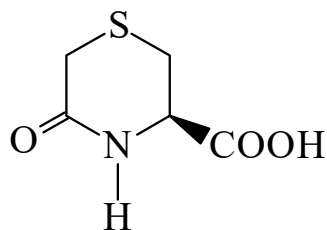




>>Entry Name: 5-Oxo-3-thiomorpholinecarboxylic acid, 9CI



CAS Registry Number: 14226-97-2

Related CAS Registry Numbers(s): 88620-38-6

Molecular Formula: C₅H₇NO₃S

Molecular Weight: 161.181

Accurate Mass: 161.014664

Percentage Composition: C 37.26%; H 4.38%; N 8.69%; O 29.78%; S 19.89%

>>Variant: (R)-form

CAS Registry Number: 62305-89-9

Molecular Formula: C₅H₇NO₃S

Molecular Weight: 161.181

Accurate Mass: 161.014664

Percentage Composition: C 37.26%; H 4.38%; N 8.69%; O 29.78%; S 19.89%

Physical Description: Oil

>>Derivative: Me ester

CAS Registry Number: 118903-82-5

Molecular Formula: C₆H₉NO₃S

Molecular Weight: 175.208

Accurate Mass: 175.030314

Percentage Composition: C 41.13%; H 5.18%; N 7.99%; O 27.39%; S 18.30%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 70-71°

Optical Rotation: [α]_D -4 (c, 1.0 in CHCl₃)

>>Derivative: S-Oxide

CAS Registry Number: 87862-95-1

Molecular Formula: C₅H₇NO₄S

Molecular Weight: 177.181

Accurate Mass: 177.009579

Percentage Composition: C 33.89%; H 3.98%; N 7.91%; O 36.12%; S 18.10%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 160-163 dec.°

References:

Levenson, C. *et al.*, *J. Med. Chem.*, 1984, **27**, 228, (*synth, oxide*)

Zanotti, G. *et al.*, *J.C.S. Perkin 1*, 1988, 2647, (*synth, ir, pmr*)