

Product Name: Kenpaullone

Catalog No.: 1398

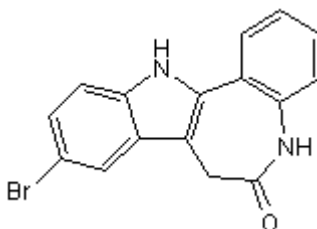
Batch No.: 2

CAS Number: 142273-20-9

IUPAC Name: 9-Bromo-7,12-dihydro-indolo[3,2-d][1]benzazepin-6(5H)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₁BrN₂O·¼H₂O
Batch Molecular Weight: 331.68
Physical Appearance: Tan solid
Solubility: DMSO to 100 mM
 ethanol to 5 mM with gentle warming
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Dichloromethane:Methanol [9:1])
Melting Point: Greater than 300°C(dec)
HPLC: Shows 98.9% purity
¹H NMR: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.94	3.49	8.45
Found	57.77	3.37	8.62

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

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Description:

Potent inhibitor of CDK1/cyclin B and GSK-3 β (IC₅₀ values are 0.4 and 0.23 μ M respectively). Also inhibits CDK2/cyclin A, CDK2/cyclin E and CDK5/cyclin/p35 (IC₅₀ values are 0.68, 7.5 and 0.85 μ M respectively). Selective over c-src (IC₅₀ = 15 μ M), casein kinase 2 (IC₅₀ = 20 μ M), ERK1 (IC₅₀ = 20 μ M), ERK2 (IC₅₀ = 9 μ M) and a range of other protein kinases (IC₅₀ values > 35 μ M). Generates induced pluripotent stem cells (iPSCs) from somatic cells when used in combination with reprogramming factors; can replace Klf4.

Physical and Chemical Properties:

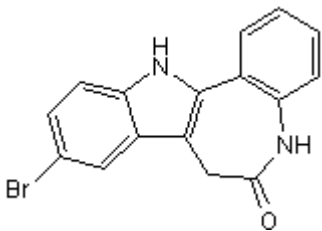
Batch Molecular Formula: C₁₆H₁₁BrN₂O.¼H₂O

Batch Molecular Weight: 331.68

Physical Appearance: Tan solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Schultz et al (1999) Paullones, a series of cyclin-dependent kinase inhibitors: synthesis, evaluation of CDK1/cyclin B inhibition, and in vitro antitumor activity. *J.Med.Chem.* **42** 2909. PMID: 10425100.

Zaharevitz et al (1999) Discovery and initial characterization of the paullones, a novel class of small-molecule inhibitors of cyclin-dependent kinases. *Cancer Res.* **59** 2566. PMID: 10363974.

Buolamwini (2000) Cell cycle targets in novel anticancer drug discovery. *Curr.Pharm.Des.* **6** 379. PMID: 10788588.

Lyssiotis et al (2009) Reprogramming of murine fibroblasts to induced pluripotent stem cells with chemical complementation of Klf4. *Proc.Natl.Acad.Sci.U.S.A.* **106** 8912. PMID: 19447925 .

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 5 mM with gentle warming

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.

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