1. GENERAL INFORMATION

**IUPAC Name:** 1-(3-chlorophenyl)-2-(methylamino)propan-1-one

**CAS#:** 1607439-32-6 (HCl)

**Synonyms:** 3-CMC; meta-chloro-N-methyl-cathinone; meta-chloromethcathinone

**Source:** DEA Reference Material Collection

**Appearance:** White powder (HCl)

**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$<em>{10}$H$</em>{12}$ClNO</td>
<td>197.66</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C$<em>{10}$H$</em>{12}$ClNO HCl</td>
<td>234.12</td>
<td>198.3</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11 mg/mL in DMSO-\(d_6\) containing TMS for 0 ppm reference and dimethylfumarate 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

\(^1\)HNMR: 3-Chloromethcathinone HCl; Lot# 0467004-25; DMSO-\(d_6\); 400MHz
3-Chloromethcathinone

The Drug Enforcement Administration's Special Testing and Research Laboratory generated this monograph using structurally confirmed reference material.

3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~2 mg/mL in CHCl₃ (base extracted)

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: 250
Tune file: stune.u  Acquisition mode: scan
Retention Time: 7.066 min

Ei Mass Spectrum: 3-Chloromethcathinone HCl; Lot# 0467004-25
3-Chloromethcathinone

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3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)
Scan Parameters: Number of scans: 32
Number of background scans: 32
Resolution: 4 cm\(^{-1}\)
Sample gain: 1
Aperture: 150

FTIR ATR (Diamond 1 Bounce): 3-Chloromethcathinone HCl; Lot# 0467004-25
3-Chloromethcathinone

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4. ADDITIONAL RESOURCES

No additional resources as of 10/2016