Product Name: PSB 10 hydrochloride

CAS Number: 591771-91-4
IUPAC Name: 8-Ethyl-1,4,7,8-tetrahydro-4-methyl-2-(2,3,5-trichlorophenyl)-5H-imidazo[2,1-i]purin-5-one monohydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{16}H_{14}Cl_{3}N_{5}O.HCl
Batch Molecular Weight: 435.14
Physical Appearance: Off-white solid
Solubility: DMSO to 25 mM
Storage: Desiccate at +4°C

2. ANALYTICAL DATA

TLC: \( R_f = 0.8 \) (Chloroform:Methanol [10:1])
Melting Point: Between 320 - 323°C
HPLC: Shows >98% purity
\(^1H\) NMR: Consistent with structure
Mass Spectrum: Consistent with structure

<table>
<thead>
<tr>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
<th>Chlorine</th>
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<td>Theoretical</td>
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<td>3.47</td>
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<td>Found</td>
<td>44.17</td>
<td>3.31</td>
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</table>
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**Description:**
Potent and highly selective antagonist for the human adenosine A3 receptor, with low affinity for the rat A2 receptor (K<sub>i</sub> values are 0.44 and > 17000 nM respectively). Displays > 3800-fold selectivity over human A<sub>1</sub>, A<sub>2A</sub> and A<sub>2B</sub> receptors (K<sub>i</sub> values are 4.1, 3.3 and 30 μM respectively) and > 1800-fold selectivity over rat A<sub>1</sub> and A<sub>2A</sub> receptors. Acts as an inverse agonist in the [35S]GTPγS binding assay in hA<sub>3</sub>-CHO cells (IC<sub>50</sub> = 4 nM). Produces thermal hyperalgesia in mice in vivo.

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C<sub>26</sub>H<sub>24</sub>Cl<sub>3</sub>N<sub>6</sub>O.HCl
- **Batch Molecular Weight:** 435.14
- **Physical Appearance:** Off-white solid
- **Minimum Purity:** >98%

**Storage:** Desiccate at +4°C

**Solubility & Usage Info:**
- DMSO to 25 mM
- Ethanol to 10 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:**