4-Chloro-α-PVP

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

1. GENERAL INFORMATION

**IUPAC Name:** 1-(4-chlorophenyl)-2-(pyrrolidin-1-yl)pentan-1-one

**CAS#:** NA

**Synonyms:** 4-chloro-alpha-PVP

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV\textsubscript{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\textsubscript{15}H\textsubscript{20}ClNO</td>
<td>266</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C\textsubscript{15}H\textsubscript{20}ClNO HCl</td>
<td>302</td>
<td>207.4</td>
</tr>
</tbody>
</table>
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3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~12 mg/mL in DMSO-$d_6$ containing TMS for 0 ppm reference and 8 drops CD$_3$OD and dimethylfumarate 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: 4-Chloro-α-PVP HCl; Lot# RM-160311-01A; 1 mL DMSO-$d_6$ with 8 drops CD$_3$OD; 400MHz

![NMR Spectrogram](image-url)
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
- 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:**
11.208 min

**EI Mass Spectrum:** 4-Chloro-α-PVP HCl; Lot# RM-160311-01A

Latest Revision: 9/6/2016  SWGDRUG.org/monographs.htm
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

FTIR ATR (Diamond 1 Bounce): 4-Chloro-α-PVP HCl; Lot# RM-160311-01A
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4. ADDITIONAL RESOURCES

Wikipedia