



>>Derivative: Et ester

CAS Registry Number: 6152-27-8

Molecular Formula: C₁₀H₁₃NO₂

Molecular Weight: 179.218

Accurate Mass: 179.094629

Percentage Composition: C 67.02%; H 7.31%; N 7.82%; O 17.85%

Boiling Point: Bp 257°. Bp₁₆ 149°. Bp₅ 114-115°

>>Derivative: 3-Methylbutyl ester

Synonym(s): Phenamacide. Aklonin

CAS Registry Number: 31031-74-0

Molecular Formula: C₁₃H₁₉NO₂

Molecular Weight: 221.299

Accurate Mass: 221.141579

Percentage Composition: C 70.56%; H 8.65%; N 6.33%; O 14.46%

Biological Use/Importance: Antispasmodic

Physical Description: Cryst. (as hydrochloride)

Melting Point: Mp 154° (as hydrochloride)

Other Data: CAS no. refers to hydrochloride

>>Derivative: Heptyl ester

Synonym(s): Aceverine

CAS Registry Number: 32560-48-8

Molecular Formula: C₁₅H₂₃NO₂

Molecular Weight: 249.352

Accurate Mass: 249.172879

Percentage Composition: C 72.25%; H 9.30%; N 5.62%; O 12.83%

Biological Use/Importance: Antispasmodic

Boiling Point: Bp_{0.3} 180°

Calculated Log P Data: Log P 3.95 (calc)

Other Data: Component of Ambridin (as hydrochloride)

Hazard & Toxicity: LD₅₀ (mus, orl) 2500 mg/kg (hydrochloride)

>>Derivative: Chloride

CAS Registry Number: 40350-93-4

Molecular Formula: C₈H₈ClNO

Molecular Weight: 169.61

Accurate Mass: 169.029441

Percentage Composition: C 56.65%; H 4.75%; Cl 20.90%; N 8.26%; O 9.43%

Physical Description: Cryst. (as hydrochloride)

Other Data: CAS no. refers to hydrochloride

>>Derivative: Nitrile

CAS Registry Number: 41804-94-8

Molecular Formula: C₈H₈N₄

Molecular Weight: 160.178

Accurate Mass: 160.074896

Percentage Composition: C 59.99%; H 5.03%; N 34.98%

Physical Description: Leaflets (petrol)

Melting Point: Mp 55°

pKa Value: pK_a 4.4 (20°)

>>Derivative: Nitrile; hydrochloride

CAS Registry Number: 53941-45-0

Physical Description: Needles

Melting Point: Mp 175-176°

Fluka: 78584