4-Hydroxy-diethyltryptamine

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

1. GENERAL INFORMATION

**IUPAC Name:** 3-(2-(diethylamino)ethyl)-1H-indol-4-ol

**CAS#:** 22204-89-3

**Synonyms:** 4-Hydroxy-DET

**Source:** DEA Reference Material Collection

**Appearance:** Off-white powder

**UV<sub>max</sub> (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&lt;sub&gt;14&lt;/sub&gt;H&lt;sub&gt;20&lt;/sub&gt;N&lt;sub&gt;2&lt;/sub&gt;O</td>
<td>232.32</td>
<td>101.3</td>
</tr>
<tr>
<td>HCl</td>
<td>C&lt;sub&gt;14&lt;/sub&gt;H&lt;sub&gt;20&lt;/sub&gt;N&lt;sub&gt;2&lt;/sub&gt;O·HCl</td>
<td>268.78</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~11 mg/mL in methanol-\textit{d}_4 containing TMS for 0 ppm reference and 1,4-BTMSB-\textit{d}_4 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: 4-Hydroxy-diethyltryptamine; Lot# 0541116-1; methanol-\textit{d}_4; 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-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 ºC/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: 12.79 min

El Mass Spectrum: 4-Hydroxy-diethyltryptamine; Lot# 0541116-1

Latest Revision: 5/14/2020
SWGDRUG.org/monographs.htm
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): 4-Hydroxy-diethyltryptamine; Lot# 0541116-1