

**Product Name:** Itraconazole

**Catalog No.:** 5981

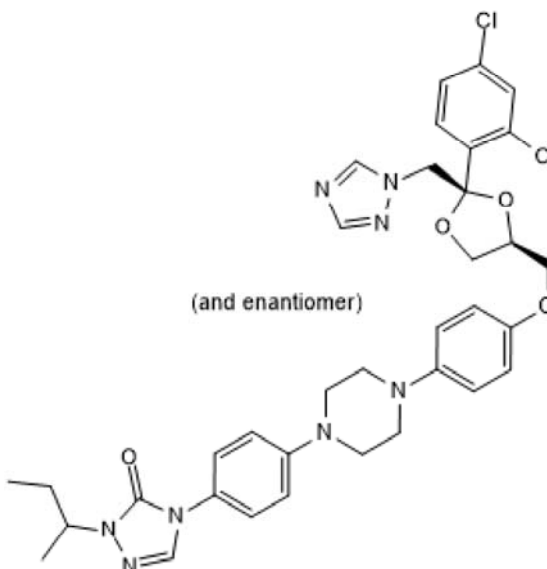
**Batch No.:** 1

CAS Number: 84625-61-6

IUPAC Name: 4-[4-[4-[2-(2,4-Dichlorophenyl)-2-(1*H*-1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]-1-piperazinyl]phenyl]-2,4-dihydro-2-(1-methylpropyl)-3*H*-1,2,4-triazol-3-one

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>35</sub>H<sub>38</sub>Cl<sub>2</sub>N<sub>8</sub>O<sub>4</sub>  
**Batch Molecular Weight:** 705.63  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 20 mM with gentle warming  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**Melting Point:** At 169°C  
**HPLC:** Shows 99.6% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	59.57	5.43	15.87
Found	59.74	5.38	16.02

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

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**Description:**

SMO antagonist (IC<sub>50</sub> = 690 nM); acts at different binding site to cyclopamine (Cat. No. 1623). Also cytochrome p450 inhibitor (IC<sub>50</sub> = 16-26 nM). Inhibits cell cycle at G<sub>1</sub> phase in vitro and blocks angiogenesis in vivo (IC<sub>50</sub> = 160 nM). Antifungal.

**Physical and Chemical Properties:**

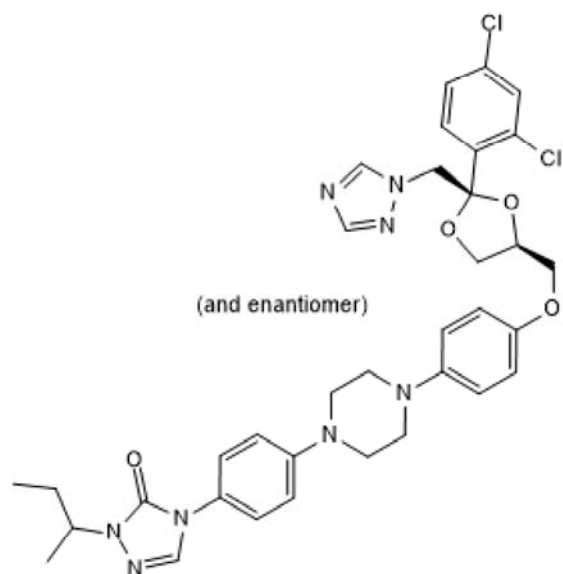
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Batch Molecular Weight: 705.63

Physical Appearance: White solid

**Minimum Purity:** ≥99%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

**Solubility & Usage Info:**

DMSO to 20 mM with gentle warming

**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:**

**Pace et al** (2016) Repurposing the clinically efficacious antifungal agent itracon. as an anticancer chemotherapeutic. *J.Med.Chem.* **59** 3635. PMID: 27014922.

**Kim et al** (2013) Itraconazole and arsenic trioxide inhibit Hedgehog pathway activation and tumor growth associated with acquired resistance to smoothened antagonists. *Cancer Cell* **23** 23. PMID: 23291299.

**Kim et al** (2010) Itraconazole, a commonly used antifungal that inhibits Hedgehog pathway activity and cancer growth. *Cancer Cell* **17** 388. PMID: 20385363.

**Chong et al** (2007) Inhibition of angiogenesis by the antifungal drug itracon. *ACS Chem.Biol.* **2** 263. PMID: 17432820.

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