dihydro-α-PPP

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

1. GENERAL INFORMATION

IUPAC Name: 1-phenyl-2-(pyrrolidin-1-yl)propan-1-ol

CAS#: Not Determined

Synonyms: dihydro-α-pyrrolidinopropiophenone

Source: DEA Reference Material Collection

Appearance: White granules (HCl)

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;13&lt;/sub&gt;H&lt;sub&gt;19&lt;/sub&gt;NO</td>
<td>205</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C&lt;sub&gt;13&lt;/sub&gt;H&lt;sub&gt;19&lt;/sub&gt;NO · HCl</td>
<td>241</td>
<td>223.3</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~13 mg/mL in deuterium oxide (D$_2$O) containing TSP 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

$^1$H NMR: dihydro-alpha-PPP HCl Lot# RM-131218-03; D$_2$O; 400MHz
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3.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~ 4 mg/mL base extracted into chloroform

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 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: 8.332 min

EI Mass Spectrum: dihydro-alpha-PPP HCl Lot# RM-131218-03
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: 4 cm⁻¹
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): dihydro-alpha-PPP HCl Lot# RM-131218-03
4. ADDITIONAL RESOURCES

Springer, D.; Fritschi, G.; Maurer, H. H. Metabolism of the new designer drug \( \alpha \)-pyrrolidinopropiophenone (PPP) and the toxicological detection of PPP and 4'-methyl-\( \alpha \)-pyrrolidinopropiophenone (MPPP) studied in rat urine using gas chromatography-mass spectrometry. Journal of Chromatography B, 796 (2003) 253-266.