1. GENERAL INFORMATION

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

**CAS#:** NA

**Synonyms:** 3-CEC

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV \( \text{max (nm)} \):** 209.7

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>{11})H(</em>{14})ClINO</td>
<td>211.69</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C(<em>{11})H(</em>{14})ClINO HCl</td>
<td>248.15</td>
<td>199.9-207.1</td>
</tr>
</tbody>
</table>
3-Chloroethcathinone

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

3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 mg/mL in D$_2$O 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

$^1$HNMR: 3-Chloroethcathinone HCl; Lot # 0523270-1; D$_2$O; 400MHz
3-Chloroethylcathinone

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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 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: 7.460 min

El Mass Spectrum: 3-Chloroethylcathinone HCl; Lot # 0523270-1
3-Chloroethylcathinone

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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-Chloroethylcathinone HCl; Lot # 0523270-1