>>**Derivative:** Et ester

**CAS Registry Number:** 6152-27-8
**Molecular Formula:** $C_{10}H_{13}NO_2$
**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°. $Bp_{16}$ 149°. $Bp_5$ 114-115°

>>**Derivative:** 3-Methylbutyl ester
**Synonym(s): Phenamacide.** Aklonin

**CAS Registry Number:** 31031-74-0

**Molecular Formula:** $C_{13}H_{19}NO_2$
**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:** $C_{15}H_{23}NO_2$
**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:** $LD_{50}$ (mus, orl) 2500 mg/kg (hydrochloride)

>>**Derivative:** Chloride

**CAS Registry Number:** 40350-93-4
**Molecular Formula:** $C_8H_8ClNO$
**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:** $C_8H_8N_4$
**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:** p$K_a$ 4.4 (20°)

>>**Derivative:** Nitrile; hydrochloride

**CAS Registry Number:** 53941-45-0
**Physical Description:** Needles
**Melting Point:** Mp 175-176°
**Fluka:** 78584