

**Product Name:** HC 030031

**Catalog No.:** 2896

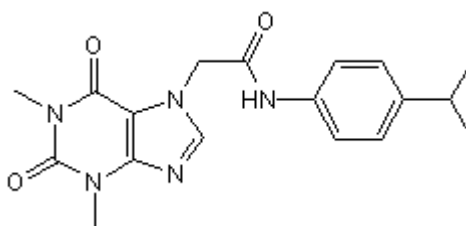
**Batch No.:** 4

**CAS Number:** 349085-38-7

**IUPAC Name:** 2-(1,3-dimethyl-2,6-dioxo-1,2,3,6-tetrahydro-7H-purin-7-yl)-N-(4-isopropylphenyl)acetamide

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>18</sub>H<sub>21</sub>N<sub>5</sub>O<sub>3</sub>  
**Batch Molecular Weight:** 355.39  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 5 mM  
**Storage:** Store at RT  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.5 (Chloroform:Methanol [9:1])  
**HPLC:** Shows 100% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	60.83	5.96	19.71
Found	60.82	5.98	19.61

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**Description:**

Selective TRPA1 channel blocker that antagonizes AITC- and formalin-evoked calcium influx ( $IC_{50}$  values are 6.2 and 5.3  $\mu$ M respectively). Does not block currents mediated by TRPV1, TRPV3, TRPV4, hERG or  $Na_v1.2$  channels. Inhibits AITC- and formalin-induced flinching in vivo.

**Physical and Chemical Properties:**

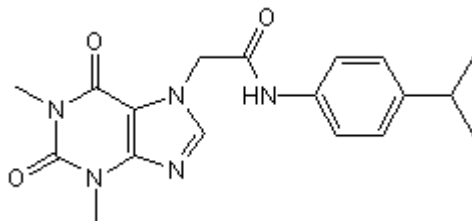
Batch Molecular Formula:  $C_{18}H_{21}N_5O_3$

Batch Molecular Weight: 355.39

Physical Appearance: White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**Storage:** Store at RT

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 5 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:**

**McNamara et al** (2007) TRPA1 mediates formalin-induced pain. *Proc.Natl.Acad.Sci.USA* **104** 13525.

**Taylor-Clark et al** (2008) Prostaglandin-induced activation of nociceptive neurons via direct interactions with TRPA1. *Mol.Pharmacol.* **73** 274. PMID: 18000030.

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