Adinazolam

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.

1. GENERAL INFORMATION

**IUPAC Name:** 1-(8-chloro-6-phenyl-4H-benzo[f][1,2,4]triazolo[4,3-a][1,4]diazepin-1-yl)-N,N-dimethylmethanamine

**CAS#:** 37115-32-5

**Synonyms:** 1-(8-chloro-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepin-1-yl)-N,N-dimethylmethanamine, 8-chloro-N,N-dimethyl-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine-1-methanamine

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV_{max} (nm):** Not determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Melting Point (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C_{19}H_{18}ClN_{5}</td>
<td>351.83</td>
<td>169.13</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11 mg/mL in CDCl$_3$ containing TMS for 0 ppm reference and 1,4-BTMSB-$d_4$ as quantitative internal standard.

Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

$^1$HNMR: Adinazolam; Lot# 0471751-27; CDCl$_3$; 400MHz

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**Diagram:**

- CHCl$_3$
- TMS
- BTMSB
- i = impurity

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Latest Revision: 4/10/2020    SWGDRUG.org/monographs.htm
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in CHCl₃

Instrument: Agilent gas chromatograph operated in split mode with MS detector

Column: HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 μm

Carrier Gas: Helium at 1.5 mL/min

Temperatures:
- Injector: 280°C
- MSD transfer line: 280°C
- MS Source: 230°C
- MS Quad: 150°C

Oven program:
1) 100°C initial temperature for 1.0 min
2) Ramp to 280°C at 12 °C/min
3) Hold final temperature for 9.0 min

Injection Parameters: Split Ratio = 25:1, 1 μL injected

MS Parameters:
- Mass scan range: 30-550 amu
- Threshold: 250
- Tune file: stune.u
- Acquisition mode: scan

Retention Time: 19.23 min

EI Mass Spectrum: Adinazolam; Lot# 0471751-27
3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)
Scan Parameters: Number of scans: 32
Number of background scans: 32
Resolution: 4 cm\(^{-1}\)
Sample gain: 1
Aperture: 150

FTIR ATR (Diamond 1 Bounce): Adinazolam; Lot# 0471751-27