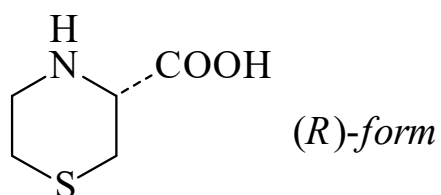




>>Entry Name: 3-Thiomorpholinecarboxylic acid, 9Cl

Synonym(s): Tetrahydro-2*H*-1,4-thiazine-3-carboxylic acid. 1,4-Thiazane-3-carboxylic acid. Deoxychondrine. Chordarine. Perhydro-1,4-thiazine-3-carboxylic acid



CAS Registry Number: 20960-92-3

Molecular Formula: C₅H₉NO₂S

Molecular Weight: 147.198

Accurate Mass: 147.035399

Percentage Composition: C 40.80%; H 6.16%; N 9.52%; O 21.74%; S 21.78%

>>Variant: (*R*)-form

Synonym(s): L-form

CAS Registry Number: 65527-54-0

Molecular Formula: C₅H₉NO₂S

Molecular Weight: 147.198

Accurate Mass: 147.035399

Percentage Composition: C 40.80%; H 6.16%; N 9.52%; O 21.74%; S 21.78%

Biological Source: Isol. from *Heterochordaria abietina*

Physical Description: Tiny needles (Me₂CO aq.)

Melting Point: Mp 270-271 dec.° (sealed tube)

Optical Rotation: $[\alpha]_{\text{D}}^{25} -54.03$ (c, 1.6 in H₂O)

>>Derivative: S-Oxide

>>Derivative: S,S-Dioxide

Molecular Formula: C₅H₉NO₄S

Molecular Weight: 179.196

Accurate Mass: 179.025229

Percentage Composition: C 33.51%; H 5.06%; N 7.82%; O 35.71%; S 17.89%

Physical Description: Cryst.

Melting Point: Mp 268-269°

Optical Rotation: $[\alpha]_{\text{D}}^{40} -3.4$ (c, 0.005 in CHCl₃)

>>Variant: (±)-form

Molecular Formula: C₅H₉NO₂S

Molecular Weight: 147.198

Accurate Mass: 147.035399

Percentage Composition: C 40.80%; H 6.16%; N 9.52%; O 21.74%; S 21.78%

Physical Description: Cryst. (EtOH aq.), prisms (Me₂CO aq.)

Melting Point: Mp 263-265° (sealed tube)

References:

Tominaga, F. *et al.*, *J. Biochem. (Tokyo)*, 1963, **54**, 222

Carson, J.F. *et al.*, *J.O.C.*, 1964, **29**, 2203, (*synth, bibl*)

Kogami, Y. *et al.*, *Bull. Chem. Soc. Jpn.*, 1987, **60**, 2963, (*synth*)

Larsson, U. *et al.*, *Acta Chem. Scand.*, 1994, **48**, 517, (*dioxide*)