

**Product Name:** NSC 109555 ditosylate

**Catalog No.:** 3034

**Batch No.:** 1

CAS Number: 66748-43-4

IUPAC Name: 2,2'-[Carbonylbis(imino-4,1-phenyleneethyldyne)]bishydrazinecarboximidamide bis(4-methylbenzenesulfonate)

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>19</sub>H<sub>24</sub>N<sub>10</sub>O<sub>2</sub>.2C<sub>7</sub>H<sub>8</sub>O<sub>3</sub>S.1¼H<sub>2</sub>O

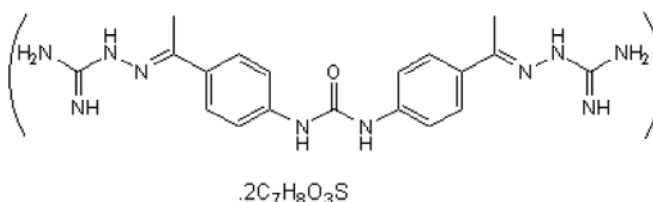
**Batch Molecular Weight:** 775.38

**Physical Appearance:** Off-white solid

**Solubility:** DMSO to 10 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.4 (Methanol:Ammonia soln. [9:1])

**HPLC:** Shows >98.4% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon Hydrogen Nitrogen		
Theoretical	51.12	5.52	18.06
Found	50.89	5.33	18.41

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IUPAC Name: 2,2'-[Carbonylbis(imino-4,1-phenyleneethyldiylidene)]bishydrazinecarboximidamide bis(4-methylbenzenesulfonate)

**Description:**

Selective, reversible, ATP-competitive Chk2 inhibitor ( $IC_{50} = 0.2 \mu M$ ) that displays no effect on a range of other kinases including Chk1 ( $IC_{50} > 10 \mu M$ ). Inhibits histone H1 phosphorylation ( $IC_{50} = 0.24 \mu M$ ) and attenuates mitochondrial ATP synthesis. Exhibits antiproliferative activity in a number of leukemias in vivo.

**Physical and Chemical Properties:**

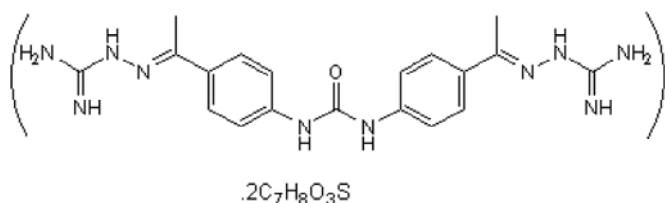
Batch Molecular Formula:  $C_{19}H_{24}N_{10}O \cdot 2C_7H_8O_3S \cdot 1\frac{1}{4}H_2O$

Batch Molecular Weight: 775.38

Physical Appearance: Off-white solid

**Minimum Purity:**  $\geq 98\%$

**Batch Molecular Structure:**



**Storage:** Store at  $-20^\circ C$

**Solubility & Usage Info:**

DMSO to 10 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  $45-60^\circ C$  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  $-20^\circ C$  or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**References:**

**Jobson et al** (2007) Identification of a bis-guanyldiylidene [4,4'-diacetyldiphenylurea-bis(guanyldiylidene)]; NSC 109555] as a novel chemotype for inhibition of Chk2 kinase. *Mol.Pharmacol.* **72** 876. PMID: 17616632.

**Byczkowski et al** (1982) Potentiation of the antimitochondrial and antiproliferative effects of bis(guanyldiylidene)s by phenethylbiguanide. *Cancer Res.* **42** 3592. PMID: 6896674.

**Byczkowski et al** (1981) Actions of bis(guanyldiylidene)s on isolated rat liver mitochondria. *Biochem.Pharmacol.* **30** 2851. PMID: 6895596.

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