Product Name: Fenobam
Catalog No.: 2386
Batch No.: 1
CAS Number: 57653-26-6
IUPAC Name: \( N-(3\text{-Chlorophenyl})-N'-(4,5\text{-dihydro-1-methyl-4-oxo-1H-imidazol-2-yl})\text{urea} \)

1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula**: \( \text{C}_{11}\text{H}_{11}\text{N}_{4}\text{O}_{2}\text{Cl} \)
- **Batch Molecular Weight**: 266.69
- **Physical Appearance**: Pale orange solid
- **Solubility**: DMSO to 100 mM
- **Storage**: Store at RT

2. ANALYTICAL DATA

- **HPLC**: Shows 99.2% purity
- **\(^1\)H NMR**: Consistent with structure
- **\(^13\)C NMR**: Consistent with structure
- **Mass Spectrum**: Consistent with structure
- **Microanalysis**:
  
<table>
<thead>
<tr>
<th>Component</th>
<th>Theoretical</th>
<th>Found</th>
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<tbody>
<tr>
<td>Carbon</td>
<td>49.54</td>
<td>49.36</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.16</td>
<td>4.12</td>
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<tr>
<td>Nitrogen</td>
<td>21.00</td>
<td>20.84</td>
</tr>
</tbody>
</table>

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Tel: +1 612 379 2956
Product Name: Fenobam
Catalog No.: 2386    Batch No.: 1

CAS Number: 57653-26-6
IUPAC Name: N-(3-Chlorophenyl)-N'-(4,5-dihydro-1-methyl-4-oxo-1H-imidazol-2-yl)urea

Description:
Potent and selective non-competitive mGlu5 negative allosteric modulator (NAM) that also displays inverse agonist properties; blocks mGlu5 constitutive activity in vitro (IC50 = 87 nM). Acts at an allosteric modulatory site shared with MPEP and binds the mGlu5 receptor with Kd values of 54 and 31 nM for rat and human receptors respectively. Displays anxiolytic activity following oral administration in vivo; also exhibits analgesic properties.

Physical and Chemical Properties:
Batch Molecular Formula: C13H11N4O2Cl
Batch Molecular Weight: 266.69
Physical Appearance: Pale orange solid
Minimum Purity: >99%

References:
Kufahl et al (2013) Positive or negative allosteric modulation of metabotropic glutamate receptor 5 (mGluR5) does not alter expression of behavioral sensitization to methamphetamine F1000Res. 10.12688/f1000resar. PMID: 24358885.

Storage: Store at RT

Solubility & Usage Info:
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.

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