

**Product Name:** PSB 12379

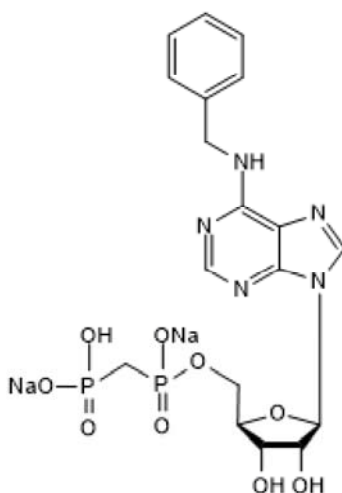
**Catalog No.:** 6083

**Batch No.:** 4

**IUPAC Name:** N<sup>6</sup>-Benzyl- $\alpha,\beta$ -methyleneadenosine 5'-diphosphate disodium salt

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>18</sub>H<sub>21</sub>N<sub>5</sub>Na<sub>2</sub>O<sub>9</sub>P<sub>2</sub>  
**Batch Molecular Weight:** 559.31  
**Physical Appearance:** White solid  
**Solubility:** Soluble in water (supplied pre-dissolved at a concentration of 10mM)  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 100% purity  
**Mass Spectrum:** Consistent with structure

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

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**IUPAC Name:** N<sup>6</sup>-Benzyl- $\alpha,\beta$ -methyleneadenosine 5'-diphosphate disodium salt

**Description:**

Selective high affinity ecto-5'-nucleotidase/CD73 inhibitor ( $K_i$  values are 2.21 and 9.03 nM at human and rat CD73, respectively). Blocks ecto-5'-nucleotidase-mediated adenosine production by preventing the conversion of AMP to adenosine. Exhibits selectivity over other ecto-nucleotidases and ADP-activated P2Y receptors tested.

**Physical and Chemical Properties:**

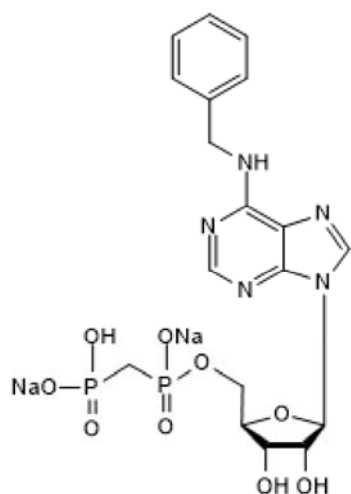
Batch Molecular Formula: C<sub>18</sub>H<sub>21</sub>N<sub>5</sub>Na<sub>2</sub>O<sub>9</sub>P<sub>2</sub>

Batch Molecular Weight: 559.31

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

Soluble in water (supplied pre-dissolved at a concentration of 10mM)

This compound is supplied in aqueous solution at a concentration of 10mM.

**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:**

**Weinmann et al** (2016) Cancer immunotherapy: selected targets and small-molecule modulators. *Chem.Med.Chem.* **11** 450. PMID: 26836578.

**Bhattarai et al** (2015)  $\alpha,\beta$ -methylene-ADP (AOPCP) derivatives and analogues: development of potent and selective ecto-5'-nucleotidase (CD73) inhibitors. *J.Med.Chem.* **58** 6248. PMID: 26147331.

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