



CAS Registry Number: 104324-18-7
Molecular Formula: C₁₃H₁₂N₂O₃S
Molecular Weight: 276.315
Accurate Mass: 276.056863
Percentage Composition: C 56.51%; H 4.38%; N 10.14%; O 17.37%; S 11.60%
Use/Importance: Used in synth. of chiral glycines
Melting Point: Mp 101°
Optical Rotation: [α]_D²⁰+92.3 (c, 1.3 in CH₂Cl₂)

>>**Derivative:** *N*-Propanoyl

CAS Registry Number: 101711-78-8
Molecular Formula: C₁₃H₁₅NO₃
Molecular Weight: 233.266
Accurate Mass: 233.105194
Percentage Composition: C 66.94%; H 6.48%; N 6.00%; O 20.58%
Melting Point: Mp 45-47°
Optical Rotation: [α]_D²²+99 (c, 1 in EtOH)

>>**Derivative:** *N*-(2*E*-Butenoyl)

CAS Registry Number: 90719-30-5
Molecular Formula: C₁₄H₁₅NO₃
Molecular Weight: 245.277
Accurate Mass: 245.105194
Percentage Composition: C 68.56%; H 6.16%; N 5.71%; O 19.57%
Melting Point: Mp 85-86°
Optical Rotation: [α]_D²⁵+77.9 (c, 2 in CHCl₃)

>>**Variant:** (±)-form

CAS Registry Number: 120574-96-1
Molecular Formula: C₁₀H₁₁NO₂
Molecular Weight: 177.202
Accurate Mass: 177.078979
Percentage Composition: C 67.78%; H 6.26%; N 7.90%; O 18.06%
Melting Point: Mp 66°

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 1431A; 1431B, (*nmr*)
Evans, D.A., *Aldrichimica Acta*, 1982, **15**, 23, (*rev*)
Evans, D.A. *et al.*, *J.A.C.S.*, 1986, **108**, 6757; 1988, **110**, 1238; 1990, **112**, 8215, (*S*-form, synth, pmr, cmr, ir, derivs, use)
Rein, K. *et al.*, *J.A.C.S.*, 1989, **111**, 2211, (*synth*)
Pridgen, L.N. *et al.*, *J.O.C.*, 1989, **54**, 3231, (*synth*, hplc)
Dharanipragada, R. *et al.*, *Tet. Lett.*, 1989, **30**, 6841, (*use*, derivs)
Org. Synth., 1990, **68**, 77, (*synth*, ir, pmr)
Greene, A.E. *et al.*, *Synth. Commun.*, 1991, **21**, 1, (*synth*)
McKillop, A. *et al.*, *Synth. Commun.*, 1995, **25**, 561, (*synth*)
Taraov, V.I. *et al.*, *J.C.S. Perkin 1*, 1997, 3101-3106, (*synth*, pmr)
Jones, G.B. *et al.*, *J.O.C.*, 1998, **63**, 2928-2938, (*synth*)
Brimble, M.A. *et al.*, *J.C.S. Perkin 1*, 2000, 697-709, (*R*-form, synth)