Heptanoyl fentanyl

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

1. GENERAL INFORMATION

**IUPAC Name:** \( N-(1\text{-phenethyl}piperidin-4-yl)-N\text{-phenylheptanamide} \)

**CAS#:** N/A

**Synonyms:** \( N\text{-phenyl-}N\text{-[1-(2-phenylethyl)piperidin-4-yl]heptanamide} \)

**Source:** DEA Reference Material Collection

**Appearance:** Off-white 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 (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>( C_{26}H_{36}N_2O )</td>
<td>392.58</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>( C_{26}H_{36}N_2O \text{ HCl} )</td>
<td>429.04</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~14 mg/mL in methanol-\(d_4\) containing TMS for 0 ppm reference and 1,4-BTMSB-\(d_4\) 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: heptanoyl fentanyl HCl; Lot# JM-N2-P90A; methanol-\(d_4\); 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

**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: 150
- Tune file: stune.u
- Acquisition mode: scan

**Retention Time:** 20.44 min

El Mass Spectrum: heptanoyl fentanyl HCl; Lot# JM-N2-P90A
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): heptanoyl fentanyl HCl; Lot# JM-N2-P90A