



CAS Registry Number: 2812-46-6
Molecular Formula: $C_9H_{17}NO_2$
Molecular Weight: 171.239
Accurate Mass: 171.125929
Percentage Composition: C 63.13%; H 10.01%; N 8.18%; O 18.69%
Physical Description: Oil
Boiling Point: $Bp_{1.5} 57^\circ$
Optical Rotation: $[\alpha]_D^{24} -40.5$ (c, 0.4 in MeOH)
Density: $d_4^{20} 0.971$
Refractive Index: $n_D^{20} 1.4421$

>>Derivative: *tert*-Butyl ester; hydrochloride

CAS Registry Number: 5497-76-7
Physical Description: Prisms (Me_2CO/Et_2O or $MeOH/Et_2O$)
Melting Point: Mp 108-111°
Optical Rotation: $[\alpha]_D^{25} -27$ (c, 1.036 in MeOH)

>>Derivative: Benzyl ester

Extra CAS Registry Numbers(s): 16652-71-4 41324-66-7
Molecular Formula: $C_{12}H_{15}NO_2$
Molecular Weight: 205.256
Accurate Mass: 205.110279
Percentage Composition: C 70.22%; H 7.37%; N 6.82%; O 15.59%
Physical Description: Cryst. ($EtOH$) (as hydrochloride)
Melting Point: Mp 148-149° (hydrochloride)
Optical Rotation: $[\alpha]_D^{25} -43.3$ (c, 1 in MeOH)
Other: PB P24940

>>Derivative: Amide

CAS Registry Number: 7531-52-4
Molecular Formula: $C_5H_{10}N_2O$
Molecular Weight: 114.147
Percentage Composition: C 52.61%; H 8.83%; N 24.54%; O 14.02%
Physical Description: Needles
Melting Point: Mp 104° (100-102°)
Optical Rotation: $[\alpha]_D^{23} -106.9$ (c, 0.9 in $EtOH$)
Aldrich: 28705-9
Fluka: 81722
Sigma: P7517

>>Derivative: Amide, hydrochloride

CAS Registry Number: 42429-27-6
Melting Point: Mp 179-181°
Other: Degussa

>>Derivative: Anilide

Molecular Formula: $C_{11}H_{14}N_2O$
Molecular Weight: 190.244
Accurate Mass: 190.110613
Percentage Composition: C 69.45%; H 7.42%; N 14.72%; O 8.41%
Physical Description: Fibrous needles (cyclohexane)
Optical Rotation: $[\alpha]_D^{20} -71.4$ (c, 1.0 in $EtOH$)

>>Derivative: Anhydride

Molecular Formula: $C_{10}H_{16}N_2O_3$
Molecular Weight: 212.248
Accurate Mass: 212.116093
Percentage Composition: C 56.59%; H 7.60%; N 13.20%; O 22.61%
Melting Point: Mp 149°
Optical Rotation: $[\alpha]_D^{19} -147.2$