α-Ethyltryptamine

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

1. GENERAL INFORMATION

**IUPAC Name:** 1-(1H-indol-3-yl)butan-2-amine

**CAS#:** 2235-90-7

**Synonyms:** alpha-Ethyltryptamine, α-ET, 3-Indolybutylamine, NSC 88061, Ro 3-1932

**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{12}H\textsubscript{16}N\textsubscript{2}</td>
<td>188</td>
<td>100.5</td>
</tr>
<tr>
<td>HCl</td>
<td>C\textsubscript{12}H\textsubscript{16}N\textsubscript{2} HCl</td>
<td>225</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 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: $90^\circ$
Delay between pulses: 45 seconds

$^1$HNMR: $\alpha$-Ethyltryptamine; Lot# 0448839-14; CD$_3$OD; 400MHz
α-Ethyltryptamine

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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: DB-5 MS (or equivalent); 15m 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) 90°C initial temperature for 1.0 min
2) Ramp to 315°C at 30 °C/min
3) Hold final temperature for 6.0 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: 5.18 min

El Mass Spectrum: α-Ethyltryptamine; Lot# 0448839-14
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): α-Ethyltryptamine; Lot# 0448839-14
4. ADDITIONAL RESOURCES

Wikipedia

Forendex