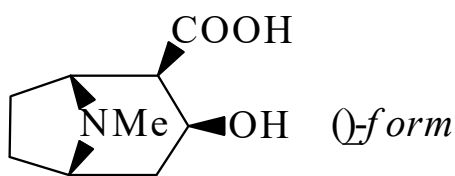




>>Entry Name: Ecgonine

Synonym(s): 3-Hydroxy-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylic acid, 9Cl. 3β-Hydroxy-1αH,5αH-tropane-2β-carboxylic acid, 8Cl



Related CAS Registry Numbers(s): 56053-45-3 56053-46-4

Molecular Formula: C₉H₁₅NO₃

Molecular Weight: 185.222

Accurate Mass: 185.105194

Percentage Composition: C 58.36%; H 8.16%; N 7.56%; O 25.91%

Hazard & Toxicity: Highly toxic by inhalation, allergen

>>Variant: (-)-form

CAS Registry Number: 481-37-8

Molecular Formula: C₉H₁₅NO₃

Molecular Weight: 185.222

Accurate Mass: 185.105194

Percentage Composition: C 58.36%; H 8.16%; N 7.56%; O 25.91%

Source/Synthesis: Obt. by hydrol. of Cocaine [BCM51-U](#)

Melting Point: Mp 205°

Optical Rotation: [α]_D -45.4 (H₂O)

>>Derivative: Me ester

Synonym(s): Methylecgonine. Ecgonine methyl ester

CAS Registry Number: 7143-09-1

Type of Compound Code(s): XA0550 VX0400

Molecular Formula: C₁₀H₁₇NO₃

Molecular Weight: 199.249

Accurate Mass: 199.120844

Percentage Composition: C 60.28%; H 8.60%; N 7.03%; O 24.09%

Biological Source: Minor alkaloid from *Erythroxylum coca* and other *Erythroxylum* spp. (Erythroxylaceae)

Use/Importance: Anaesthetic

Physical Description: Oil (synthetic)

Boiling Point: Bp_{0.2} 84-88°

Density: d₂₀ 1.15

Refractive Index: n_D²⁰ 1.4890

Calculated Log P Data: Log P 0.13 (calc)

Other Data: Poorly characterized as a natural alkaloid

>>Derivative: Me ester; hydrochloride

CAS Registry Number: 38969-40-3

Melting Point: Mp 212 dec.° (199-200°) (synthetic)

>>Derivative: O-Benzoyl

Synonym(s): Benzoylecgonine

CAS Registry Number: 519-09-5

Type of Compound Code(s): VX0400

Molecular Formula: C₁₆H₁₉NO₄

Molecular Weight: 289.33

Accurate Mass: 289.131409

Percentage Composition: C 66.42%; H 6.62%; N 4.84%; O 22.12%

Biological Source: Alkaloid from *Erythroxylum* spp. Major metab. of Cocaine

Melting Point: Mp 195°

Optical Rotation: [α]_D -63.3 (H₂O)

Sigma: B8900

>>Derivative: O-Benzoyl, Me ester

see Cocaine, [BCM51-U](#)