

## Certificate of Analysis

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**Product Name:** 8-Cyclopentyl-1,3-dimethylxanthine

**Catalog No.:** 6137

**Batch No.:** 1

CAS Number: 35873-49-5

IUPAC Name: 8-Cyclopentyltheophylline

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{12}H_{16}N_4O_2 \cdot \frac{1}{2}H_2O$

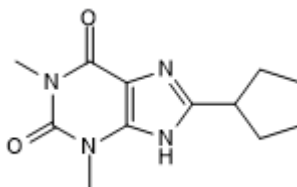
**Batch Molecular Weight:** 257.29

**Physical Appearance:** Pale yellow solid

**Solubility:** DMSO to 100 mM  
ethanol to 10 mM

**Storage:** Store at RT

**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.13$  (Ethyl acetate:Petroleum ether [1:1])

**HPLC:** Shows 99.6% purity

**$^1H$  NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

	Carbon Hydrogen Nitrogen		
	Theoretical	Found	
	56.02	56.29	21.78
		6.57	21.6

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

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**Batch No.:** 1

CAS Number: 35873-49-5

IUPAC Name: 8-Cyclopentyltheophylline

**Description:**

High affinity adenosine A<sub>1</sub> receptor antagonist (pK<sub>i</sub> = 7.5-8).

**Physical and Chemical Properties:**

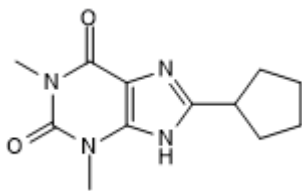
Batch Molecular Formula: C<sub>12</sub>H<sub>16</sub>N<sub>4</sub>O<sub>2</sub>·½H<sub>2</sub>O

Batch Molecular Weight: 257.29

Physical Appearance: Pale yellow solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**Storage:** Store at RT

**Solubility & Usage Info:**

DMSO to 100 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:**

**Dalpiatz et al** (1998) Thermodynamics of full agonist, partial agonist, and antagonist binding to wild-type and mutant adenosine A<sub>1</sub> receptors. *Biochem.Pharmacol.* **56** 1437. PMID: 9827575.

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