

Product Name: MDL 11,939

Catalog No.: 0870

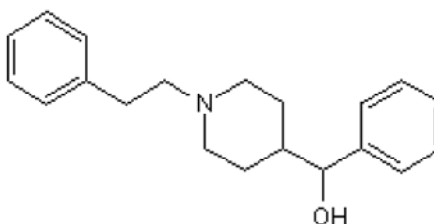
Batch No.: 2

CAS Number: 107703-78-6

IUPAC Name: α -Phenyl-1-(2-phenylethyl)-4-piperidinemethanol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₅NO
Batch Molecular Weight: 295.42
Physical Appearance: White solid
Solubility: 1eq. HCl to 50 mM
 ethanol to 50 mM
 DMSO to 50 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.38 (Chloroform:Methanol [95:5])
Melting Point: Greater than 128 - 129°C
HPLC: Shows 98.9% purity
¹H NMR: Consistent with structure

	Carbon Hydrogen Nitrogen		
	Carbon	Hydrogen	Nitrogen
Theoretical	81.31	8.53	4.74
Found	81.23	8.6	4.71

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

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Description:

Orally active 5-HT_{2A} receptor antagonist; displays selectivity for 5-HT_{2A} receptors over 5-HT_{2C} receptors (K_i values are 0.54, 2.5, 81.6 and ~10,000 nM at rabbit 5-HT_{2A}, human 5-HT_{2A}, rabbit 5-HT_{2C} and human 5-HT_{2C} receptors respectively).

Physical and Chemical Properties:

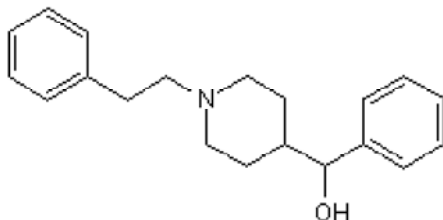
Batch Molecular Formula: C₂₀H₂₅NO

Batch Molecular Weight: 295.42

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

1eq. HCl to 50 mM
ethanol to 50 mM
DMSO 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:

Jensen et al (2013) Design, synthesis, and pharmacological characterization of *N*- and *O*-substituted 5,6,7,8-tetrahydro-4*H*-isoxazolo [4,5-*d*]azepin-3-ol analogues: novel 5-HT_{2A}/5-HT_{2C} receptor agonists with pro-cognitive J.Med.Chem. **56** 1211. PMID: 23301527.

Aloyo and Harvey (2000) Antagonist binding at 5-HT_{2A} and 5-HT_{2C} receptors in the rabbit: high correlation with the profile for the human receptors. Eur.J.Pharmacol. **406** 163. PMID: 11020478.

Dudley et al (1988) Pharmacological effects of MDL 11,939: a selective, centrally acting antagonist of 5-HT₂ receptors. Drug Dev.Res. **13** 29.

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