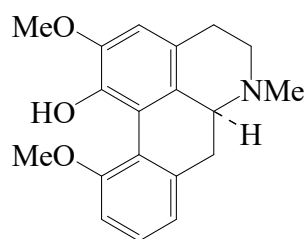




>>Entry Name: Isothebaine

Synonym(s): 1-Hydroxy-2,11-dimethoxyaporphine



CAS Registry Number: 568-21-8

Molecular Formula: C₁₉H₂₁NO₃

Molecular Weight: 311.38

Accurate Mass: 311.152144

Percentage Composition: C 73.29%; H 6.80%; N 4.50%; O 15.41%

>>Variant: (S)-form

Molecular Formula: C₁₉H₂₁NO₃

Molecular Weight: 311.38

Accurate Mass: 311.152144

Percentage Composition: C 73.29%; H 6.80%; N 4.50%; O 15.41%

Biological Source: Alkaloid from *Papaver orientale* and *Papaver bracteatum* (Papaveraceae)

Use/Importance: Convulsive agent in high doses. Small doses increase muscle tonus in intestinal tissue, higher doses produce relaxation. Increases tonus in uterine tissue. Respiratory depressant, shows analgesic and some antiinflammatory action

Melting Point: Mp 164-166° (203-204°)

Optical Rotation: $[\alpha]_D^{21} +281$ (c, 1.11 in CHCl₃)

Hazard & Toxicity: LD₅₀ (mus, scu) 26 mg/kg

>>Derivative: N-Oxide

Synonym(s): Isothebaine N-oxide

Molecular Formula: C₁₉H₂₁NO₄

Molecular Weight: 327.379

Accurate Mass: 327.147059

Percentage Composition: C 69.71%; H 6.47%; N 4.28%; O 19.55%

Biological Source: Alkaloid from *Papaver pseudo-orientale*

Physical Description: Amorph.

Optical Rotation: $[\alpha]_D +260$ (CHCl₃)

>>Derivative: N-Me

Synonym(s): N-Methylisothebainium

CAS Registry Number: 25651-02-9

Molecular Formula: C₂₀H₂₄NO₃⁽⁺⁾

Molecular Weight: 326.414

Accurate Mass: 326.175619

Percentage Composition: C 73.59%; H 7.41%; N 4.29%; O 14.70%

Biological Source: Alkaloid from *Papaver orientale*, *Papaver pseudo-orientale* and *Papaver bracteatum*

Physical Description: Needles (MeOH) (as iodide)

Melting Point: Mp 254-256° (249-253°) (iodide)

Optical Rotation: $[\alpha]_D^{21} +194$ (c, 0.51 in MeOH)

Other Data: CAS no. refers to iodide

>>Derivative: Me ether

Synonym(s): O-Methylisothebaine

CAS Registry Number: 90275-86-8