



CAS Registry Number: 188447-91-8
Molecular Formula: C₇H₉NOS
Molecular Weight: 155.22
Accurate Mass: 155.040484
Percentage Composition: C 54.17%; H 5.84%; N 9.02%; O 10.31%; S 20.66%
Physical Description: Solid
Melting Point: Mp 110-112°
Optical Rotation: [α]_D²⁰ +79.7 (c, 1.2 in CHCl₃)

>>Variant: (±)-form

Molecular Formula: C₇H₈O₂S
Molecular Weight: 156.205
Accurate Mass: 156.0245
Percentage Composition: C 53.82%; H 5.16%; O 20.49%; S 20.53%

>>Derivative: Chloride

CAS Registry Number: 10439-23-3
Molecular Formula: C₇H₇ClOS
Molecular Weight: 174.65
Accurate Mass: 173.990612
Percentage Composition: C 48.14%; H 4.04%; Cl 20.30%; O 9.16%; S 18.36%
Physical Description: Needles
Melting Point: Mp 54-58°
Boiling Point: Bp₄ 115°

>>Derivative: Amide

CAS Registry Number: 6873-55-8
Molecular Formula: C₇H₉NOS
Molecular Weight: 155.22
Percentage Composition: C 54.17%; H 5.84%; N 9.02%; O 10.31%; S 20.66%
Physical Description: Needles
Melting Point: Mp 120°

References:

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Douglass, I.B., *J.O.C.*, 1965, **30**, 633, (*esters*)
Kobayashi, M. *et al.*, *Bull. Chem. Soc. Jpn.*, 1966, **39**, 1788, (*uv*)
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Evans, D.A. *et al.*, *J.A.C.S.*, 1992, **114**, 5977-5985, (*S-form, Me ester*)
Davis, F.A. *et al.*, *J.O.C.*, 1997, **62**, 2555-2563, (*amide, synth, pmr, cmr*)
Schwan, A.L. *et al.*, *Eur. J. Org. Chem.*, 2001, 1643-1654, (*chloride*)