3,4-Dimethylmethcathinone

1. GENERAL INFORMATION

**IUPAC Name:** 1-(3,4-dimethylphenyl)-2-(methylamino)propan-1-one  
**CFR:** Not Scheduled (7/2013)  
**CAS#:** 1081772-06-6 (HCl)  
**Synonyms:** 3,4-DMMC  
**Source:** DEA Reference Material Collection  
**Appearance:** White powder (HCl)  
**Kovat's Index:** Pending  
**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_{17}NO</td>
<td>191</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C_{12}H_{17}NO \cdot HCl</td>
<td>227</td>
<td>216.4</td>
</tr>
</tbody>
</table>

3. ADDITIONAL RESOURCES

Locos, O; Reynolds, D. The Characterization of 3,4-Dimethylmethcathinone (3,4-DMMC). *J. Forensic Sci.* 2012, 57(5), 1303-1306.

*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: 3,4-Dimethylmethcathinone HCl; Lot N17-P79A; 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: 8.337 min

EI Mass Spectrum: 3,4-Dimethylmethcathinone HCl; Lot N17-P79A
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: 100

FTIR ATR (Diamond, 3 Bounce): 3,4-Dimethylmethcathinone HCl; Lot N17-P79A