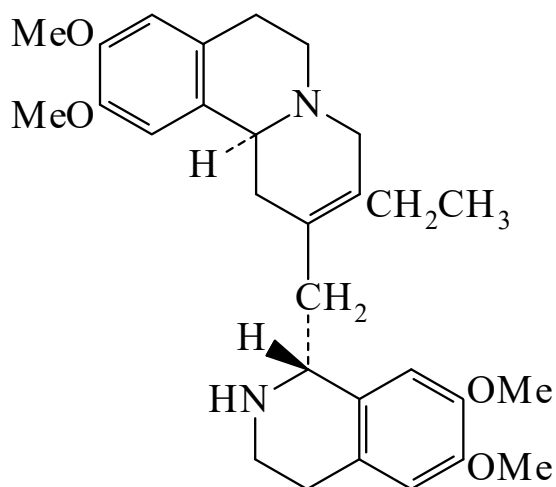




>>Entry Name: Dehydroemetine, BAN, INN

Synonym(s): 2,3-Didehydro-6',7',10,11-tetramethoxyemetan, 9Cl. Dametin. Efemetin. Mebadin. Ro 1-9334. DHE. BT 436



CAS Registry Number: 4914-30-1

Molecular Formula: C₂₉H₃₈N₂O₄

Molecular Weight: 478.63

Accurate Mass: 478.283158

Percentage Composition: C 72.77%; H 8.00%; N 5.85%; O 13.37%

Use/Importance: Amoebicide

Calculated Log P Data: Log P 4.06 (calc)

Hazard & Toxicity: Mutagenic props.

>>Variant: (+)-form

Molecular Formula: C₂₉H₃₈N₂O₄

Molecular Weight: 478.63

Accurate Mass: 478.283158

Percentage Composition: C 72.77%; H 8.00%; N 5.85%; O 13.37%

>>Derivative: Hydrobromide (1:2)

Physical Description: Cryst.

Melting Point: Mp 241-243°

Optical Rotation: [α]_D +95 (MeOH)

>>Variant: (–)-form

Molecular Formula: C₂₉H₃₈N₂O₄

Molecular Weight: 478.63

Accurate Mass: 478.283158

Percentage Composition: C 72.77%; H 8.00%; N 5.85%; O 13.37%

Physical Description: Cryst. (diisopropyl ether)

Melting Point: Mp 94-96°

Optical Rotation: [α]_D –183

>>Derivative: Hydrobromide (1:2)

Physical Description: Cryst.

Melting Point: Mp 243-245°

Optical Rotation: [α]_D –97 (MeOH)

>>Variant: (±)-form

CAS Registry Number: 1986-67-0

Molecular Formula: C₂₉H₃₈N₂O₄

Molecular Weight: 478.63

Accurate Mass: 478.283158

Percentage Composition: C 72.77%; H 8.00%; N 5.85%; O 13.37%