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

1. GENERAL INFORMATION

**IUPAC Name:** 1-(1,3-benzodioxol-5-yl)-2-(diethylamino)pentan-1-one

**CAS#:** 17763-15-4 (HCl)

**Synonyms:**
- 1-(2H-1,3-benzodioxol-5-yl)-2-(diethylamino)pentan-1-one,
- 1-(1,3-benzodioxol-5-yl)-2-(diethylamino)-1-pentanone

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV\(_{\text{max}}\) (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>{16})H(</em>{23})NO(_{3})</td>
<td>277.36</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C(<em>{16})H(</em>{23})NO(_{3}) HCl</td>
<td>313.82</td>
<td>159.13</td>
</tr>
</tbody>
</table>

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3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11 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

¹HNMR: N,N-Diethylpentylone HCl; Lot# 0563933-3; D₂O; 400MHz

![NMR Spectrogram](image-url)
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in CHCl₃; base 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 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: 11.17 min

EI Mass Spectrum: N,N-Diethylpentylone HCl; Lot# 0563933-3
N,N-Diethylpentylone

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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): N,N-Diethylpentylone HCl; Lot# 0563933-3

[Image of FTIR spectrum]

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