1. GENERAL INFORMATION

IUPAC Name: (3β)-3-hydroxyandrost-4-en-17-one

CAS#: N/A

Synonyms: 3β-hydroxy-4-androstenone

Source: DEA Reference Material Collection

Appearance: White powder

\( UV_{max}(nm): \) 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_{19}H_{20}O_2 )</td>
<td>288.42</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3β-Hydroxyandrost-4-en-17-one

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

3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~12 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: 3β-Hydroxyandrost-4-en-17-one; Lot# 13-ISU-157-1; CDCl$_3$; 400MHz
3β-Hydroxyandrost-4-en-17-one

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3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 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: 3β-Hydroxyandrost-4-en-17-one; Lot# 13-ISU-157-1
3β-Hydroxyandrost-4-en-17-one

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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: 1
- Aperture: 150

FTIR ATR (Diamond 1 Bounce): 3β-Hydroxyandrost-4-en-17-one; Lot# 13-ISU-157-1