Isovaleryl fentanyl

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

1. GENERAL INFORMATION

**IUPAC Name:** 3-methyl-N-(1-phenethylpiperidin-4-yl)-N-phenylbutanamide

**CAS#:** N/A

**Synonyms:** β'-methyl butyryl fentanyl, 3-methyl-N-phenyl-N-[1-(2-phenylethyl)piperidin-4-yl]butanamide

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV\text{\textsubscript{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\textsubscript{24}H\textsubscript{32}N\textsubscript{2}O</td>
<td>364.52</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C\textsubscript{24}H\textsubscript{32}N\textsubscript{2}O·HCl</td>
<td>400.98</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~13 mg/mL in methanol-\textit{d}_4 containing TMS for 0 ppm reference and dimethylfumarate 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

\textsuperscript{1}HNMR: Isovaleryl fentanyl HCl; Lot# 0550263-1; methanol-\textit{d}_4; 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in CHCl₃

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: 17.37 min

EI Mass Spectrum: Isovaleryl fentanyl HCl; Lot# 0550263-1

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): Isovaleryl fentanyl HCl; Lot# 0550263-1