1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_7\text{H}_8\text{N}_4\text{O}_2 \)

Batch Molecular Weight: 180.16

Physical Appearance: White solid

Solubility:
- water to 25 mM
- DMSO to 100 mM
- 1.1eq. NaOH to 100 mM
- 1eq. HCl to 25 mM
- ethanol to 10 mM

Storage: Store at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

Melting Point: At 272°C

HPLC: Shows 100% purity

\(^1\text{H} NMR: \) Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>46.67</td>
<td>46.67</td>
</tr>
<tr>
<td>H</td>
<td>4.48</td>
<td>4.44</td>
</tr>
<tr>
<td>N</td>
<td>31.09</td>
<td>30.59</td>
</tr>
</tbody>
</table>

Certificate of Analysis

Print Date: Jul 28th, 2018

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Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
**Product Name:** Theophylline  
**Catalog No.:** 2795  
**Batch No.:** 1  
**EC Number:** 200-385-7  
**CAS Number:** 58-55-9  
**IUPAC Name:** 3,7-Dihydro-1,3-dimethyl-1H-purine-2,6-dione

<table>
<thead>
<tr>
<th>Description</th>
<th>Storage: Store at RT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bronchodilator, anti-inflammatory and immunomodulator. Antagonizes adenosine receptors and is a weak non-selective inhibitor of phosphodiesterases (PDEs).</td>
<td>Solubility &amp; Usage Info:</td>
</tr>
<tr>
<td>Physical and Chemical Properties:</td>
<td>water to 25 mM</td>
</tr>
<tr>
<td>Batch Molecular Formula: C$_7$H$_8$N$_4$O$_2$</td>
<td>DMSO to 100 mM</td>
</tr>
<tr>
<td>Batch Molecular Weight: 180.16</td>
<td>1.1eq. NaOH to 100 mM</td>
</tr>
<tr>
<td>Physical Appearance: White solid</td>
<td>1eq. HCl to 25 mM</td>
</tr>
<tr>
<td>Minimum Purity: &gt;99%</td>
<td>ethanol to 10 mM</td>
</tr>
<tr>
<td>Batch Molecular Structure:</td>
<td>Stability and Solubility Advice:</td>
</tr>
</tbody>
</table>

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:**