4-Fluoropentedrone

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-fluorophenyl)-2-(methylamino)pentan-1-one  
**CAS#:** N/A  
**Synonyms:** 4-FPD, 4-Fluoro-α-methylamino-Valerophenone  
**Source:** DEA Reference Material Collection  
**Appearance:** White powder  
**$UV_{max}$ (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>$C_{12}H_{16}FNO$</td>
<td>209.26</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>$C_{12}H_{16}FNO\text{ HCl}$</td>
<td>245.72</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>

Latest Revision: 10/25/2017    SWGDRUG.org/monographs.htm
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~4 mg/mL in D₂O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

Instrument: 400 MHz NMR spectrometer

Parameters: Spectral width: at least containing -2.9 ppm through 13.1 ppm
Pulse angle: 90°
Delay between pulses: 45 seconds

¹HNMR: 4-Fluoropentedrone HCl; Lot 0464459-21; D₂O; 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

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: 100
- Tune file: stune.u
- Acquisition mode: scan

Retention Time:
6.744 min

EI Mass Spectrum: 4-Fluoropentedrone HCl; Lot 0464459-21
3.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with Golden Gate diamond ATR attachment (1 bounce)

**Scan Parameters:**
- Number of scans: 16
- Number of background scans: 16
- Resolution: 4 cm$^{-1}$
- Sample gain: 8
- Aperture: 150

FTIR (Golden Gate with ATR, 1 Bounce): 4-Fluoropentedrone HCl; Lot 0464459-21

![FTIR Spectrum](image-url)
4. ADDITIONAL RESOURCES

*No Literature as of 08/2017*