applicable

• **Evaporation rate:** N/A

• **Flammability (solid, gas):** N/A

• **Flammability (liquids):** N/A

• **Burning rate:** N/A

• **Upper/Lower explosion limit:** N/A

• **Vapor pressure:** N/A

• **Relative vapour density:** N/A

• **Relative density:** N/A

• **Density:** N/A

• **Water solubility:** N/A

• **Partition coefficient: n-octanol/water:** log Pow: 1.808

• **Autoignition temperature:** N/A

• **Decomposition temperature:** N/A

• **Viscosity:** N/A

• **Explosive properties:** N/A

• **Oxidizing properties:** none

• **Molecular weight:** 504.49 g/mol

• **Particle size:** N/A

10. STABILITY AND REACTIVITY

- **Reactivity:** Flammable organic substances in fine distribution may generally assume a powder explosion potential when whirled up.
- **Chemical stability:** The product is chemically stable under standard ambient conditions (room temperature).
- **Possibility of hazardous reactions:** Violent reactions possible with strong oxidizing agents.
- **Conditions to avoid:** No information available.
- **Incompatible materials:** Strong oxidizing agents.
- **Hazardous decomposition products:** In the event of fire, see section 5.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

- **Acute toxicity:**
 - Acute toxicity estimate Oral: 500.1 mg/kg (Expert judgement).
 - LD50 Oral - Rat: 500 mg/kg (External MSDS).
 - Inhalation/Dermal: N/A.
- **Skin corrosion/irritation:** N/A.
- **Serious eye damage/eye irritation:** N/A.
- **Respiratory or skin sensitization:** Local lymph node assay (LLNA) - Mouse: Result: negative (External MSDS).
- **Germ cell mutagenicity:** N/A.
- **Carcinogenicity:** No component of this product present at levels greater than or equal to 0.1% is identified as a probable, possible, or confirmed human carcinogen by IARC, NTP, or OSHA.
- **Reproductive toxicity:** Suspected of damaging the unborn child. Suspected of damaging fertility.
- **STOT - single/repeated exposure:** N/A.
- **Aspiration hazard:** N/A.

11.2 Additional Information

- Repeated dose toxicity - Rat - Oral - No observed adverse effect level: 1 mg/kg (External MSDS).
- To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

Ecotoxicity

- **Components:**
3-((3R,4R)-4-methyl-3-(methyl(7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino)piperidin-1-yl)-3-oxopropanenitrile citrate
- **Toxicity to fish:** LC50 (Cyprinodon variegatus): > 1 mg/l; Exposure time: 96 h. Remarks: No toxicity at the limit of solubility.
- **Toxicity to daphnia and other aquatic invertebrates:** LC50 (Mysidopsis bahia): > 1 mg/l; Exposure time: 96 h. Remarks: No toxicity at the limit of solubility.

Persistence and degradability

N/A.

Bioaccumulative potential

- **Components:**

3-((3R,4R)-4-methyl-3-(methyl(7H-pyrrolo[2,3-d]pyrimidin-4-yl)amino)piperidin-1-yl)-3-oxopropanenitrile citrate

- **Partition coefficient: n-octanol/water:** log Pow: 1.808.

Mobility in soil

N/A.

Other adverse effects

N/A.

13. DISPOSAL CONSIDERATIONS

Disposal methods

- **Waste from residues:** Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

14. TRANSPORT INFORMATION

- **IATA-DGR:** Not regulated as a dangerous good.
- **IMDG-Code:** Not regulated as a dangerous good.
- **Transport in bulk according to IMO instruments:** Not applicable for product as supplied.
- **49 CFR Road:** Not regulated as a dangerous good.
- **Poison Inhalation Hazard:** No.
- **Special precautions for user:** Not classified as dangerous in the meaning of transport regulations.

15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards

No SARA Hazards

SARA 313

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

US State Regulations

- **Massachusetts Right To Know:** No components are subject to the Massachusetts Right to Know Act.
- **Maine Chemicals of High Concern:** Product does not contain any listed chemicals.
- **Vermont Chemicals of High Concern:** Product does not contain any listed chemicals.
- **Washington Chemicals of High Concern:** Product does not contain any listed chemicals.

The components of this product are reported in the following inventories:

- **TSCA:** Product contains substance(s) not listed on TSCA inventory.

TSCA list

- No substances are subject to a Significant New Use Rule.
- No substances are subject to TSCA 12(b) export notification requirements.

16. OTHER INFORMATION

Revision Date: 2026/07/03

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.