

**Product Name:** IT1t

**Catalog No.:** 4596

**Batch No.:** 1

**CAS Number:** 1092776-63-0

**IUPAC Name:** *N,N*-Dicyclohexylcarbamimidothioic acid (5,6-dihydro-6,6-dimethylimidazo[2,1-*b*]thiazol-3-yl)methyl ester dihydrochloride

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:**  $C_{21}H_{34}N_4S_2 \cdot 2HCl \cdot \frac{1}{2}H_2O$

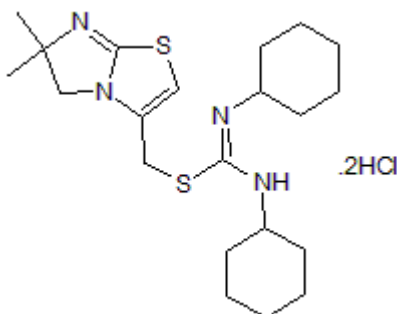
**Batch Molecular Weight:** 488.58

**Physical Appearance:** Off-white solid

**Solubility:** DMSO to 100 mM  
ethanol to 100 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 100% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	51.63	7.63	11.47
Found	51.6	7.52	11.36

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

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**Description:**

Potent CXCR4 antagonist ( $IC_{50}$  = 1.1 nM in calcium mobilization assays). Orally available. Blocks interaction with the HIV envelope protein, gp120 ( $IC_{50}$  = 7 nM, inhibition of X4-tropic HIV-1IIIB attachment).

**Physical and Chemical Properties:**

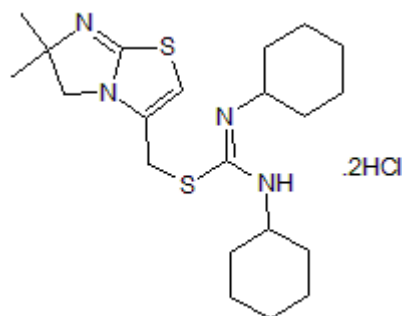
Batch Molecular Formula:  $C_{21}H_{34}N_4S_2 \cdot 2HCl \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 488.58

Physical Appearance: Off-white solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM  
ethanol to 100 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:**

**Thoma et al** (2008) Orally bioavailable isothioureas block function of the chemokine receptor CXCR4 *in vitro* and *in vivo*. *J.Med.Chem.* **51** 7915. PMID: 19053768.

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