

Name: Cocaine

Formula: C₁₇H₂₁NO₄

MW: 303 CAS#: 50-36-2 NIST#: 334447 ID#: 23085 DB: replib

Other DBs: RTECS, USP, HODOC, EINECS, IRDB

Contributor: Frank Antolasic, RMIT Applied Chemistry Department, Victoria Australia 3001

10 largest peaks:

182 999 | 82 805 | 83 364 | 303 312 | 105 275 | 94 267 | 77 241 | 96 229 | 42 143 | 198 129 |

Synonyms:

1.8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, [1R-(exo,exo)]-

2.1 α H,5 α H-Tropane-2 β -carboxylic acid, 3 β -hydroxy-, methyl ester, benzoate (ester)

3.L-Cocaine

4.Benzoylmethylecgonine

5.Ecgonine, methyl ester, benzoate (ester)

6.Neurocaine

7.2 β -Carbomethoxy-3 β -benzoxytropane

8.2 β -Tropanecarboxylic acid, 3 β -hydroxy-, methyl ester, benzoate (ester)

9.1- α -H,5- α -H-Tropane-2- β -carboxylic acid, 3- β -hydroxy-, methyl ester, benzoate

10.Bernice

11.Bernies

12.Burese

13."C" Carrie

14.Cecil

15.Cholly

16. β -Cocaine

17.1-Cocaine

18.Coke

19.Corine

20.Ecgonine, methyl ester, benzoate

21.Eritroxilina

22.Erytroxylin

23.Girl

24.Gold dust

25.Happy dust

26.Kokain

27.Kokan

28.Kokayeen

29.Methyl 3- β -hydroxy-1- α -H,5- α -H-tropane-2- β -carboxylate benzoate

30.Star dust

31.2- β -Tropanecarboxylic acid, 3- β -hydroxy-, methyl ester, benzoate

32.3-Tropanylbenzoate-2-carboxylic acid methyl ester

33.Methyl 3 β -hydroxy-1 α H,5 α H-tropane-2 β -carboxylate benzoate (ester)

34.3 β -Hydroxy-2 β -tropanecarboxylic acid methyl ester, benzoate

35.2-Methyl-3 β -hydroxy-1 α H,5 α H-tropane-2 β -carboxylate benzoate (ester)

Estimated non-polar retention index (n-alkane scale):

Value: 2204 iu

Confidence interval (Diverse functional groups): 89(50%) 382(95%) iu

Retention index

1. Value: 2186 iu

Column Type: Capillary

Column Class: Standard non-polar

Active Phase: SPB-1

Column Length: 30 m
Carrier Gas: He
Column Diameter: 0.75 mm
Phase Thickness: 1.0 µm
Data Type: Linear RI
Program Type: Ramp
Start T: 160 C
End T: 280 C
Heat Rate: 10 K/min
End Time: 12 min
Source: Christ, D.W.; Noomano, P.; Rosas, M.; Rhone, D., Retention indices by wide-bore capillary gas chromatography with nitrogen-phosphorus detection, J. Anal. Toxicol., 12, 1988, 84-88.

2. Value: 2179 iu
Column Type: Capillary
Column Class: Standard non-polar
Active Phase: BP-1
Column Length: 12 m
Carrier Gas: He
Column Diameter: 0.22 mm
Phase Thickness: 0.25 µm
Data Type: Linear RI
Program Type: Complex
Description: 120C=>8C/min=>270C=>25C/min=>300C
Source: Stowell, A.; Wilson, L.W., A simple approach to the interlaboratory transfer of drug retention indices determined by temperature programmed capillary gas chromatography, J. Forensic Sci., 32(5), 1987, 1214-1220.

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