Molecular Formula: $C_7H_{11}NO_3$
Molecular Weight: 157.169
Accurate Mass: 157.073894
Percentage Composition: C 53.49%; H 7.05%; N 8.91%; O 30.54%
Physical Description: Cryst.
Melting Point: Mp 118°
Optical Rotation: $[\alpha]_D^{23}$ –115 (c, 2 in H_2O)
Sigma: A0783

>>**Derivative:** *N*-Ac, Me ester

CAS Registry Number: 27460-51-1
Molecular Formula: $C_8H_{13}NO_3$
Molecular Weight: 171.196
Accurate Mass: 171.089544
Percentage Composition: C 56.13%; H 7.65%; N 8.18%; O 28.04%
Physical Description: Liq.
Boiling Point: $Bp_{0.2}$ 100-104°
Optical Rotation: $[\alpha]_D^{20}$ –105.9 (c, 1.6 in MeOH)

>>**Derivative:** *N*-*tert*-Butyloxycarbonyl

>>**Derivative:** *N*-Benzoyl

CAS Registry Number: 5874-58-8
Molecular Formula: $C_{12}H_{13}NO_3$
Molecular Weight: 219.24
Accurate Mass: 219.089544
Percentage Composition: C 65.74%; H 5.98%; N 6.39%; O 21.89%
Physical Description: Cryst. (hexane/2-propanol)
Melting Point: Mp 158-159° (153-157°)
Optical Rotation: $[\alpha]_D^{21}$ –99 (c, 1.0 in EtOH)

>>**Derivative:** *N*-(4-Methylbenzenesulfonyl)

CAS Registry Number: 51077-01-1
Molecular Formula: $C_{12}H_{15}NO_4S$
Molecular Weight: 269.321
Accurate Mass: 269.072179
Percentage Composition: C 53.52%; H 5.61%; N 5.20%; O 23.76%; S 11.91%
Melting Point: Mp 130-133°

>>**Derivative:** *N*-Me

>>**Derivative:** *N*-(2,4-Dinitrophenyl)

CAS Registry Number: 1655-55-6
Molecular Formula: $C_{11}H_{11}N_3O_6$
Molecular Weight: 281.224
Accurate Mass: 281.064787
Percentage Composition: C 46.98%; H 3.94%; N 14.94%; O 34.14%
Melting Point: Mp 137°
Sigma: D1505

>>**Derivative:** *N*-Nitroso

CAS Registry Number: 7519-36-0
Molecular Formula: $C_5H_8N_2O_3$
Molecular Weight: 144.13
Accurate Mass: 144.053493
Percentage Composition: C 41.67%; H 5.59%; N 19.44%; O 33.30%
Use/Importance: Used as a non-invasive marker for endogenous *N*-nitrosamine synthesis