1. GENERAL INFORMATION

**IUPAC Name:** 2-(methylamino)-1-(4-methylphenyl)butan-1-one

**CAS#:** 1336911-98-8 (HCl)

**Synonyms:** BZ-6378, 4-methyl BP, 4-methyl-N-methylbutiophenone

**Source:** DEA Reference Material Collection

**Appearance:** Beige powder

**$UV_{max}$(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 ($^\circ$C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C$<em>{12}$H$</em>{17}$NO</td>
<td>191</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C$<em>{12}$H$</em>{17}$NO HCl</td>
<td>228</td>
<td>224.3</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~6 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: 4-Methylbuphedrone HCl; Lot# 0452569-8; D$_2$O; 400MHz

![NMR spectrum of 4-Methylbuphedrone HCl](image-url)
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~5 mg/mL in CHCl₃ (1N NaOH extraction)

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 0.8 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 = 25:1, 1 µL injected
MS Parameters:
   Mass scan range: 30-550 amu
   Threshold: 150
   Tune file: stune.u
   Acquisition mode: scan
Retention Time: 8.134 min

El Mass Spectrum: 4-Methylbuphedrone HCl; Lot# 0452569-8
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: 8
- Aperture: 150

FTIR ATR (Diamond 1 Bounce): 4-Methylbuphedrone HCl; Lot# 0452569-8
4-Methylbuphedrone

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

4. ADDITIONAL RESOURCES

   Wikipedia

   Forendex