MDPBP

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

1. GENERAL INFORMATION

**IUPAC Name:** 1-(1,3-benzodioxol-5-yl)-2-(1-pyrrolidinyl)-1-butanone

**CAS #:** 24622-60-4

**Synonyms:** 3,4-methylenedioxy-α-pyrrolidinobutiophenone; 3,4-MD-α-PBP; 3,4-MDPBP

**Source:** DEA Reference Material Collection

**Appearance:** White powder (HCl)

**UV<sub>max</sub>:** 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&lt;sub&gt;15&lt;/sub&gt;H&lt;sub&gt;19&lt;/sub&gt;NO&lt;sub&gt;3&lt;/sub&gt;</td>
<td>261</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C&lt;sub&gt;15&lt;/sub&gt;H&lt;sub&gt;19&lt;/sub&gt;NO&lt;sub&gt;3&lt;/sub&gt;HCl</td>
<td>297</td>
<td>241.9</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

**Method NMR D$_2$O**

*Sample Preparation:* Dilute analyte to $\sim$5 mg/mL in D$_2$O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

**Instrument:** Varian Mercury 400 MHz NMR spectrometer with proton detection probe

**Parameters:**
- Spectral width: at least containing -3 ppm through 13 ppm
- Pulse angle: 90°
- Delay between pulses: 45 seconds
- Number of scans (NT): 8
- Number of steady state scans: 0
- Oversampling: 4 or more
- Shimming: automatic gradient shimming of Z1-4 shims
- Phasing, Drift Correction: automatic or manual

1H NMR: MDPBP HCl Lot #0435471-8, D$_2$O, 400MHz
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1H NMR: MDPBP HCl Lot #0435471-8, D₂O, 400MHz

[Graph showing 1H NMR spectrum]

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1H NMR: MDPBP HCl Lot #0435471-8, D₂O, 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

Instrument: Gas chromatograph operated in split mode with MS detector

Column: DB-1 MS or equivalent; 30m x 0.25mm x 0.25µm

Carrier Gas: Helium at 1 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 300°C at 12°C/min
3) Hold final temperature for 9.0 min

Injection Parameters: Split Ratio = 20:1, 1 µL injected

MS Parameters:
- Mass scan range: 30-550 amu
- Threshold: 100
- Tune file: stune.u
- Acquisition mode: scan

Retention Time: 12.799 minutes

EI Mass Spectrum: MDPBP HCl Lot # 0435471-8
3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (3 bounce)

**Scan Parameters:**
- Number of scans: 32
- Number of background scans: 32
- Resolution: 4cm\(^{-1}\)
- Sample gain: 8
- Aperture: 150

FTIR ATR (Diamond, 3 Bounce): MDPBP HCl Lot # 0435471-8
4. ADDITIONAL RESOURCES