

Regorafenib

Multi-kinase inhibitor (Including KDR-Tie2)

Catalog # K01-900

Lot # K4554-18

CAS # 755037-03-7

Product Description

Molecular Formula: C₂₁H₁₅ClF₄N₄O₃

Appearance: Off-White powder

Molecular Weight: 482.80

Purity: >98% (HPLC/TLC); NMR (conforms)

Solubilization: May be dissolved in DMSO (50 mg/ml)

Alias

4-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]-3-fluorophenoxy]-N-methyl-2-pyridinecarboxamide; BAY 73-4506

Specific Activity

Multi-kinase inhibitor (Including KDR-Tie2)

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.

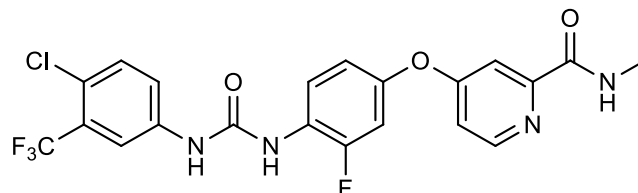
Scientific Background

A multi-kinase inhibitor related to sorafenib¹. Inhibits c-Raf, B-Raf, VEGFR1, VEGFR2, VEGFR3, Tie2, PDGFRβ, FGFR1, c-Kit, and RET with IC₅₀s=2.5, 28, 13, 4.2, 46, 311, 22, 202, 7 and 1.5 nM respectively¹⁻². Enhances SHP-1 activity³. Also inhibits soluble epoxide hydrolase (IC₅₀=0.5 nM)⁴. Clinically useful anticancer agent.

References

1. SM Wilhelm *et al.* *Int. J. Cancer* 2011 129:245
2. JCM Uitdehaag *et al.* *PLoS One* 2014 9(3):e92146
3. LC Fan *et al.* *Oncotarget* 2014 5:6243
4. SH Huang *et al.* *Bioorg. Med. Chem. Lett.* 2013 23:3732

Molecular Structure



Regorafenib

Multi-kinase inhibitor (Including KDR-Tie2)

| | |
|--------------------|---|
| Catalog # | K01-900 |
| CAS # | 755037-03-7 |
| Lot # | K4554-18 |
| Purity | >98% (HPLC/TLC); NMR (conforms) |
| Format | Off-White powder |
| Solubilization | May be dissolved in DMSO (50 mg/ml) |
| Storage & Shipping | Store desiccated as supplied at -20°C for up to 1 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: Regorafenib

Catalog # K01-900

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.

Supplier'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)

Toxic to Reproduction, Category 1B

Specific target organ toxicity – (repeated exposure) Category 1

2.2 Label Elements

Classification according to Regulation (EC) No 1272/2008



GHS Signal Word: DANGER

GHS Hazard Phrases:

| | |
|-------------|--|
| H360 + H362 | May damage fertility or the unborn child. May cause harm to breast-fed children. |
| H372 | Causes damage to organs through prolonged or repeated exposure. Route of exposure: Oral, Dermal. |
| H400 | Very toxic to aquatic life. |
| H410 | Very toxic to aquatic life with long lasting effects. |

GHS Precaution Phrases:

| | |
|------|--|
| P201 | Obtain special instructions before use. |
| P202 | Do not handle until all safety precautions have been read and understood. |
| P260 | Do not breathe dust/fume/gas/mist/vapors/spray. |
| P263 | Avoid contact during pregnancy and while nursing. |
| P264 | Wash thoroughly after handling. |
| P270 | Do not eat, drink, or smoke when using this product. |
| P273 | Avoid release to the environment. |
| P280 | Wear protective gloves/protective clothing/eye protection/face protection. |

GHS Response Phrases:

| | |
|----------|---|
| P308+313 | IF exposed or concerned: Get medical attention/advice. |
| P314 | Get medical advice/attention if you feel unwell. |
| P391 | Collect spillage. |
| P405 | Store locked up. |
| P501 | Dispose of contents/container in accordance with local/regional/national/international regulations. |

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.

