1-Dehydro Epiandrosterone

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

1. GENERAL INFORMATION

*IUPAC Name:* (3β,5α)-3-hydroxyandrost-1-en-17-one

*CAS#:* 23633-63-8

*Synonyms:* 1-Androsterone

*Source:* DEA Reference Material Collection

*Appearance:* White Powder

*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{19}H\textsubscript{28}O\textsubscript{2}</td>
<td>288.42</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. **QUALITATIVE DATA**

3.1 **NUCLEAR MAGNETIC RESONANCE**

**Sample Preparation:** Dilute analyte to ~14 mg/mL in CDCl$_3$ containing TMS for 0 ppm reference and dimethylfumarate 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: 1-Dehydro Epiandrosterone; Lot# 21-SHG-11-1; CDCl$_3$; 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

**Sample Preparation:** Dilute analyte ~3 mg/mL in CHCl₃

**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: 150
- Tune file: stune.u
- Acquisition mode: scan

**Retention Time:**
- 15.20 min

**EI Mass Spectrum:** 1-Dehydro Epiandrosterone; Lot# 21-SHG-11-1

![Mass Spectrum Image]
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: 1
Aperture: 150

FTIR ATR (Diamond 1 Bounce): 1-Dehydro Epiandrosterone; Lot# 21-SHG-11-1