

Product Name: Ciliobrevin A

Catalog No.: 4529

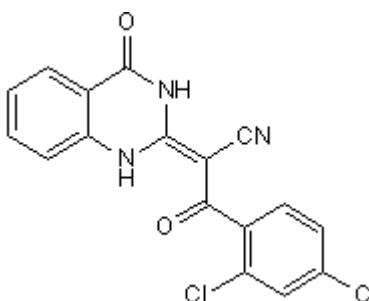
Batch No.: 1

CAS Number: 302803-72-1

IUPAC Name: 2,4-Dichloro- α -(3,4,4-oxo-2(1*H*)-quinazolinylidene)- β -oxobenzeneprapanenitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₉Cl₂N₃O₂
Batch Molecular Weight: 358.18
Physical Appearance: Yellow solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

Melting Point: At 266°C
HPLC: Shows 98.5% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.01	2.53	11.73
Found	57.09	2.51	11.82

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

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IUPAC Name: 2,4-Dichloro- α -(3,4,4-oxo-2(1H)-quinazolinylidene)- β -oxobenzeneprapanenitrile

Description:

Hedgehog (Hh) pathway antagonist; blocks Sonic hedgehog (Shh)-induced Hh pathway activation ($IC_{50} = 7 \mu M$) downstream of Smo. Perturbs primary cilia formation; inhibits cytoplasmic AAA+ ATPase dynein-dependent microtubule gliding and ATPase activity.

Physical and Chemical Properties:

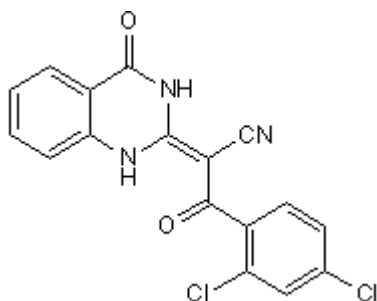
Batch Molecular Formula: $C_{17}H_9Cl_2N_3O_2$

Batch Molecular Weight: 358.18

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°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:

Hyman *et al* (2009) Small-molecule inhibitors reveal multiple strategies for Hedgehog pathway blockade. *Proc.Natl.Acad.Sci.U.S.A.* **106** 14132. PMID: 19666565.

Firestone *et al* (2012) Small-molecule inhibitors of the AAA+ ATPase motor cytoplasmic dynein. *Nature* **484** 7392. PMID: 22425997.

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