1. GENERAL INFORMATION

IUPAC Name: 2-(diethylamino)-1-phenyl-hexan-1-one

InChI String: InChI=1S/C16H25NO/c1-4-7-13-15(17(5-2)6-3)16(18)14-11-9-8-10-12-14/h8-12,15H,4-7,13H2,1-3H3

CFR: Not Scheduled (03/2019)

CAS#: Not Available

Synonyms: Diethylhexedrone, α-Diethylaminohexanophenone

Source: Department of Homeland Security

Appearance: White Solid Material

Important Note: All identifications were made based on evaluation of analytical data (GC-MS and LC-QTOF) in comparison to analysis of acquired reference material.

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2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Molecular Ion [M⁺]</th>
<th>Exact Mass [M+H]+</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C₁₆H₂₅NO</td>
<td>247.37</td>
<td>247</td>
<td>248.2009</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

N,N-Diethyl Hexedrone is classified as a synthetic (or novel) stimulant and substituted cathinone. Substituted cathinones are modified based on the structure of cathinone, an alkaloid found in the Khat plant. Synthetic stimulants have been reported to cause stimulant-like effects, similar to amphetamines. Synthetic stimulants have also caused adverse events, including death, as described in the literature. Structurally similar compounds include pentedrone, hexedrone, and N-ethyl hexedrone. In the United States, hexedrone, N-ethyl hexedrone, and N,N-diethyl hexedrone are not scheduled substances; however, pentedrone is a Schedule I substance.

4. ADDITIONAL RESOURCES

No additional resources are available at this time.

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At: NMS Labs (Willow Grove, PA)
Sample Preparation: Acid/Base extraction
Instrument: Agilent 5975 Series GC/MSD System
Column: Zebron™ Inferno™ ZB-35HT (15 m x 250 µm x 0.25 µm)
Carrier Gas: Helium (Flow: 1 mL/min)
Temperatures: Injection Port: 265 °C
Transfer Line: 300 °C
MS Source: 230 °C
MS Quad: 150 °C
Oven Program: 60 °C for 0.5 min, 35 °C/min to 340 °C for 6.5 min

**Injection Parameters:**
- Injection Type: Splitless
- Injection Volume: 1 µL

**MS Parameters:**
- Mass Scan Range: 40-550 m/z
- Threshold: 250

**Retention Time:**
- 4.997 min

**Chromatogram: N,N-Diethyl Hexedrone**

*Additional peaks present in chromatogram: internal standard (3.213 min), not a controlled substance (4.922 min), and internal standard (6.294 min)*
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): N,N-Diethyl Hexedron
5.2 LIQUID CHROMATOGRAPHY QUADRUPOLE TIME OF FLIGHT MASS SPECTROMETRY (LC-QTOF)

Testing Performed At: The Center for Forensic Science Research and Education at the Fredric Rieders Family Foundation (Willow Grove, PA)

Sample Preparation: 1:100 dilution of acid/base extract in mobile phase

Instrument: Sciex TripleTOF® 5600+, Shimadzu Nexera XR UHPLC

Column: Phenomenex® Kinetex C18 (50 mm x 3.0 mm, 2.6 µm)

Mobile Phase: A: Ammonium formate (10 mM, pH 3.0)

B: Methanol/acetonitrile (50:50)

Flow rate: 0.4 mL/min

Gradient: Initial: 95A:5B; 5A:95B over 13 min; 95A:5B at 15.5 min

Temperatures: Autosampler: 15 °C

Column Oven: 30 °C

Source Heater: 600 °C

Injection Parameters: Injection Volume: 10 µL

QTOF Parameters: TOF MS Scan Range: 100-510 Da

Precursor Isolation: SWATH® acquisition (27 windows)

Fragmentation: Collision Energy Spread (35±15 eV)

MS/MS Scan Range: 50-510 Da

Retention Time: 6.64 min
Chromatogram: *N,N*-Diethyl Hexedrone

Additional peak present in chromatogram: internal standards (4.90 min and 7.24 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: *N,N*-Diethyl Hexedrone
5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Dilute powder in CDCl₃

Instrument: 300 MHz INOVA VARIAN Spectrometer

Parameters:
- Pulse Sequence: Proton
- Solvent: CDCl₃
- Spectral Width: 4798.5 Hz for 1D (-2 – 14 ppm) and 3773.6 for 2D
- Delay between pulses: 1st delay, d₁ = 1.000

¹H NMR: N,N-Diethyl Hexedrone

¹H NMR (300 MHz, CHLOROFORM-d) δ ppm 0.81 - 0.93 (m, 6 H) 1.18 - 1.55 (m, 9 H) 1.64 - 1.88 (m, 2 H) 2.41 - 2.59 (m, 2 H) 4.18 (dd, J=6.74, 4.98 Hz, 1 H) 7.45 - 7.62 (m, 3 H) 7.94 - 7.99 (m, 2 H)