Methoxpropamine (MXPr)

Sample Type: Seized Material

Latest Revision: April 13, 2020
Date Received: November 13, 2019
Date of Report: April 13, 2020

1. GENERAL INFORMATION

IUPAC Name: 2-(3-methoxyphenyl)-2-(propylamino)cyclohexanone

InChI String: InChI=1S/C16H23NO2/c1-3-11-17-16(10-5-4-9-15(16)18)13-7-6-8-14(12-13)19-2/h6-8,12,17H,3-5,9-11H2,1-2H3

CFR: Not Scheduled (04/2020)

CAS#: Not Available

Synonyms: MXPr, 3-methoxy-2-oxo-PCPr, 3-MeO-2'-OxO-PCPr

Source: Department of Homeland Security

Appearance: White Solid Material

Important Note: All identifications were made based on evaluation of analytical data (GC-MS, LC-QTOF-MS, and NMR), as no standard reference material was available at the time of testing. Delay between date of receipt and date of report may be due to the requirement of complex analytical testing for confirmation.

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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>C₁₆H₂₃NO₂</td>
<td>261.4</td>
<td>261</td>
<td>262.1802</td>
</tr>
</tbody>
</table>

3. BRIEF DESCRIPTION

Methoxpropamine (MXPr) is classified as a novel hallucinogen, with subclassification as an arylcyclohexylamine. Novel hallucinogens have been reported to cause effects similar to ketamine and phencyclidine (PCP). Novel hallucinogens have caused adverse events, including deaths, as described in the literature. Structurally similar arylcyclohexylamines include methoxetamine (MXE) and methoxmetamine (MXM). Analogues in this series are not scheduled in the United States.

4. ADDITIONAL RESOURCES

https://www.wikiwand.com/en/Arylcyclohexylamine

No other resources 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:**
- 5.73 min

**Chromatogram: Methoxpropamine**

*Additional peaks present in chromatogram: internal standards (3.18 and 6.28 min)*
EI (70 eV) Mass Spectrum (Top) and 10x (Bottom): Methoxpropamine
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: 5.44 min
Chromatogram: Methoxpropamine

Additional peaks present in chromatogram: internal standards (4.93 min and 7.29 min)
TOF MS (Top) and MS/MS (Bottom) Spectra: Methoxpropamine
5.3 NUCLEAR MAGNETIC RESONANCE (NMR)

Testing Performed At: IteraMed™ (Doylestown, PA)

Sample Preparation: Powder dissolved in CD$_3$OD

Instrument: 600 MHz Bruker AVANCE™ III Spectrometer

Parameters: Pulse Sequence: Proton

Solvent: CD$_3$OD

Spectral Width: 12019.23 Hz = 20.0276 ppm = 0.183399 Hz/pt for $^1$H; 36231.88 Hz = 240.0768 ppm = 0.552855 Hz/pt for $^{13}$C;
5319.15 Hz = 8.8633 ppm = 2.5972 Hz/pt for COSY; 5319.15 Hz = 8.8633 ppm = 2.5972 Hz/pt for HSQC; 5319.15 Hz = 8.8633 ppm = 1.7315 Hz/pt for HMBC

Number of Scans: 8 for $^1$H; 2987 for $^{13}$C; 4 for COSY; 8 for HSQC; 20 for HMBC

Delay Between Pulses: 1.000 second for $^1$H, 2.000 seconds for $^{13}$C

$^1$H NMR: Methoxpropamine
\textbf{\(^{13}\)C NMR: Methoxpropamine}

\textbf{COSY NMR: Methoxpropamine}
HSQC NMR: Methoxpropamine

HMBC NMR: Methoxpropamine