17-beta-hydroxy-17-alpha-methylandrost-1-en-3-one

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

1. GENERAL INFORMATION

**IUPAC Name:** 17-beta-hydroxy-17-alpha-methylandrost-1-en-3-one

**CAS#:** 65-04-3

**Synonyms:**
1, (5-alpha)-Androsten-17-alpha-methyl-17-beta-ol-3-one;
17-beta-hydroxy-17-alpha-methyl-5-alpha-androst-1-en-3-one;
17-alpha-methyl-1Delta-dihydrotestosterone;
1, (5-alpha)-Androsten-17-alpha-methyl-17-beta-ol-3-one;
Methyl-1-testosterone;
1-dehydromethandrostenolone (Steraloids)

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV\text{\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>Neutral</td>
<td>C\textsubscript{20}H\textsubscript{30}O\textsubscript{2}</td>
<td>302.45</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>

Latest Revision: 11/22/2016

SWGDRUG.org/monographs.htm
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in CDCl₃ 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

¹HNMR: 17-beta-hydroxy-17-alpha-methylandrost-1-en-3-one; Lot # B0365; CDCl₃; 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: HP-1 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: 250°C  MS Quad: 150°C
Oven program:
   1) 100°C initial temperature for 1.0 min
   2) Ramp to 300°C at 14 °C/min
   3) Hold final temperature for 25.0 min
Injection Parameters: Split Ratio = 20:1, 1 μL injected
MS Parameters:
   Mass scan range: 30-550 amu  Threshold: 90
   Tune file: stune.u  Acquisition mode: scan
Retention Time: 15.915 min

El Mass Spectrum: 17-beta-hydroxy-17-alpha-methylandrost-1-en-3-one; Lot# B0365
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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: 150

FTIR ATR (Diamond 1 Bounce): 17-beta-hydroxy-17-alpha-methylandrost-1-en-3-one; Lot# B0365
4. ADDITIONAL RESOURCES

No additional resources as of 03/2016