Product Name: Ro 19-4603  
Catalog No.: 1995  
Batch No.: 1  
CAS Number: 99632-94-7  
IUPAC Name: 5,6-Dihydro-5-methyl-6-oxo-4H-imidazo[1,5-a]thieno[2,3-f][1,4]diazepine-3-carboxylic acid 1,1-dimethylethyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $\text{C}_{15}\text{H}_{17}\text{N}_{3}\text{O}_{3}\text{S}$  
Batch Molecular Weight: 319.38  
Physical Appearance: Light yellow solid  
Solubility: ethanol to 100 mM  
DMSO to 100 mM  
Storage: Store at RT  
Batch Molecular Structure:

![Molecular Structure](image)

2. ANALYTICAL DATA

TLC: $R_f = 0.25$ (Ethyl acetate:Petroleum ether [3:7])  
HPLC: Shows 99% purity  
$^1\text{H NMR}$: Consistent with structure  
Microanalysis:  

<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
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<td>Nitrogen</td>
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Description:
Benzodiazepine inverse agonist. Binds with high affinity to both diazepam-sensitive (DS) and diazepam-insensitive (DI) GABA<sub>A</sub> receptors (K<sub>i</sub> values are ~ 0.2 and ~ 2.6 nM for DS and DI receptors respectively). Antagonizes effects of ethanol on locomotor behavior and suppresses ethanol intake in alcohol-prefering rats.

Physical and Chemical Properties:
Batch Molecular Formula: C<sub>19</sub>H<sub>17</sub>N<sub>3</sub>O<sub>3</sub>S
Batch Molecular Weight: 319.38
Physical Appearance: Light yellow solid
Minimum Purity: >99%

Storage: Store at RT

Solubility & Usage Info:
ethanol 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: