Benzyl 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-benzylpiperidin-4-yl)-N-phenylpropanamide

**CAS#:**  
5156-58-1 (HCl)

**Synonyms:**  
1-benzyl-4-(N-phenylpropionamido)piperidine,  
N-phenyl-N-(1-(phenylmethyl)-4-piperidinyl)-propanamide

**Source:**  
DEA Reference Material Collection

**Appearance:**  
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$<em>{21}$H$</em>{26}$N$_2$O</td>
<td>322.44</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C$<em>{21}$H$</em>{26}$N$_2$O HCl</td>
<td>358.90</td>
<td>241.55</td>
</tr>
</tbody>
</table>

Latest Revision: 1/28/2020 SWGDRUG.org/monographs.htm
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11 mg/mL in methanol-$d_4$ 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

$^1$HNMR: Benzyl fentanyl HCl; Lot# ALB25-6; 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: 250
- Tune file: stune.u
- Acquisition mode: scan

**Retention Time:** 15.77 min

**EI Mass Spectrum:** Benzyl fentanyl HCl; Lot# ALB25-6
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): Benzyl fentanyl HCl; Lot# ALB25-6