

Certificate of Analysis

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Product Name: Febuxostat

Catalog No.: 4427

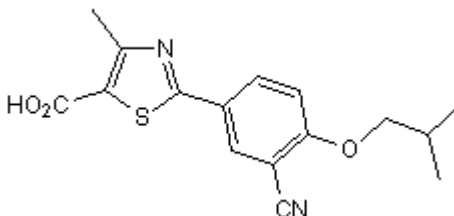
Batch No.: 1

CAS Number: 144060-53-7

IUPAC Name: 2-[3-Cyano-4-(2-methylpropoxy)phenyl]-4-methyl-5-thiazolecarboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₆N₂O₃S
Batch Molecular Weight: 316.37
Physical Appearance: White solid
Solubility: DMSO to 75 mM
ethanol to 50 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.74	5.1	8.85
Found	60.49	5.37	8.96

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Non-purine inhibitor of xanthine oxidase ($K_i = 1.2 \text{ nM}$). Binds to a channel leading to the enzyme active site; obstructs substrate binding.

Physical and Chemical Properties:

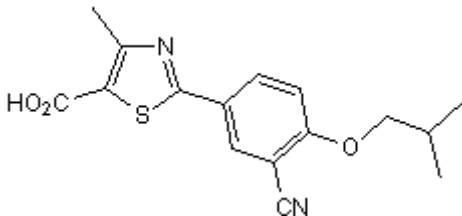
Batch Molecular Formula: $C_{16}H_{16}N_2O_3S$

Batch Molecular Weight: 316.37

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 75 mM

ethanol to 50 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Osada et al (1993) Hypouricemic effect of the novel xanthine oxidase inhibitor, TEI-6720, in rodents. *Eur.J.Pharmacol.* **241** 183. PMID: 8243554.

Okamoto et al (2003) An extremely potent inhibitor of xanthine oxidoreductase. Crystal structure of the enzyme-inhibitor complex and mechanism of inhibition. *J.Biol.Chem.* **278** 1848. PMID: 12421831.

Xu et al (2008) Xanthine oxidase inhibition with febuxostat attenuates systolic overload-induced left ventricular hypertrophy and dysfunction in mice. *J.Card.Fail.* **14** 746. PMID: 18995179.

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