1. GENERAL INFORMATION

**IUPAC Name:** 1-(4-fluorophenyl)propan-2-amine

**CFR:** Not Scheduled (6/2013)

**CAS#:** 459-02-9 (base), 64609-06-9 (HCl)

**Synonyms:** 4-FA, p-FA, PFA, para-fluoroamphetamine, PAL-303, 4-fluoro-α-methyl-benzeneethanamine

**Source:** DEA Reference Material Collection

**Appearance:** White powder (HCl)

**Kovat's Index:** Pending

**UV$_{max}$ (nm):** 264.0

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$<em>9$H$</em>{12}$FN</td>
<td>153</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C$<em>9$H$</em>{12}$FN·HCl</td>
<td>189</td>
<td>156.9</td>
</tr>
</tbody>
</table>

3. ADDITIONAL RESOURCES

*Forendex*

*Wikipedia*
4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D₂O

Sample Preparation: Dilute analyte to ~10 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 -3 ppm through 13 ppm
- Pulse angle: 90°
- Delay between pulses: 45 seconds

¹H NMR: 4-Fluoroamphetamine HCl; Lot N17-P13D; D₂O; 400 MHz
4.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~ 1 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: 3.929 min

EI Mass Spectrum: 4-Fluoroamphetamine HCl; Lot N17-P13D
4.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:**
FTIR with diamond ATR attachment (3 bounce)

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

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<table>
<thead>
<tr>
<th>Wavenumber (cm(^{-1}))</th>
<th>% Transmittance</th>
</tr>
</thead>
<tbody>
<tr>
<td>3500</td>
<td>20</td>
</tr>
<tr>
<td>3000</td>
<td>30</td>
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<tr>
<td>2500</td>
<td>40</td>
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<tr>
<td>2000</td>
<td>50</td>
</tr>
<tr>
<td>1500</td>
<td>60</td>
</tr>
<tr>
<td>1000</td>
<td>70</td>
</tr>
</tbody>
</table>

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FTIR ATR (Diamond, 3 Bounce): 4-Fluoroamphetamine HCl; Lot N17-P13D