

**Product Name:** TCB-2

**Catalog No.:** 2592

**Batch No.:** 4

CAS Number: 912342-28-0

IUPAC Name: (4-Bromo-3,6-dimethoxybenzocyclobuten-1-yl)methylamine hydrobromide

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>11</sub>H<sub>14</sub>BrNO<sub>2</sub>.HBr

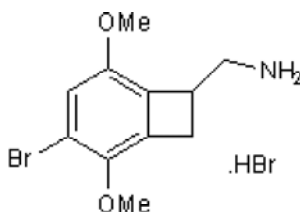
**Batch Molecular Weight:** 353.05

**Physical Appearance:** White solid

**Solubility:** water to 25 mM  
DMSO to 100 mM  
ethanol to 10 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.47 (80:20:1MeOH:DCM:AcOH)

**HPLC:** Shows 99.5% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	37.42	4.28	3.97
Found	37.47	4.24	3.87

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**Description:**

High affinity 5-HT<sub>2A</sub> receptor agonist (K<sub>i</sub> values are 0.73 and 0.75 nM for rat and human receptors respectively). Potently stimulates IP<sub>3</sub> accumulation in NIH3T3 cells stably expressing rat 5-HT<sub>2A</sub> receptors (EC<sub>50</sub> = 36 nM). Induces head twitches and hyperthermia in mice following i.p. administration.

**Physical and Chemical Properties:**

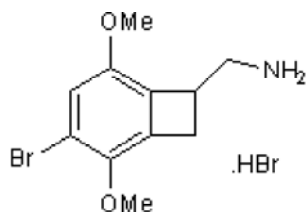
Batch Molecular Formula: C<sub>11</sub>H<sub>14</sub>BrNO<sub>2</sub>.HBr

Batch Molecular Weight: 353.05

Physical Appearance: White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

water to 25 mM

DMSO to 100 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:**

**Niebert *et al*** (2011) Expression and function of serotonin 2A and 2B receptors in the mammalian respiratory network. *PLoS One* **6** e21395. PMID: 21789169.

**Fox *et al*** (2010) The serotonin 5-HT<sub>2A</sub> receptor agonist TCB-2: a behavioral and neurophysiological analysis. *Psychopharmacology* **212** 13. PMID: 19823806.

**McLean *et al*** (2006) 1-Aminomethylbenzocycloalkanes: conformationally restricted hallucinogenic phenethylamine analogues as functionally selective 5-HT<sub>2A</sub> receptor agonists. *J.Med.Chem.* **49** 5794. PMID: 16970404.

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