**N-ethyl Hexylone**

Sample Type: Seized Material

Latest Revision: May 18th, 2018
Date Received: February 12th, 2018
Date of Report: April 19th, 2018

1. GENERAL INFORMATION

IUPAC Name: 1-(1,3-benzodioxol-5-yl)-2-(ethylamino)hexan-1-one

InChI String: InChI=1S/C15H21NO3/c1-3-5-6-12(16-4-2)15(17)11-7-8-13-14(9-11)19-10-18-13/h7-9,12,16H,3-6,10H2,1-2H3

CFR: Not Scheduled (04/2018)

CAS#: Not Available

Synonyms: Not Available

Source: Department of Homeland Security

Appearance: Off-White Solid Material

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>C₁₅H₂₁NO₃</td>
<td>263.33</td>
<td>263</td>
<td>264.1594</td>
</tr>
</tbody>
</table>

**Important Note:** All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF, and NMR), as no standard reference material was available at the time of testing.

**Prepared By:** Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, and Barry K. Logan, PhD, F-ABFT
3. BRIEF DESCRIPTION

*N*-ethyl Hexylone is classified as a novel stimulant and substituted cathinone. Substituted cathinones are modified based on the structure of cathinone, an alkaloid found in the Khat plant. Novel stimulants have been reported to cause stimulant-like effects, similar to amphetamines. Novel stimulants have also caused adverse events, including deaths, as described in the literature. Structurally similar compounds include *N*-ethyl pentylone, pentylone, methyline, and butylone. Pentylone, methyline, and butylone are all Schedule I substances in the United States, while *N*-ethyl pentylone is not scheduled in the United States.

4. ADDITIONAL RESOURCES


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: 5.728 min

Chromatogram: N-ethyl Hexylone

Additional peaks present in chromatogram: internal standard 1 (3.205 min), N-ethyl pentyline (5.479 min), and internal standard 2 (6.289 min)
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): N-ethyl Hexylone
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 extraction 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: 5.93 min
Chromatogram: N-ethyl Hexylone

Additional peaks present in chromatogram: internal standard 1 (4.95 min), N-ethyl pentyline (5.27 min), and internal standard 2 (7.27 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: N-ethyl Hexylone
5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Dilute powder in CDCl$_3$

Instrument: 300 MHz INOVA VARIAN Spectrometer

Parameters: Pulse Sequence: Proton

Solvent: CDCl$_3$

Spectral Width: 4798.5 Hz for 1D (-2 – 14 ppm) and 3773.6 for 2D

Delay between pulses: 1st delay, d1 = 1.000

$^1$H NMR: N-ethyl Hexylone
6. REVISION HISTORY

<table>
<thead>
<tr>
<th>Date</th>
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<tr>
<td>05/18/2018</td>
<td>Added “Sample Type: Seized Material” to Page 1.</td>
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