1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{11}\text{H}_{13}\text{BrN}_{2}\text{O} \)

Batch Molecular Weight: 269.14

Physical Appearance: White solid

Solubility:
- Water to 100 mM
- DMSO to 100 mM

Storage: Store at -20°C

2. ANALYTICAL DATA

TLC: \( R_f = 0.25 \) (Chloroform:Methanol [9:1])

HPLC: Shows 99.9% purity

\(^1\text{H} \text{NMR}: \) Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>49.09</td>
<td>48.94</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.87</td>
<td>4.85</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>10.41</td>
<td>10.41</td>
</tr>
</tbody>
</table>
Product Name: 3-Bromocytisine
CAS Number: 207390-14-5
IUPAC Name: \((1\text{R},5\text{S})\)-9-Bromo-1,2,3,4,5,6-hexahydro-1,5-methano-8\(H\)-pyrido[1,2-\(a\)][1,5]diazocin-8-one

Description:
Potent agonist of \(\alpha_4\beta_4\), \(\alpha_4\beta_2\) and \(\alpha_7\) nACh receptors (IC\(_{50}\) values are 0.28, 0.30 and 31.6 nM respectively). Displays different effects on high (HS) and low (LS) ACh sensitivity \(\alpha_4\beta_2\) nAChRs (EC\(_{50}\) values are 0.008 and 0.05 \(\mu\)M respectively).

Physical and Chemical Properties:
Batch Molecular Formula: C\(_{11}\)H\(_{13}\)BrN\(_2\)O
Batch Molecular Weight: 269.14
Physical Appearance: White solid
Minimum Purity: >98%

Storage: Store at -20°C
CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:
water to 100 mM
DMSO 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.

References:
Houlihan et al (2001) Activity of cytisine and its brominated isoteres on recombinant human \(\alpha_7\), \(\alpha_4\beta_2\) and \(\alpha_4\beta_4\) nicotinic acetylcholine receptors. J.Neurochem. 78 1029. PMID: 11553677.