Fentanyl Carbamate

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

1. GENERAL INFORMATION

**IUPAC Name:** ethyl (1-phenethylpiperidin-4-yl)(phenyl)carbamate

**CAS#:** 1465-20-9 (base)

**Synonyms:** ethyl phenyl[1-(2-phenylethyl)piperidin-4-yl]carbamate

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV<sub>max</sub>(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&lt;sub&gt;22&lt;/sub&gt;H&lt;sub&gt;28&lt;/sub&gt;N&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt;</td>
<td>352.47</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>C&lt;sub&gt;22&lt;/sub&gt;H&lt;sub&gt;28&lt;/sub&gt;N&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;2&lt;/sub&gt; HCl</td>
<td>388.93</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: Fentanyl Carbamate; Lot# 0551590-1; 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: 16.80 min

EI Mass Spectrum: Fentanyl Carbamate; Lot# 0551590-1
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): Fentanyl Carbamate; Lot# 0551590-1