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Article 3 – Composition/Information on Ingredients

3.1 Substance

| | |
|---------------------------|--|
| Product Name(s): | Regorafenib |
| Chemical Name: | 4-[4-[[[4-chloro-3-(trifluoromethyl)phenyl]amino]carbonyl]amino]-3-fluorophenoxy]-N-methyl-2-pyridinecarboxamide |
| Molecular Formula: | C ₂₁ H ₁₅ ClF ₄ N ₄ O ₃ |
| CAS Number: | 755037-03-7 |
| Concentration: | 100% |

Article 4 – First Aid

4.1 Description of First Aid Measures

General: Symptoms of poisoning may even occur after several hours; therefore, medical observation for at least 48 hours after the accident.

If Inhaled: Supply fresh air; consult a doctor in case of complaints.

In Case of Skin Contact: Generally, the product does not irritate the skin.

In Case of Eye Contact: Rinse opened eye for several minutes under running water.

If Swallowed: If symptoms persist, consult a doctor.

4.2 Important Symptoms and Effects: May cause anemia, cough, CNS depression, drowsiness, headache, heart damage, lassitude (weakness, exhaustion), liver damage, narcosis, reproductive effects, teratogenic effects. No further relevant information available.

Article 5 – Fire Fighting Measures

5.1 Extinguishing Media

Use fire fighting measures that suit the environment. A solid water stream may be inefficient.

5.2 Special Hazards

No further relevant information available.

5.3 Precautions for Fire Fighters

No special measures required.

Article 6 – Accidental Release Measures

6.1 Personal Precautions

Not required.

6.2 Environmental Precautions

Inform respective authorities in case of seepage into water course or sewage system. Do not allow to enter sewers/surface or ground water.

6.3 Methods for Containment and Clean-up

Dispose contaminated material as waste according to Article 13.

Article 7 – Handling and Storage

7.1 Handling Precautions

No special precautions are necessary if used correctly. Avoid breathing dust/fume/gas/mist/vapours/spray. Avoid prolonged or repeated exposure. Keep away from sources of ignition. Take precautionary measures against static discharge.

7.2 Safe Storage Measures

Keep container tightly closed. Store in accordance with information listed on the product insert.

Article 8 – Exposure Controls/Personal Protection

8.1 Control Parameters

Contains no substances with occupational exposure limit values.

8.2 Specific Engineering Controls

Not required.

8.3 Personal Protection

Eye/Face Protection: Tightly sealed goggles.

Skin Protection: Use chemical resistant gloves. Remove and dispose of gloves properly after use. Wash hands thoroughly after use.

Body Protection: Wear a lab coat.

Respiratory Protection: Not required.

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Article 9 – Physical and Chemical Properties

Appearance: Off-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 (50 mg/ml)

Article 10 – Stability and Reactivity

10.1 Stability: No further relevant information available
10.2 Conditions to Avoid: No further relevant information available
10.3 Incompatibility – Materials to Avoid: strong oxidizing agents
10.4 Hazardous Decomposition Products: carbon oxides, hydrogen chloride, hydrogen fluoride, nitrogen oxides

Article 11– Toxicological Information

11.1 Toxicological Effects: The toxicological effects of this product have not been thoroughly studied.
Acute Toxicity:
Chronic Toxicity:
For complete information, see Registry of Toxic Effects of Chemical Substances (RTECS) entry. Regorafenib RTECS Number: US4588810
Skin Corrosion/Irritation: No irritant effect
Eye Damage/Irritation: No irritant effect
Respiratory or Skin Sensitization: No sensitizing effects known
Germ Cell Mutagenicity: data not available
Carcinogenicity: None according to NIOSH

Article 12 – Ecological Information

12.1 Toxicity
Water hazard class 3 (self-assessment): extremely hazardous for water. Do not allow product to reach ground water, water course or sewage system, even in small quantities. Danger to drinking water if even extremely small quantities leak into the ground. Also poisonous for fish and plankton in water bodies. Very toxic for aquatic organisms.
12.2 Degradability
Data not available

Article 13 – Disposal Considerations

13.1 Waste Treatment
Must not be disposed together with household garbage. Do not allow product to reach sewage system. Disposal must be made according to official regulations.

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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