Desmethylflunitrazepam

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

1. GENERAL INFORMATION

**IUPAC Name:** 5-(2-fluorophenyl)-7-nitro-1,3-dihydro-2H-benzo[e][1,4]-diazepin-2-one

**CAS#:** 2558-30-7

**Synonyms:** 5-(2-fluorophenyl)-7-nitro-1,3-dihydro-2H-1,4-benzodiazepin-2-one

**Source:** DEA Reference Material Collection

**Appearance:** Yellow 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_{15}H_{10}FN_{3}O_{3}</td>
<td>299.26</td>
<td>223.71</td>
</tr>
</tbody>
</table>

Latest Revision: 7/2/2019

SWGDRUG.org/monographs.htm
3. **QUALITATIVE DATA**

3.1 **NUCLEAR MAGNETIC RESONANCE**

*Sample Preparation:* Dilute analyte to ~14 mg/mL in DMSO-$d_6$ containing TMS for 0 ppm reference and maleic acid 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: Desmethylflunitrazepam; Lot# 71.1B0.3; DMSO-$d_6$; 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: 16.91 min

EI Mass Spectrum: Desmethylflunitrazepam; Lot# 71.1B0.3
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: $4 \text{ cm}^{-1}$
- Sample gain: 8
- Aperture: 80

FTIR ATR (Diamond 1 Bounce): Desmethylflunitrazepam; Lot# 71.1B0.3

![FTIR Spectroscopy Graph](image-url)