1. GENERAL INFORMATION

IUPAC Name: {1-[1-methylpiperidin-2-yl]-1H-indol-3-yl}(tricyclo[3.3.1.1^3,7]dec-1-yl)methanone

CFR: Not Scheduled (as of 2/2013)

CAS #: 335160-66-2

Synonyms: 1-[(N-methylpiperidin-2-yl)methyl]-3-(adamant-1-oyl)indole, Adamantan-1-yl[1-[(1-methyl-2-piperidinyl)methyl]-1H-indol-3-yl]methanone

Source: DEA Reference Material Collection

Appearance: White powder

Kovat’s Index: Pending

UV$_{\text{max}}$ (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$<em>{26}$H$</em>{34}$N$_2$O</td>
<td>390</td>
<td>143.1</td>
</tr>
</tbody>
</table>

3. ADDITIONAL RESOURCES

Forendex

Wikipedia
4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR CDCl₃

Sample Preparation: Dilute analyte to ~10 mg/mL in deuterochloroform (CDCl₃) containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

Instrument: Varian Mercury 400 MHz NMR spectrometer with proton detection probe

Parameters:
- Spectral width: at least containing -3 ppm through 13 ppm
- Pulse angle: 90°
- Delay between pulses: 45 seconds
- Number of scans (NT): 8
- Number of steady state scans: 0
- Oversampling: 4 or more
- Shimming: automatic gradient shimming of Z1-4 shims
- Phasing, Drift Correction: automatic or manual

¹H NMR: AM1248 Lot NIP21; CDCl₃; 400 MHz
\[ ^1H\text{ NMR: AM1248 Lot N1P21; CDCl}_3; 400\text{ MHz} \]

\[ \text{CHCl}_3 \]

\[ 8.5 \quad 8.0 \quad 7.5 \quad \text{Chemical Shift (ppm)} \]

\[ 0.15 \quad 0.10 \quad 0.05 \]

\[ 1 \]

\[ 3 \]

\[ ^1H\text{ NMR: AM1248 Lot N1P21; CDCl}_3; 400\text{ MHz} \]

\[ 4.6 \quad 4.5 \quad 4.4 \quad 4.3 \quad 4.2 \quad 4.1 \quad \text{Chemical Shift (ppm)} \]

\[ 0.15 \quad 0.10 \quad 0.05 \]

\[ 1 \]

\[ 1 \]

\[ ^1H\text{ NMR: AM1248 Lot N1P21; CDCl}_3; 400\text{ MHz} \]

\[ 3.0 \quad 2.5 \quad 2.0 \quad 1.5 \quad \text{Chemical Shift (ppm)} \]

\[ 0.15 \quad 0.10 \quad 0.05 \]

\[ 1 \quad 4 \quad 10 \quad 6 \quad 3 \quad 3 \]
4.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte to ~1 mg/mL in 9:1 CHCl₃:MeOH.

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

**Column:**
DB-1 MS; 30m x 0.25 mm x 0.25 µm

**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) 100°C initial temperature for 1.0 min
  2) Ramp to 300°C at 12°C/min
  3) Hold final temperature for 9.0 min

**Injection Parameters:**
- Split Ratio = 20:1, 1 µL injected

**MS Parameters:**
- Mass scan range: 30-550 amu
- Threshold: 100
- Tune file: stune.u
- Acquisition mode: scan

**Retention Time:**
- AM1248 peak at 24.019 min; Impurity peak at 24.114 min

GC/MS TIC: AM1248, Lot N1P21
GC/MS Observation:

The GC/MS TIC of AM1248 has a shoulder on the right with a dissimilar mass spectrum but the same molecular weight. The major peak at retention time 24.019 minutes is AM1248; while the shoulder at retention time 24.114 minutes is a suspected synthesis byproduct consisting of an azepane isomer. (Citation: “Identification
of the cannabimimetic AM-1220 and its azepane isomer (N-methylazepan-3-yl)-3-(1-naphthoyl)indole in a research chemical and several herbal mixtures.” Forensic Toxicol (2012) 30:126-134

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

FTIR ATR (Diamond, 3 bounce): AM1248; Lot N1P21

![FTIR ATR spectra](image_url)