5-Acetoxy-N,N-dimethyltryptamine

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

1. GENERAL INFORMATION

IUPAC Name: 3-[2-(dimethylamino)ethyl]-1H-indol-5-yl acetate

CAS#: NA

Synonyms: 5-Acetoxy-DMT, 5-AcO-DMT

Source: DEA Reference Material Collection

Appearance: White Powder (Oxalate)

UV\textsubscript{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\textsubscript{14}H\textsubscript{18}N\textsubscript{2}O\textsubscript{2}</td>
<td>246</td>
<td>Not Determined</td>
</tr>
<tr>
<td>Oxalate</td>
<td>C\textsubscript{14}H\textsubscript{18}N\textsubscript{2}O\textsubscript{2} C\textsubscript{2}H\textsubscript{2}O\textsubscript{4}</td>
<td>336</td>
<td>151.7</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~10 mg/mL in CD$_3$OD containing TMS for 0 ppm reference and maleic acid 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: 5-Acetoxy-N,N-dimethyltryptamine Oxalate; Lot# TAD121908; CD$_3$OD; 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

**Sample Preparation:** Dilute analyte ~4 mg/mL in MeOH

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

**Column:**
DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25 μm

**Carrier Gas:**
Helium at 1.0 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 = 25:1, 1 μL injected

**MS Parameters:**
- Mass scan range: 30-550 amu
- Threshold: 150
- Tune file: stune.u
- Acquisition mode: scan

**Retention Time:**
13.75 min

El Mass Spectrum: 5-Acetoxy-N,N-dimethyltryptamine Oxalate; Lot# TAD121908
5-Acetoxy-N,N-dimethyltryptamine
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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: 8
- Aperture: 80

FTIR ATR (Diamond 1 Bounce): 5-Acetoxy-N,N-dimethyltryptamine Oxalate; Lot# TAD121908

[Graph showing infrared spectra]
4. ADDITIONAL RESOURCES

No additional resources as of 07/2016