

## Certificate of Analysis

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**Product Name:** 3-Cyano-7-ethoxycoumarin

**Catalog No.:** 4815

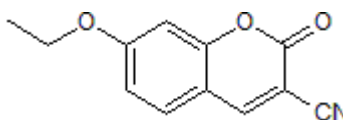
**Batch No.:** 1

CAS Number: 117620-77-6

IUPAC Name: 7-Ethoxy-2-oxo-2H-1-benzopyran-3-carbonitrile

### 1. PHYSICAL AND CHEMICAL PROPERTIES

<b>Batch Molecular Formula:</b>	C <sub>12</sub> H <sub>9</sub> NO <sub>3</sub>
<b>Batch Molecular Weight:</b>	215.2
<b>Physical Appearance:</b>	Purple solid
<b>Solubility:</b>	DMSO to 50 mM
<b>Storage:</b>	Store at +4°C
<b>Batch Molecular Structure:</b>	



### 2. ANALYTICAL DATA

<b>HPLC:</b>	Shows 99.2% purity
<b><sup>1</sup>H NMR:</b>	Consistent with structure
<b>Mass Spectrum:</b>	Consistent with structure

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

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IUPAC Name: 7-Ethoxy-2-oxo-2H-1-benzopyran-3-carbonitrile

**Description:**

Fluorescent P450 substrate (excitation/emission wavelengths = 408/455 nm); metabolized to cyano-hydroxycoumarin.

**Physical and Chemical Properties:**

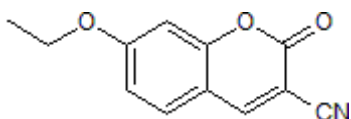
Batch Molecular Formula: C<sub>12</sub>H<sub>9</sub>NO<sub>3</sub>

Batch Molecular Weight: 215.2

Physical Appearance: Purple solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 50 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:**

**White et al** (1988) A continuous fluorometric assay for cytochrome P-450-dependent mixed function oxidases using 3-cyano-7-ethoxycoumarin. *Anal.Biochem.* **172** 304. PMID: 3189781.

**Donato et al** (2004) Fluorescence-based assays for screening nine cytochrome P450 (P450) activities in intact cells expressing individual human P450 enzymes. *Drug Metab.Dispos.* **32** 699. PMID: 15205384.

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