Isobutryl fentanyl

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

1. GENERAL INFORMATION

**IUPAC Name:** 2-methyl-N-phenyl-N-[1-(2-phenylethyl)piperidin-4-yl]propanamide

**CAS#:** 117332-90-8 (HCl)

**Synonyms:** N-(1-Phenethylpiperidin-4-yl)N-phenylisobutyramide, NIH 10487

**Source:** DEA Reference Material Collection

**Appearance:** white powder

**UV$_{max}$(nm):** NA

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$<em>{23}$H$</em>{30}$N$_2$O</td>
<td>350.50</td>
<td>NA</td>
</tr>
<tr>
<td>HCl</td>
<td>C$<em>{23}$H$</em>{30}$N$_2$O · HCl</td>
<td>386.96</td>
<td>NA</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11 mg/mL in DMSO-d$_6$ containing TMS for 0 ppm reference and maleic acid 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: Isobutyryl fentanyl HCl Lot# ALB-235-7; DMSO-d$_6$; 400 MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL into methanol.

Instrument: Agilent gas chromatograph operated in split mode with MS detector
Column: HP-5; 30m x 0.25 mm x 0.25 μm
Carrier Gas: Helium at 1 mL/min
Temperatures:
- 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: 100
- Tune file: stune.u
- Acquisition mode: scan

Retention Time:
16.946 min

EI Mass Spectrum: Isobutyryl fentanyl HCl Lot# ALB-235-7
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

FTIR-ATR: Isobutyryl fentanyl HCl Lot# ALB-235-7

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4. ADDITIONAL RESOURCES

No additional resources as of 05/30/17