1. GENERAL INFORMATION

**IUPAC Name:** 1-(1,3-benzodioxol-5-yl)-2-(methylamino)propan-1-one

**CFR:** Schedule I

**CAS#:** 186028-79-5 (base), 186028-80-8 (HCl)

**Synonyms:** bk-MDMA, β-ketone-MDMA, bk-methylenedioxymethamphetamine, MDMC, 3,4-methylenedioxyethylcathinone, N-methyl-MDC, 3,4-methylenedioxy-N-methylcathinone, N-methyl-3,4-methylenedioxyethylcathinone

**Source:** DEA Reference Material Collection

**Appearance:** White powder (HCl)

**Kovat's Index:** Pending

**UV_{max} (nm):** 234.0, 281.9, 320.1

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_{11}H_{13}NO_3</td>
<td>207</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C_{11}H_{13}NO_3·HCl</td>
<td>243</td>
<td>248.4</td>
</tr>
</tbody>
</table>

3. ADDITIONAL RESOURCES

Forendex

Wikipedia
4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR D$_2$O

Sample Preparation: Dilute analyte to ~25 mg/mL in deuterium oxide (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

$^1$H NMR: Methylene HCl; Lot N1P25; D$_2$O; 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: 9.462 min

EI Mass Spectrum: Methylone HCl; Lot N1P25
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