N-ethyl Heptedrone

Sample Type: Seized Material

Latest Revision: September 30, 2019
Date Received: June 13, 2019
Date of Report: September 30, 2019

1. GENERAL INFORMATION

IUPAC Name: 2-(ethylamino)-1-phenyl-heptan-1-one

InChI String: InChI=1S/C15H23NO/c1-3-5-7-12-14(16-4-2)15(17)13-10-8-6-9-11-13/h6,8-11,14,16H,3-5,7,12H2,1-2H3

CFR: Not Scheduled (09/2019)

CAS#: Not Available

Synonyms: Ethyl-Heptedrone

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>C₁₅H₂₃NO</td>
<td>233.4</td>
<td>233</td>
<td>234.1852</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

*N*-ethyl Heptedrone 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 hexedrone, hexedrone, and pentedrone. Pentedrone and *N*-ethyl hexedrone are Schedule I substances in the United States; however, hexedrone and *N*-ethyl heptedrone are not scheduled.

In September 2019, NMS Labs confirmed two additional seized drug materials positive for *N*-ethyl heptedrone.

4. ADDITIONAL RESOURCES


https://www.caymanchem.com/product/27327/

5. QUALITATIVE DATA

5.1 GAS CHROMATOGRAPHY MASS SPECTROMETRY (GC-MS)

Testing Performed At: NMS Labs (Willow Grove, PA)
Sample Preparation: Acid/Base extraction (1:10 dilution)
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:**
- 4.738 min

**Standard Comparison:**
Reference material for N-ethyl heptadone (Batch: 0549986-6) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as N-ethyl heptadone, based on retention time (4.736 min) and mass spectral data. (https://www.caymanchem.com/product/27327/)
Chromatogram: \textit{N-ethyl Heptedrone}

Additional peaks present in chromatogram: internal standard (3.205 min), not a controlled substance (4.703 min), internal standard (6.279 min)
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): N-ethyl Heptedrone
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: Collison Energy Spread (35±15 eV)

MS/MS Scan Range: 50-510 Da

Retention Time: 6.44 min

Standard Comparison: Reference material for N-ethyl heptedrone (Batch: 0549986-6) was purchased from Cayman Chemical (Ann Arbor, MI, USA). Analysis of this standard resulted in positive identification of the analyte in the exhibit as N-ethyl heptedrone, based on retention time (6.45 min) and mass spectral data. (https://www.caymanchem.com/product/27327/)
Chromatogram: *N*-ethyl Heptedrone

Additional peak present in chromatogram: internal standards (4.88 min and 7.26 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: N-ethyl Heptedrone