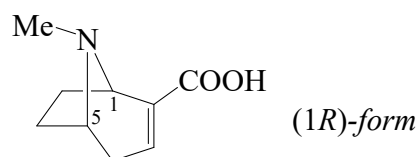




>>Entry Name: 8-Methyl-8-azabicyclo[3.2.1]oct-2-ene-2-carboxylic acid

Synonym(s): Anhydroecgonine. Ecgonidine



Molecular Formula: C₉H₁₃NO₂

Molecular Weight: 167.207

Accurate Mass: 167.094629

Percentage Composition: C 64.65%; H 7.84%; N 8.38%; O 19.14%

Biological Use/Importance: Topical anaesthetic

pKa Value: p*K*_{a1} 3.8; p*K*_{a2} 9.8

>>Variant: (1*R*)-form

Synonym(s): (–)-form

CAS Registry Number: 484-93-5

Molecular Formula: C₉H₁₃NO₂

Molecular Weight: 167.207

Accurate Mass: 167.094629

Percentage Composition: C 64.65%; H 7.84%; N 8.38%; O 19.14%

Source/Synthesis: Obt. semisynthetically from Cocaine

Physical Description: Cryst. (MeOH/EtOH)

Melting Point: Mp 235 dec.°

Optical Rotation: [α]_D¹⁴ –84.6

>>Derivative: Hydrochloride

CAS Registry Number: 74242-55-0

Physical Description: Needles (EtOH) or tablets (H₂O)

Melting Point: Mp 240-241°

Optical Rotation: [α]_D²⁵ –62.7 (H₂O)

>>Derivative: Me ester

CAS Registry Number: 43021-26-7

Molecular Formula: C₁₀H₁₅NO₂

Molecular Weight: 181.234

Accurate Mass: 181.110279

Percentage Composition: C 66.27%; H 8.34%; N 7.73%; O 17.66%

Boiling Point: Bp₇ 107°

>>Derivative: Et ester

CAS Registry Number: 73045-45-1

Molecular Formula: C₁₁H₁₇NO₂

Molecular Weight: 195.261

Accurate Mass: 195.125929

Percentage Composition: C 67.66%; H 8.78%; N 7.17%; O 16.39%

Boiling Point: Bp₁₆ 136-139°

Solubility: Sol. cold H₂O, spar. sol. hot

>>Variant: (1*S*)-form

Synonym(s): (+)-form

Molecular Formula: C₉H₁₃NO₂

Molecular Weight: 167.207

Accurate Mass: 167.094629

Percentage Composition: C 64.65%; H 7.84%; N 8.38%; O 19.14%

Physical Description: Cryst. + 1H₂O (MeOH or MeOH/Et₂O)

Melting Point: Mp 226-230°

Solubility: Sol. H₂O; spar. sol. EtOH

>>Derivative: Me ester