**meta-Fluoroisobutyryl fentanyl**

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

![Chemical Structure of meta-Fluoroisobutyryl fentanyl](image)

### 1. GENERAL INFORMATION

**IUPAC Name:**  
\( N-(3\text{-fluorophenyl})-N-(1\text{-phenethylpiperidin-4-yl})\text{isobutyramide} \)

**CAS#:**  
N/A

**Synonyms:**  
3-FIBF, m-FIBF, 3-fluoroisobutyryl fentanyl, m-fluoroisobutyryl fentanyl,  
\( N\text{-}(3\text{-fluorophenyl})\text{-2-methyl-}N\text{-}[1\text{-}(2\text{-phenylethyl)piperidin-4-yl}]\text{propanamide} \)

**Source:**  
DEA Reference Material Collection

**Appearance:**  
White powder

**\( UV_{\text{max}}(\text{nm}) \):**  
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>( \text{C}<em>{23}\text{H}</em>{29}\text{FN}_{2}\text{O} )</td>
<td>368.49</td>
<td>Not Determined</td>
</tr>
<tr>
<td>HCl</td>
<td>( \text{C}<em>{23}\text{H}</em>{29}\text{FN}_{2}\text{O} \text{ HCl} )</td>
<td>404.95</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~12 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: meta-fluoroisobutyryl fentanyl HCl; Lot# 0538870-1; methanol-$d_4$; 400MHz

![NMR spectrum diagram]

i = residual solvent

Latest Revision: 5/14/2020  SWGDRUG.org/monographs.htm
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### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

**Sample Preparation:** Dilute analyte ~5 mg/mL in MeOH

**Instrument:** Agilent gas chromatograph operated in split mode with MS detector

**Column:** HP-5 MS (or equivalent); 30 m 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:** 16.34 min

EI Mass Spectrum: *meta-*fluoroisobutyryl fentanyl HCl; Lot# 0538870-1
**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): *meta*-fluoroisobutyryl fentanyl HCl; Lot# 0538870-1