1. GENERAL INFORMATION

**IUPAC Name:** 7-Chloro-5-(2-chlorophenyl)-1-methyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one

**CAS#:** 2894-68-0

**Synonyms:** 2'-Chloro-diazepam, chlorodiazepam, Ro5-3448

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV\(_{\text{max}}\) (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(<em>{16})H(</em>{12})Cl(_2)N(_2)O</td>
<td>319.19</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~12 mg/mL in CD$_3$OD 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: Diclazepam; Lot# RM-161026-03; CD$_3$OD; 400MHz
Diclazepam

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

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: 100
Tune file: stune.u
Acquisition mode: scan

**Retention Time:**
15.882 min

EI Mass Spectrum: Diclazepam; Lot# RM-161026-03
Diclazepam

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

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): Diclazepam; Lot# RM-161026-03

![FTIR ATR Spectrum](image)
4. ADDITIONAL RESOURCES

Forendex

Wikipedia