

**Product Name:** TY 52156

**Catalog No.:** 5328

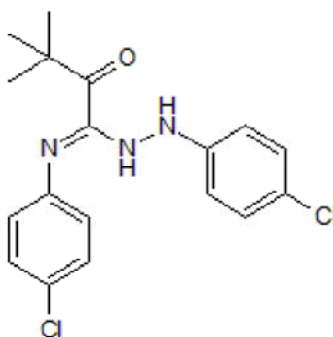
**Batch No.:** 2

CAS Number: 934369-14-9

IUPAC Name: *N*-(4-Chlorophenyl)-3,3-dimethyl-2-oxobutanimidic 2-(4-chlorophenyl) hydrazide

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>18</sub>H<sub>19</sub>Cl<sub>2</sub>N<sub>3</sub>O  
**Batch Molecular Weight:** 364.27  
**Physical Appearance:** Yellow solid  
**Solubility:** DMSO to 100 mM  
ethanol to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.5 (Ethyl acetate:Petroleum ether [9:1])  
**HPLC:** Shows 99.6% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	59.35	5.26	11.54
Found	59.57	5.26	11.53

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

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**Description:**

S1P<sub>3</sub> receptor antagonist ( $K_i = 110$  nM); inhibits S1P-induced Ca<sup>2+</sup> release in HUVEC cells. Suppresses FTY-720-induced S1P<sub>3</sub> receptor-mediated bradycardia in vivo. Also inhibits S1P-induced breast cancer stem cell expansion in vitro. Orally bioavailable.

**Physical and Chemical Properties:**

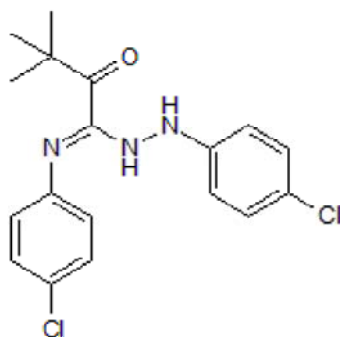
Batch Molecular Formula: C<sub>18</sub>H<sub>19</sub>Cl<sub>2</sub>N<sub>3</sub>O

Batch Molecular Weight: 364.27

Physical Appearance: Yellow solid

**Minimum Purity:** ≥98%

**Batch Molecular Structure:**



**Storage:** Store at -20°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:**

**Hirata *et al*** (2014) Sphingosine-1-phosphate promotes expansion of cancer stem cells via S1PR<sub>3</sub> by a ligand-independent Notch activation. *Nat. Commun.* **25** 4806. PMID: 25254944.

**Murakami *et al*** (2010) Sphingosine 1-phosphate (S1P) regulates vascular contraction via S1P<sub>3</sub> receptor: investigation based on a new S1P<sub>3</sub> receptor antagonist. *Mol. Pharmacol.* **77** 704. PMID: 20097776.

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