Pyrovalerone

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

1. GENERAL INFORMATION

*IUPAC Name:* 1-(4-methylphenyl)-2-(pyrrolidin-1-yl)pentan-1-one

*CAS#:* 3563-49-3

*Synonyms:* Centroton, 4-Methyl-B-detone-prolintane, Thymergix, O-2371, Valerophenone

*Source:* DEA Reference Material Collection

*Appearance:* NA (sample in solution)

*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 (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C_{16}H_{23}NO</td>
<td>245</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C_{16}H_{23}NO HCl</td>
<td>281</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~9 mg/mL in CDCl$_3$ containing TMS for 0 ppm reference.

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: Pyrovalerone; Lot# 0427898-21; CDCl$_3$; 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

**Sample Preparation:** Dilute analyte ~ 2 drops in 1 mL CHCl₃

**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 1.0 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 30.0 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:** 11.332 min

**EI Mass Spectrum:** Pyrovalerone; Lot# 0427898-21
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): Pyrovalerone; Lot# 0427898-21 (dried down)
4. ADDITIONAL RESOURCES

Wikipedia

Forendex