ANALYTICAL REPORT

Ethylone (C12H15NO3)

(RS)-1-(1,3-benzodioxol-5-yl)-2-(ethylamino)propan-1-one

Remark – other active cpd. detected: none

Sample ID: 1107-14A
Sample description: powder - white
Sample type: RM-reference material
Comments: LGC Lot#24827;
Date of entry: 9/22/2014

Substance identified-structure1 (base form)

Systematic name: (RS)-1-(1,3-benzodioxol-5-yl)-2-(ethylamino)propan-1-one

Other names:

Formula (per base form) C12H15NO3
Mw (g/mol) 221,25
Salt form: HCl
StdInChIKey MJEMIOXXNZZK-UHFFFAOYSA-N
Compound Class Cathinones
Other active cpd. detected: none
Add.info (purity..) 98,40%

1 Created by OPSIN free tool: http://opsin.ch.cam.ac.uk/ DOI: 10.1021/ci100384d
Report updates

<table>
<thead>
<tr>
<th>date</th>
<th>comments (explanation)</th>
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<tbody>
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Supporting information

<table>
<thead>
<tr>
<th>Analytical technique:</th>
<th>applied</th>
<th>remarks</th>
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<tbody>
<tr>
<td>GC-MS (EI ionization)</td>
<td>+</td>
<td>NFL GC-RT (min): 5,53</td>
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<td>BP(1): 72; BP(2): 44, BP(3) :149,</td>
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<tr>
<td>FTIR-ATR</td>
<td>+</td>
<td>direct measurement</td>
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**GC-MS** (Agilent):
GC-method is RT locked to tetracosane (RT=9.53 min).
Injection volume 1 ml and split mode (1:50).
Injector temperature: 280 °C.
Chromatographic separation
Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 mm.
Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, than heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal.
MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadropole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (40) to 550 amu.

**FTIR-ATR** (Perkin Elmer): scan range 4000-400 cm-1; resolution 4cm-1

**GC- (MS)-IR condensed phase** (GC-MS (Agilent) & IR (Spectra analyses-Danny) IR scan range 4000 to 700, resolution 4cm-1

**GC-method:**
Injection volume 1 ml and split mode (1:5).
Injector temperature: 280 °C.
Chromatographic separation
Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 mm.
Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, than heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal.
Split MS : IR : (1:9)
MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadropole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (40) to 550 amu.
IR (condensed phase): IR scan range 4000 to 700, resolution 4cm-1
FIGURES OF SPECTRA

MS (EI)

Abundance

FTIR-ATR

Name | Description
--- | ---
Ethylene HCl, LOC | Ethylene HCl, LOC
Ethylene HCl, ATR | Ethylene HCl, ATR