1. GENERAL INFORMATION

**IUPAC Name:** 1-(1,3-benzodioxol-5-yl)-2-(butylamino)pentan-1-one

**InChI String:** InChI=1S/C16H23NO3/c1-3-5-9-17-13(6-4-2)16(18)12-7-8-14-15(10-12)20-11-19-14/h7-8,10,13,17H,3-6,9,11H2,1-2H3

**CFR:** Not Scheduled (04/2019)

**CAS#** 17763-10-9

**Synonyms:** N-butylpentylone, bk-BBDP, bk-Butyl-K

**Source:** Department of Homeland Security

**Appearance:** Pink 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.

*Prepared By:* Alex J. Krotulski, MSFS, Melissa F. Fogarty, MSFS, D-ABFT-FT, and Barry K. Logan, PhD, F-ABFT
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>C₁₆H₂₃NO₃</td>
<td>277.4</td>
<td>277</td>
<td>278.1751</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

N-butyl Pentylone 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, methylene, and butylone. N-ethyl Pentylone, pentylone, methylene, and butylone are Schedule I substances in the United States; however, N-butyl pentylone is not scheduled.

4. ADDITIONAL RESOURCES


https://www.caymanchem.com/product/26701

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:**

5.940 min

**Standard Comparison:**

Reference material for N-butyl pentylone (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-butyl pentylone, based on retention time (5.981 min) and mass spectral data. ([https://www.caymanchem.com/product/26701](https://www.caymanchem.com/product/26701))

**Chromatogram: N-butyl Pentylone**
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): N-butyl Pentyline
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: 6.20 min

Standard Comparison: Reference material for N-butyl pentyline (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-butyl pentyline, based on retention time (6.20 min) and mass spectral data.
(https://www.caymanchem.com/product/26701)
Chromatogram: N-butyl Pencylone

Additional peak present in chromatogram: internal standard (4.93 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: N-butyl Pencylone