MPHP

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

![Chemical Structure](image)

1. GENERAL INFORMATION

**IUPAC Name:** 1-(4-methylphenyl)-2-(pyrrolidin-1-yl)hexan-1-one

**CAS#:** 34138-58-4

**Synonyms:** 4'-Methyl-α-pyrrolidinohexiophenone, 4'-Me-α-PHP,
4'-Methyl-α-pyrrolidinohexanophenone, PV-4, 4'-MePHP

**Source:** DEAReferenceMaterialCollection

**Appearance:** WhitePowder

**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$<em>{17}$H$</em>{25}$NO</td>
<td>259</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C$<em>{17}$H$</em>{25}$NO·HCl</td>
<td>295</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in D$_2$O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard. Note: sample was hygroscopic.

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: MPHP HCl; Lot# 0431333-14; D$_2$O; 400MHz
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: DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 µm
Carrier Gas: Helium at 1.0 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: 150
- Tune file: stune.u
- Acquisition mode: scan

Retention Time: 10.846 min

EI Mass Spectrum: MPHP HCl; Lot# 0431333-14
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: 8
- Aperture: 150

Note: sample was hygroscopic
4. ADDITIONAL RESOURCES

Wikipedia

Forendex