1. GENERAL INFORMATION

IUPAC Name: 1-(3-fluorophenyl)-2-methylaminopropan-1-one

CFR: Not Scheduled (3/2013)

CAS #: 1049677-77-1

Synonyms: 3-FMC

Source: DEA Reference Material Collection

Appearance: White powder (HCl)

Kovat’s Index: Pending

UV max (nm): 247.5, 291.1

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_{10}H_{12}FNO</td>
<td>181</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C_{10}H_{12}FNO \cdot HCl</td>
<td>217</td>
<td>169.3</td>
</tr>
</tbody>
</table>
3. ADDITIONAL RESOURCES


Wikipedia
4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR (CDCl₃)

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: 3-Fluoromethcathinone HCl; lot TAD3FLU1; 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: 5.692 min

EI Mass Spectrum: 3-Fluoromethacinone HCl; lot TAD3FLU1
4.3 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): 3-Fluoromethcathinone HCl; lot TAD3FLU1