3,4-MDPV

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-(pyrrolidin-1-yl)pentan-1-one

**CFR:** Schedule I

**CAS #:** 687603-66-3 (Base) 24622-62-6 (HCl)

**Synonyms:** 3,4-methylenedioxypyrovalerone

**Source:** DEA Reference Material Collection

**Appearance:** White powder (HCl)

**$UV_{max}$:** 235.8, 283.1, 322.6

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$</em>{21}$NO$_3$</td>
<td>274</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C$<em>{16}$H$</em>{21}$NO$_3$·HCl</td>
<td>311</td>
<td>238-239 decomposes</td>
</tr>
</tbody>
</table>

3. QUALITATIVE DATA
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3.1 NUCLEAR MAGNETIC RESONANCE

Method NMR $D_2O$

Sample Preparation: Dilute analyte to ~10 mg/mL in $D_2O$ containing TSP for 0 ppm reference and maleic acid as quantitative internal standard.

Instrument: Varian Mercury 400 MHz NMR spectrometer with proton detection probe

Parameters: Spectral width: at least containing -3 ppm through 13 ppm
Pulse angle: $90^\circ$
Delay between pulses: 45 seconds
Number of scans (NT): 8
Number of steady state scans: 0
Oversampling: 4 or more
Shimming: automatic gradient shimming of Z1-4 shims
Phasing, Drift Correction: automatic or manual

![1H NMR: 3,4-MDPV HCl Lot # TAD0531A; D$_2$O; 400 MHz](image)
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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

**Sample Preparation:** Dilute analyte to ~4 mg/mL in MeOH.

**Instrument:** Gas chromatograph operated in split mode with MS detector

**Column:** DB-1 MS or equivalent; 30m x 0.25mm x 0.25μm

**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 = 25:1, 1 µL injected

**MS Parameters:**
- Mass scan range: 30-550 amu
- Threshold: 100
- Tune file: stune.u
- Acquisition mode: scan

**Retention Time:** 13.500 minutes
3.3 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
4. ADDITIONAL RESOURCES


Forendex

Wikipedia