Oxazepam

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

1. GENERAL INFORMATION

**IUPAC Name:** 7-chloro-3-hydroxy-5-phenyl-1,3-dihydro-2H-benzo[e][1,4]diazepin-2-one

**CAS#:** 604-75-1

**Synonyms:** 7-chloro-3-hydroxy-5-phenyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one, Serex, Benzotran, Sobril, Tazepam, Serenid-D

**Source:** DEA Reference Material Collection

**Appearance:** Yellow 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}ClN_{2}O_{2}</td>
<td>286.71</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~14 mg/mL in DMSO-\textit{d}_6 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

\(^1\text{HNMR: Oxazepam; Lot# C-002668; DMSO-\textit{d}_6 ; 400MHz}\)

![NMR Spectrum](image-url)
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

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: 14.16 min

EI Mass Spectrum: Oxazepam; Lot# C-002668
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): Oxazepam; Lot# C-002668