

**Product Name:** LUF 5834

**Catalog No.:** 4603

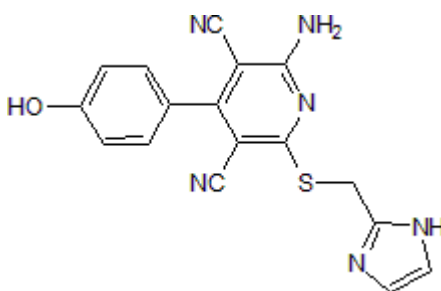
**Batch No.:** 2

**CAS Number:** 333962-91-7

**IUPAC Name:** 2-Amino-4-(4-hydroxyphenyl)-6-[(1*H*-imidazol-2-ylmethyl)thio]-3,5-pyridinecarbonitrile

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>17</sub>H<sub>12</sub>N<sub>6</sub>OS.0.2C<sub>2</sub>H<sub>5</sub>OH.¼H<sub>2</sub>O  
**Batch Molecular Weight:** 362.09  
**Physical Appearance:** Yellow solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.65 (Dichloromethane:Methanol:Ammonia soln. [80:19:1])  
**HPLC:** Shows 100% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	57.72	3.81	23.21
Found	57.89	3.74	23.22

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

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**Catalog No.:** 4603

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CAS Number: 333962-91-7

EC Number:

IUPAC Name: 2-Amino-4-(4-hydroxyphenyl)-6-[(1*H*-imidazol-2-ylmethyl)thio]-3,5-pyridinecarbonitrile

**Description:**

Potent A<sub>2A</sub> and A<sub>2B</sub> adenosine receptor partial agonist ( K<sub>i</sub> = 2.6 nM and EC<sub>50</sub> = 12 nM respectively). Also exhibits selectivity for A<sub>1</sub> over A<sub>3</sub> (K<sub>i</sub> values are 2.6 and 538 nM respectively).

**Physical and Chemical Properties:**

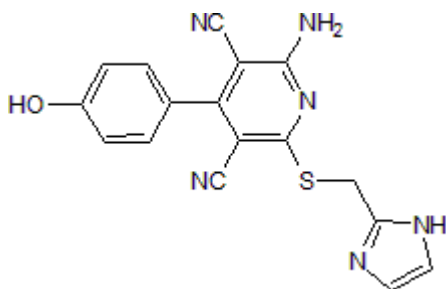
Batch Molecular Formula: C<sub>17</sub>H<sub>12</sub>N<sub>6</sub>OS.0.2C<sub>2</sub>H<sub>5</sub>OH.¼H<sub>2</sub>O

Batch Molecular Weight: 362.09

Physical Appearance: Yellow solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 100 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:**

**Beukers et al** (2004) New, non-adenosine, high potency agonists for the human adenosine A<sub>2B</sub> receptor with an improved selectivity profile compared to the reference agonist *N*-ethylcarboxamidoadenosine J.Med.Chem **47** (15) 3707. PMID: 15239649.

**Lane et al** (2012) A novel nonribose agonist, LUF5834, engages residues that are distinct from those of adenosine-like ligands to activate the adenosine A<sub>2a</sub> receptor Mol.Pharmacol. **81** (3) 475. PMID: 22188926.

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