1. GENERAL INFORMATION

**IUPAC Name:** 2α,3α-epithio-17α-methyl-5α-androstan-17β-ol

**CAS#:** NA

**Synonyms:** (2α,3α,5α,17β)-17-methyl-2,3-epithioandrostan-17-ol, methylepitiostanol, 17α-methylepitiostanol

**Source:** DEA Reference Material Collection

**Appearance:** white powder

**UV<sub>max</sub>(nm):** NA

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&lt;sub&gt;20&lt;/sub&gt;H&lt;sub&gt;32&lt;/sub&gt;OS</td>
<td>320.53</td>
<td>NA</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation:  Dilute analyte to ~18mg/mL in CDCl \textsubscript{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

\textsuperscript{1}HNMR: Methylepitiostanol Lot\#RM-170728-01; CDCl \textsubscript{3}; 400MHz

![NMR Spectrum](image-url)
**Methylepitiostanol**

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

### 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

***Methylepitiostanol breakdown on GC-FID and GC/MS***

Sample Preparation: Dilute analyte ∼4 mg/mL into methanol.

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

**Column:**
HP-5; 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 30.0 min

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

**MS Parameters:**
Mass scan range: 30-550 amu
Threshold: 250
Tune file: stune.u
Acquisition mode: scan

**Retention Time:**
17.101 min

**El Mass Spectrum:** Methylepitiostanol Lot# RM-170728-01
3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR (Smart Golden Gate ATR Accessory)

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): Methylepitiostanol Lot# RM-170728-01

![FTIR Spectrum](attachment:image.png)
4. ADDITIONAL RESOURCES