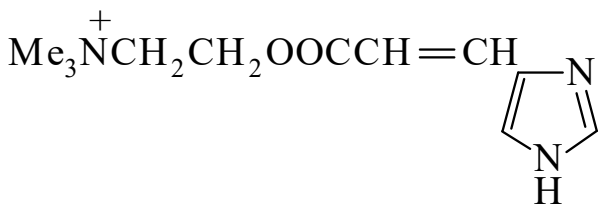
>>**Entry Name: Murexine**
Synonym(s): 2-[[3-(1*H*-Imidazol-4-yl)-1-oxo-2-propenyl]oxy]-*N*,*N*,*N*-trimethylethanaminium(1+), $_{9}Cl$. Choline imidazole-4-acrylate. Choline urocanate



CAS Registry Number: 20284-40-6

Molecular Formula: $C_{11}H_{18}N_3O_2^{(+)}$
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. H_2O
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: $C_{11}H_{18}ClN_3O_2$
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. + $1H_2O$
Other Data: Unstable, instantly hydrol. by H_2O

>>**Derivative:** Chloride; hydrochloride

Physical Description: Microcryst. powder + ½ H_2O
Melting Point: Mp 219-221 dec.°
Other Data: Hygroscopic

>>**Derivative:** Dipicrate

Physical Description: Yellow needles (H_2O)
Melting Point: Mp 221-222 dec.°

>>**Derivative:** *N*-Me
Synonym(s): ***N*-Methylmurexine**

Molecular Formula: $C_{12}H_{20}N_3O_2^{(+)}$
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: