



Tofacitinib

JAK Inhibitor

Catalog # J01-900

Lot # O3936-12

CAS # 477600-75-2

Product Description

Molecular Formula: $C_{16}H_{20}N_6O$

Appearance: White powder

Molecular Weight: 312.4

Purity: >99% (HPLC, TLC); NMR (conforms)

Solubility: May be dissolved DMSO (100 mg/ml); ethanol (100 mg/ml)

Alias

(3R,4R)-4-Methyl-3-(methyl-7H-pyrrolo[2,3-d]pyrimidin-4-ylamino)- β -oxo-1-piperidine-propanenitrile; CP-690550

Specific Activity

JAK Inhibitor

Storage and Stability

Store desiccated as supplied at -20°C for up to 2 years.

Store solutions at -20°C for up to 3 months.

Scientific Background

Tofacitinib is a potent pan-JAK inhibitor (IC_{50} s=1, 20, and 112 nM for JAK3, JAK2, and JAK1) (1). It is a strong anti-inflammatory and immunosuppressant (2, 3). Induces white-to-brown metabolic conversion in human adipocytes (4). In therapeutic use for rheumatoid arthritis (5).

References

1. Jiang JK et al. J. Med. Chem. 2008 51:8012
2. Cutolo M & Meroni M J. Inflamm. Res. 2013 6:129
3. Martina M et al. Transplant. Proc. 2016 48:3046
4. Moisan A et al. Nat. Cell Biol. 2015 17:57
5. Dowty ME et al. J. Pharmacol. Exp. Ther. 2014 348:165

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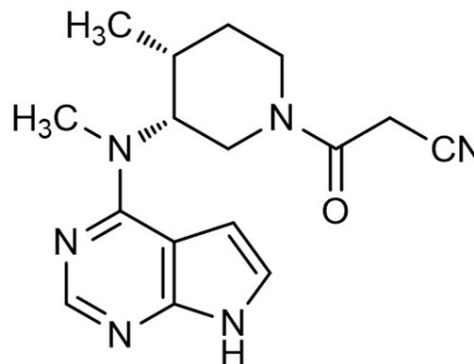
J01-900

Aliquot Size

5 mg

25 mg

Molecular Structure



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Purity

>99% (HPLC, TLC); NMR (conforms)

Format

White powder

Solubility

May be dissolved DMSO (100 mg/ml); ethanol (100 mg/ml)

Storage & Shipping

Store desiccated as supplied at -20°C for up to 2 years. Store solutions at -20°C for up to 3 months.

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SAFETY DATA SHEET

Article 1 – Identification of the Substance

Product Name: Tofacitinib**Catalog # J01-900**

This product is sold only for research use by qualified laboratory personnel, and is not to be used as a drug, medical device, food additive, cosmetic, nor household chemical. It is not to be used in diagnostic, therapeutic, consumer, agricultural, nor pesticidal applications.

Manufacturer's Name: SignalChem Biotech Inc.
Street Address: 110-13120 Vanier Place
City, Prov. Postal Code: Richmond, BC, V6V 2J2
Fax: 604-232-4601
EMERGENCY PHONE: 604-232-4600

Article 2 - Hazardous Identification

2.1 Classification of Substance (GHS)

Acute toxicity, Oral (Category 3)
Reproductive toxicity (Category 1B)

2.2 Label Elements

Classification according to Regulation (EC) No 1272/2008

**GHS Signal Word: DANGER****GHS Hazard Phrases:**

H302	Harmful if swallowed
H360	May damage fertility or the unborn child.

GHS Precaution Phrases:

P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P264	Wash hands thoroughly after handling.
P281	Use personal protective equipment.
P301 + P312	IF SWALLOWED: call a POISON CENTER or doctor/physician if you feel unwell.
P330	Rinse mouth.
P308 + P313	IF exposed or concerned: Get medical attention/advice.

GHS Storage and Disposal Phrases:

Please refer to Section 7 for Storage and Section 13 for Disposal Information

2.3 Other hazards: To the best of our knowledge, the toxicological properties have not been thoroughly investigated.

Article 3 – Composition/Information on Ingredients

3.1 Substance

Product Name(s): Tofacitinib
Chemical Name: (3R,4R)-4-Methyl-3-(methyl-7H-pyrrolo[2,3-d]pyrimidin-4-ylamino)-β-oxo-1-piperidine-propanenitrile
Molecular Formula: C₁₆H₂₀N₆O
CAS Number: 477600-75-2
Concentration: 100%

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SAFETY DATA SHEET

Article 4 – First Aid

4.1 Description of First Aid Measures

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

If Inhaled: Move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In Case of Skin Contact: Wash off with soap and plenty of water.

In Case of Eye Contact: Flush eyes with water as a precaution. Consult a physician.

If Swallowed: Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2 Important Symptoms and Effects: The most important known symptoms and effects are described in section 2.2.

Article 5 – Fire Fighting Measures

5.1 Extinguishing Media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special Hazards:

Combustion products are carbon oxides, nitrogen oxides.

5.3 Precautions for Fire Fighters

Wear self-contained breathing apparatus for firefighting if necessary.

Article 6 – Accidental Release Measures

6.1 Personal Precautions

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

6.2 Environmental Precautions

Do not let product enter drains.

6.3 Methods for Containment and Clean-up

Pick up and arrange disposal without creating dust using wet towels for small properties, for example. Keep in suitable, closed containers for disposal. Offer surplus and non-recyclable solutions to a licensed disposal company.

Article 7 – Handling and Storage

7.1 Handling Precautions

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

7.2 Safe Storage Measures

Keep container tightly closed in a dry and well-ventilated place. Non-combustible.

Article 8 – Exposure Controls/Personal Protection

8.1 Control Parameters

The product does not contain any hazardous materials with occupational exposure limits established by region-specific regulatory bodies.

8.2 Specific Engineering Controls

Keep airborne levels low by using a fumehood or local exhaust.

8.3 Personal Protection

Eye/Face Protection: Tightly fitting safety goggles. Face shield.

Skin Protection: Handle with gloves.

Body Protection: Impervious clothing.

Respiratory Protection: Wear NIOSH / MSHA-approved respirator if required.

Personal Hygiene Measures: When using this product, do not eat, drink or smoke. Remove and wash contaminated clothing before re-use. Provide regular cleaning of equipment, work area and clothing.

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Article 9 – Physical and Chemical Properties

Appearance: White powder
Odour: data not available
Odour Threshold: data not available
pH: data not available
Melting/Freezing Pt: data not available
Boiling Pt: data not available
Flash Pt: data not available
Explosive Properties: data not available
Solubility notes: May be dissolved in DMSO (100 mg/ml); or ethanol (100 mg/ml)

Article 10 – Stability and Reactivity

10.1 Stability: Stable under recommended transport or storage conditions
10.2 Conditions to Avoid: Avoid heat, moisture.
10.3 Incompatibility – Materials to Avoid: Strong oxidizing agents, strong acids/alkalis.
10.4 Hazardous Decomposition Products: Carbon oxides, nitrogen oxides.

Article 11– Toxicological Information

11.1 Toxicological Effects: The toxicological effects of this product have not been thoroughly studied.

Article 12 – Ecological Information

12.1 Toxicity
Avoid release into the environment.
12.2 Degradability
Data not available

Article 13 – Disposal Considerations

13.1 Waste Treatment
Product and Contaminated Packaging: Dispose according to national legislation. Contact a licensed chemical disposal company.

Article 14 – Transport Information

14.1 DOT
Not dangerous goods
14.2 IMDG
Not dangerous goods
14.2 IATA
Not dangerous goods

Article 15 – Regulatory Information

This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the SDS contains all the information required by the Controlled Products Regulations.

Article 16 – Other Information

The above information is believed to be correct but does not purport to be all-inclusive and shall be used only as a guide. SignalChem shall not be held liable for any damage resulting from handling or from contact with the above product. See the Technical Specification, Packing Slip, Invoice, and Product Catalog for additional terms and conditions of sale.

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