1. GENERAL INFORMATION

**IUPAC Name:** 2-(ethylamino)-1-(3-methylphenyl)propan-1-one

**CFR:** Not Scheduled (4/2013)

**CAS#:** Not Available

**Synonyms:** 3-MEC, 3-methyl-N-ethylcathinone

**Source:** DEA Reference Material Collection

**Appearance:** White powder (HCl)

**Kovat's Index:** Pending

**UV max:** 254.8, 294.2

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{12}H\textsubscript{17}NO</td>
<td>191</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C\textsubscript{12}H\textsubscript{17}NO \cdot HCl</td>
<td>227</td>
<td>212.9</td>
</tr>
</tbody>
</table>

3. ADDITIONAL RESOURCES

4. **QUALITATIVE DATA**

4.1 **NUCLEAR MAGNETIC RESONANCE**

**Method NMR D₂O**

*Sample Preparation:* Dilute analyte to ~5 mg/mL in D₂O containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

**Instrument:** 600 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-methylethcathinone HCl; lot 0435404-15; D₂O; 600 MHz
4.2 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 30.0 min

**Injection Parameters:** Split Ratio = 25:1, 1 µL injected

**MS Parameters:**
- Mass scan range: 34-550 amu
- Threshold: 100
- Tune file: stune.u
- Acquisition mode: scan

**Retention Time:** 7.654 min

EI Mass Spectrum: 3-methylethcathinone HCl; lot 0435404-15
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-methylethcathinone HCl; lot 0435404-15