1. GENERAL INFORMATION

**IUPAC Name:**  
N-(2-chlorophenyl)-N-(1-phenethylpiperidin-4-yl)propionamide

**CAS#:**  
N/A

**Synonyms:**  
N-(2-chlorophenyl)-N-[1-(2-phenylethyl)piperidin-4-yl]propanamide, o-Chlorofentanyl

**Source:**  
DEA Reference Material Collection

**Appearance:**  
white powder

**UV\textsubscript{max}(nm):**  
N/A

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\textsubscript{22}H\textsubscript{27}ClN\textsubscript{2}O</td>
<td>370.92</td>
<td>NA</td>
</tr>
<tr>
<td>HCl</td>
<td>C\textsubscript{22}H\textsubscript{25}ClN\textsubscript{2}O \cdot HCl</td>
<td>407.38</td>
<td>NA</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~4 mg/mL in CD3OD containing TMS for 0 ppm reference and 1,4-BTMSB-d₄ 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

¹HNMR: ortho-Chlorofentanyl HCl; Lot# 0600281-13; CD3OD; 400MHz
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 1.5mL/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: 100
   - Tune file: stune.u
   - Acquisition mode: scan

Retention Time:
   17.594 min

EI Mass Spectrum: ortho-Chlorofentanyl HCl; Lot# 0600281-13

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[Graph showing mass spectrum]
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: 4
- Aperture: 150

FTIR ATR (Diamond 1 Bounce): ortho-Chlorofentanyl HCl; Lot# 0600281-13
3.4. GAS CHROMATOGRAPHY /INFRARED DETECTION:

Sample Preparation: Dilute analyte 1mg/ml in CHCl₃

Instrument: Gas Chromatograph in split mode with Infrared Detection

Column: HP-5; 30m x 0.32 mm id x 0.25 μm

Carrier Gas: Helium at 2.0mL/min

Temperature: Injector: 280°C   Split ratio: 2:1, 2μl injection

65°C hold 1.5min., ramp to 310°C at 20°C/min., hold 5min.

IRD: Detector: Transfer line

Temp 280°C

Flow Cell Temp 280°C

Resolution 8 cm⁻¹

GC-IRD: ortho-Chlorofentanyl HCl; Lot# 0600281-13
4. ADDITIONAL RESOURCES

No additional resources as of 07/16/2021