Nitrazepam

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

1. GENERAL INFORMATION

**IUPAC Name:** 7-nitro-5-phenyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one

**CAS#:** 146-22-5

**Synonyms:** Mogadon, Benzalin, Insomin

**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_{15}H_{11}N_{3}O_{3}</td>
<td>281.27</td>
<td>229.2</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 mg/2mL in methanol-d$_4$ containing TMS for 0 ppm reference and dimethylsulfone 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: Nitrazepam; Lot# 27F0248; methanol-d$_4$; 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

**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: 150
- Tune file: stune.u
- Acquisition mode: scan

**Retention Time:**
17.83 min

EI Mass Spectrum: Nitrazepam; Lot# 27F0248
Nitrazepam

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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): Nitrazepam; Lot# 27F0248