1. GENERAL INFORMATION

**IUPAC Name:** 2-(2-methoxyphenyl)-1-(1-pentyl-1H-indol-3-yl)ethanone

**CFR:** Schedule I

**CAS #:** 864445-43-2

**Synonyms:** 1-pentyl-3-(2-methoxyphenylacetyl)indole

**Source:** DEA Reference Material Collection

**Appearance:** Pink powder

**Kovat’s Index:** Pending

**UV\text{max} (\text{nm}):** 218.1, 245.0, 296.7

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_{22}H_{25}NO_{2}</td>
<td>335</td>
<td>82.6</td>
</tr>
</tbody>
</table>
3. ADDITIONAL RESOURCES


4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CDCl$_3$

Sample Preparation: Dilute analyte to ~10 mg/mL in deuterochloroform (CDCl$_3$) containing TMS for 0 ppm reference and dimethylsulfone 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
4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 mg/mL in MeOH.

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

Column: DB-1 MS or equivalent; 30m x .25mm x .25µm

Carrier Gas: Helium at 1 mL/min

Temperatures:
- Injector: 280°C
- MSD transfer line: 280°C
- MS Source: 230°C
- MS Quad: 150°C

Oven program:
1) 90°C initial temperature for 2.0 min
2) Ramp to 300°C at 14°C/min
3) Hold final temperature for 10.0 min

Injection Parameters: Split Ratio = 25:1, 1 µL injected

MS Parameters:
- Mass scan range: 34-550 amu
- Threshold: 100
- Tune file: stune.u
- Acquisition mode: scan

Retention Time: 18.249 minutes

El Mass Spectrum: JWH-250 Lot # ALB055RC
4.3 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