t-boc Norfentanyl

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

1. GENERAL INFORMATION

**IUPAC Name:** tert-butyl 4-(N-phenylpropanamido)piperidine-1-carboxylate

**CAS#:** 2665695-47-4

**Synonyms:** N-boc Norfentanyl

**Source:** DEA Reference Materials Collection

**Appearance:** tan 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_{19}H_{28}N_{2}O_{3}</td>
<td>332.44</td>
<td>N/A</td>
</tr>
</tbody>
</table>

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3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

*Sample Preparation:* Dilute analyte to ~12 mg/mL in CD$_3$OD 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

$^1$HNMR; T-boc Norfentanyl; Lot JM-N3-58-1; CD$_3$OD; 400 MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in CH$_3$OH.

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: 100
  - Tune file: stune.u
  - Acquisition mode: scan
Retention Time: 14.103 min

EI Mass Spectrum: T-boc Norfentanyl; Lot #JM-N3-58-1
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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): T-boc Norfentanyl; Lot JM-N3-58-1

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