

**Product Name:** W146

**Catalog No.:** 3602

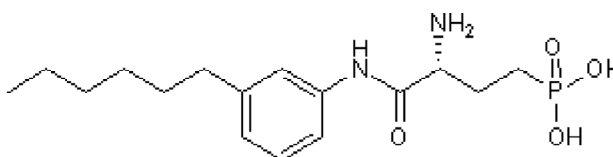
**Batch No.:** 2

CAS Number: 909725-61-7

IUPAC Name: [(3*R*)-3-amino-4-[(3-hexylphenyl)amino]-4-oxobutyl]-phosphonic acid

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>16</sub>H<sub>27</sub>N<sub>2</sub>O<sub>4</sub>P  
**Batch Molecular Weight:** 342.37  
**Physical Appearance:** White solid  
**Solubility:** 3eq. NaOH to 20 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.05 (Pyridine:Acetic acid:Water [3:8:11])  
**HPLC:** Shows >99.6% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = -3.2 (Concentration = 3.4, Solvent = 0.1M NaOH)  
**Microanalysis:**

	Carbon Hydrogen Nitrogen		
Theoretical	56.13	7.95	8.18
Found	55.79	7.9	8.21

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

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**2**

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IUPAC Name: [(3R)-3-amino-4-[(3-hexylphenyl)amino]-4-oxobutyl]-phosphonic acid

**Description:**

W146 is a potent sphingosine-1-phosphate receptor S1P<sub>1</sub> selective antagonist (K<sub>i</sub> = 18 nM); displays no effect at S1P<sub>2</sub>, S1P<sub>3</sub> or S1P<sub>5</sub>. Enhances capillary leakage and restores lymphocyte egress *in vivo*.

**Physical and Chemical Properties:**

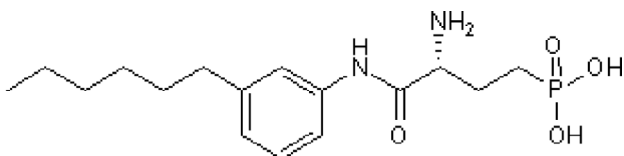
Batch Molecular Formula: C<sub>16</sub>H<sub>27</sub>N<sub>2</sub>O<sub>4</sub>P

Batch Molecular Weight: 342.37

Physical Appearance: White solid

**Minimum Purity:** ≥98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

3eq. NaOH to 20 mM

This product is supplied in lyophilized form. It may appear as a solid, gel or film and be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

**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. \*Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

**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:**

**Gonzalez-Cabrera et al (2008)** Full pharmacological efficacy of a novel S1P<sub>1</sub> agonist that does not require S1P-like headgroup interactions. *Mol.Pharmacol.* **74** 1308. PMID: 18708635.

**Sanna et al (2006)** Enhancement of capillary leakage and restoration of lymphocyte egress by a chiral S1P<sub>1</sub> antagonist *in vivo*. *Nat.Chem.Biol.* **8** 434. PMID: 16829954.

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**bio-techne.com**

info@bio-techne.com  
techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com  
Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

www.tocris.com/distributors  
Tel:+1 612 379 2956