3,4-Methylenedioxy-α-Pyrrolidinoheptanophenone

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-(pyrrolidin-1-yl)hexan-1-one

**CAS#:** 24622-61-5

**Synonyms:** 3,4-MD-α-PHP; 3,4-MDPHP; 3,4-Methylenedioxy-α-PHP

**Source:** DEA Reference Material Collection

**Appearance:** Tan powder

**UV<sub>max</sub> (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&lt;sub&gt;17&lt;/sub&gt;H&lt;sub&gt;23&lt;/sub&gt;NO&lt;sub&gt;3&lt;/sub&gt;</td>
<td>289.37</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C&lt;sub&gt;17&lt;/sub&gt;H&lt;sub&gt;23&lt;/sub&gt;NO&lt;sub&gt;3&lt;/sub&gt; HCl</td>
<td>325.83</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~17 mg/mL in methanol-$d_4$ containing TMS for 0 ppm reference and 1,4-BTMSB-$d_4$ 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: 3,4-Methylenedioxy-$\alpha$-Pyrrolidinohexanophenone HCl; Lot# 0464802-38; methanol-$d_4$; 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4.7 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: 250
- Tune file: stune.u
- Acquisition mode: scan

**Retention Time:** 13.21 min

EI Mass Spectrum: 3,4-Methylenedioxy-α-PyrrolidinoHexanophenone HCl; Lot# 0464802-38
3.4-Methylenedioxy-\(\alpha\)-Pyrrolidinohexanophenone

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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): 3,4-Methylenedioxy-\(\alpha\)-Pyrrolidinohexanophenone HCl; Lot# 0464802-38
4. ADDITIONAL RESOURCES

Kaizaki-Mitsumoto, A.; Noguchi, N.; Yamaguchi, S.; et. al. Three 25-NBOMe-type drugs, three other phenethylamine-type drugs (25I-NBMD, RH34, and escaline), eight cathinone derivatives, and a phencyclidine analog MMXE, newly identified in ingredients of drug products before they were sold on the drug market. Forensic Toxicology. DOI 10.1007/s11419-015-0293-6.