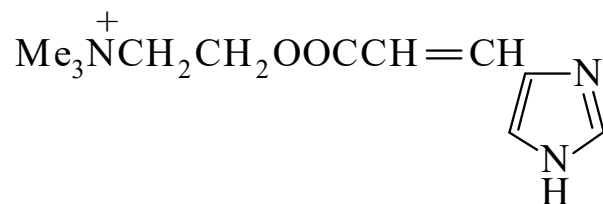




>>Entry Name: Murexine

Synonym(s): 2-[[3-(1*H*-Imidazol-4-yl)-1-oxo-2-propenyl]oxy]-*N,N,N*-trimethylethanaminium(1+), 9Cl. Choline imidazole-4-acrylate. Choline urocanate



CAS Registry Number: 20284-40-6

Molecular Formula: C₁₁H₁₈N₃O₂⁽⁺⁾

Molecular Weight: 224.282

Accurate Mass: 224.139902

Percentage Composition: C 58.91%; H 8.09%; N 18.74%; O 14.27%

Biological Source: Found in large amts. in the hypobranchial glands of molluscs, esp. *Murex* spp., and also *Concholepas concholepas* and *Tritonalia erinacea*

Use/Importance: Muscle relaxant with strong curariform action

Solubility: BERDY SOL: Sol. H₂O

pKa Value: pK_a 4.6

UV: [acid] λ_{max} 285 (ε 16700) (pH 4.5 buffer) (Berdy)

>>Derivative: Chloride

CAS Registry Number: 6209-43-4

Molecular Formula: C₁₁H₁₈ClN₃O₂

Molecular Weight: 259.735

Accurate Mass: 259.108754

Percentage Composition: C 50.87%; H 6.98%; Cl 13.65%; N 16.18%; O 12.32%

Physical Description: Hygroscopic cryst. + 1H₂O

Other Data: Unstable, instantly hydrol. by H₂O

>>Derivative: Chloride; hydrochloride

Physical Description: Microcryst. powder + ½ H₂O

Melting Point: Mp 219-221 dec.°

Other Data: Hygroscopic

>>Derivative: Dipicrate

Physical Description: Yellow needles (H₂O)

Melting Point: Mp 221-222 dec.°

>>Derivative: *N*-Me

Synonym(s): *N*-Methylmurexine

Molecular Formula: C₁₂H₂₀N₃O₂⁽⁺⁾

Molecular Weight: 238.309

Accurate Mass: 238.155552

Percentage Composition: C 60.48%; H 8.46%; N 17.63%; O 13.43%

Biological Source: Reported to occur in the marine gastropod mollusc *Nucella emarginata*

Other Data: Struct. assignment prob. incorrect. A recent unambiguous synth. of the two possible *N*-Me derivs. of Murexine indicates that the natural compd. is neither of these

>>Derivative: 1-Me, iodide

Source/Synthesis: Synthetic

Physical Description: Cryst. (MeOH)

Melting Point: Mp 224-225°

>>Derivative: 3-Me, iodide

Source/Synthesis: Synthetic

Melting Point: Mp 224°

References: