

Product Name: KC 12291 hydrochloride

Catalog No.: 3251

Batch No.: 1

CAS Number: 181936-98-1

IUPAC Name: 3,4-Dimethoxy-N-methyl-N-[3-[(5-phenyl-1,2,4-thiadiazol-3-yl)oxy]propyl]benzeneethanamine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₇N₃O₃S.HCl.¼H₂O

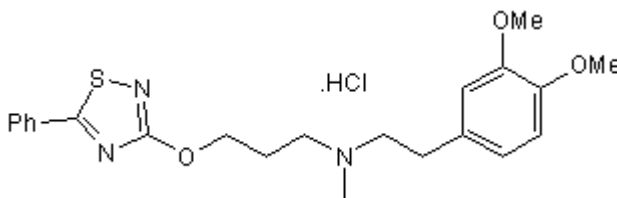
Batch Molecular Weight: 454.49

Physical Appearance: off-white solid

Solubility: water to 25 mM
DMSO to 50 mM
ethanol to 10 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.14	6.32	9.25
Found	58.08	6.18	9.16

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Description:

Orally active atypical voltage-gated sodium channel blocker. Inhibits sustained sodium currents (I_{NaL}) and prevents diastolic contracture in isolated atria in vitro (IC_{50} values are 9.6 and 0.55 - 0.79 μ M respectively). Displays anti-ischemic, bradycardic and cardioprotective activity in vivo.

Physical and Chemical Properties:

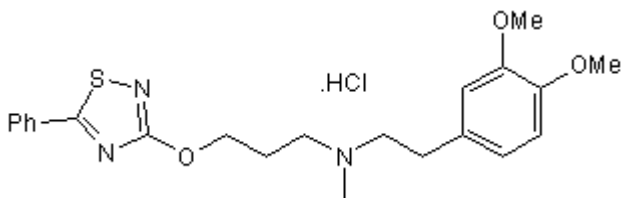
Batch Molecular Formula: $C_{22}H_{27}N_3O_3S.HCl. \frac{1}{4}H_2O$

Batch Molecular Weight: 454.49

Physical Appearance: off-white solid

Minimum Purity: >97%

Batch Molecular Structure:



Storage: Desiccate at +4°C

Solubility & Usage Info:

water to 25 mM
DMSO to 50 mM
ethanol 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°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:

Decking et al (1998) Cardioprotective actions of KC 12291. *Naunyn-Schmied.Arch.Pharmacol.* **358** 547.

Tamareille et al (2002) Anti-ischemic compound KC 12291 prevents diastolic contracture in isolated atria by blockade of voltage-gated sodium channels. *J.Cardiovasc.Pharmacol.* **40** 346. PMID: 12198320.

John et al (2004) KC 12291: an atypical sodium channel blocker with myocardial antiischemic properties. *Cardiovasc.Drug Rev.* **22** 17. PMID: 14978516.

Letienne et al (2006) Pharmacological characterisation of sodium channels in sinoatrial node pacemaking in the rat heart. *Eur.J.Pharmacol.* **530** 243. PMID: 16368090.

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