MDPEP

1-(1,3-benzodioxol-5-yl)-2-pyrrolidin-1-yl-heptan-1-one

GC-MS

Rt.: 10.97 min

An Agilent 6890N Network GC system set up with Agilent HP-5MS (length: 30 m, diameter: 0.25 mm, film: 0.25 mm) coupled to an Agilent 5973 Network Mass Selective Detector (scan range m/z 35 – m/z 500) was used. Samples were subjected to electron ionization (EI) mode. GC-MS conditions: HP-5MS column was temperature programmed from 100 °C (which was held for 2 minutes) to 280 °C at 20 °C/min, 280 °C was held for 3 minutes, then to 315 °C at 25 °C/min, the temperature was stated at 315 °C for 12 minutes. The carrier gas was helium. Tribenzyl-amine was applied as an internal standard (locked to 10.8 minutes). Data handling was carried out with GC/MSD ChemStation sofware.
ATR-FTIR (powder)

![ATR-FTIR spectrum](image-url)
Hungarian Institute for Forensic Science

Analytical data for MDPEP

NMR

**MDPEP**
3,4-methylenedioxy-PV8
in DMSO-d$_6$ solution

$^1$H-NMR chemical shifts $\delta$ [ppm]

1-(1,3-benzoxol-5-yl)-2-pyrroldin-1-yl-heptan-1-one

$^1$H-$^1$H coupling constants $J$ [Hz]

$^{13}$C-NMR chemical shifts $\delta$ [ppm]

CAS No.: 24646-39-7
Formula Weight: 303.386 (base)
Exact Mass: 303.18344367
Molecular Formula: C$_{20}$H$_{22}$NO$_3$
Formula Weight: 339.85694 (HCl salt)

07-10-2019

3/9
$^1$H NMR (overview and characteristic parts)

Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-$d_6$
Hungarian Institute for Forensic Science

Analytical data for MDPEP

**zqs-clip-COSY**

**zqs-TOCSY**

Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d$_6$
**zqs-easy-ROESY**

Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d$_6$
Hungarian Institute for Forensic Science

Analytical data for MDPEP

\[ ^{13} \text{C NMR} \]

Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d\textsubscript{6}
ed-HSQC

Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-\textsubscript{d\textregistered}
ed-HSQC-zqs-TOCSY-ed3

HMBC

Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d6