

**Product Name:** CGP 78608 hydrochloride

**Catalog No.:** 1493

**Batch No.:** 2

CAS Number: 1135278-54-4

IUPAC Name: [(1S)-1-[[[7-Bromo-1,2,3,4-tetrahydro-2,3-dioxo-5-quinoxaliny]methyl]amino]ethyl]phosphonic acid hydrochloride

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>11</sub>H<sub>13</sub>BrN<sub>3</sub>O<sub>5</sub>P.HCl.½H<sub>2</sub>O

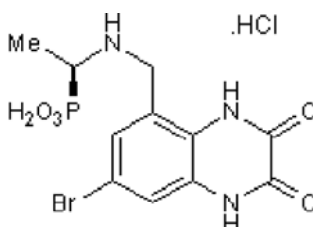
**Batch Molecular Weight:** 423.59

**Physical Appearance:** White solid

**Solubility:** 2.2eq. NaOH to 100 mM

**Storage:** Store at RT

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.3 (Butanol:Acetic acid:Water [40:10:25])

**Melting Point:** At 260°C(dec)

**HPLC:** Shows 98.6% purity

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

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	31.19	3.57	9.92
Found	31.21	3.44	9.73

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**Description:**

Potent and selective NMDA antagonist that acts through the glycine site ( $IC_{50} = 5$  nM). Displays > 500-fold selectivity over kainate and AMPA receptors ( $IC_{50}$  values are 2.7 and 3  $\mu$ M respectively). Also potentiates GluN1/GluN3A-mediated glycine currents ( $EC_{50} = 26.3$  nM). Anticonvulsant in vivo following systemic administration.

**Physical and Chemical Properties:**

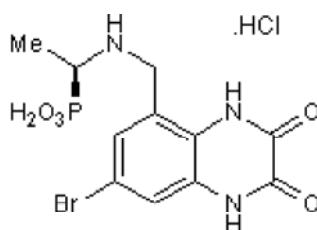
Batch Molecular Formula:  $C_{11}H_{13}BrN_3O_5P \cdot HCl \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 423.59

Physical Appearance: White solid

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

**Batch Molecular Structure:**



**References:**

**Grand et al** (2018) Unmasking GluN1/GluN3A excitatory glycine NMDA receptors. *Nat. Commun.* **9** 4769. PMID: 30425244.

**Ametamey et al** (2000) Synthesis, radiolabelling and biological characterization of (D)-7-iodo-N-(1-phosphonoethyl)-5-aminomethylquinoxaline-2,3-dione, a glycine-binding site antagonist of NMDA receptors. *Bioorg. Med. Chem. Lett.* **10** 75. PMID: 10636248.

**Auberson et al** (1999) N-phosphonoalkyl-5-aminomethylquinoxaline-2,3-diones: *in vivo* active AMPA and NMDA(glycine) antagonists. *Bioorg. Med. Chem. Lett.* **9** 249. PMID: 10021939.

**Storage:** Store at RT

**Solubility & Usage Info:**

2.2eq. NaOH 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.

**Licensing Information:**

Sold with the permission of Novartis Pharma AG

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