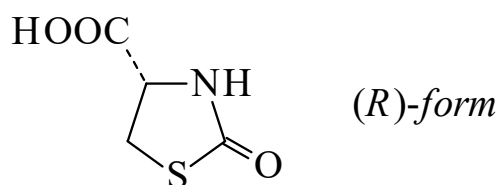




>>Entry Name: 2-Oxo-4-thiazolidinecarboxylic acid, 9CI



CAS Registry Number: 19750-45-9

Related CAS Registry Numbers(s): 77273-78-0

Molecular Formula: C₄H₅NO₃S

Molecular Weight: 147.154

Accurate Mass: 146.999014

Percentage Composition: C 32.65%; H 3.42%; N 9.52%; O 32.62%; S 21.79%

>>Variant: (R)-form

Synonym(s): L-form

CAS Registry Number: 19771-63-2

Molecular Formula: C₄H₅NO₃S

Molecular Weight: 147.154

Accurate Mass: 146.999014

Percentage Composition: C 32.65%; H 3.42%; N 9.52%; O 32.62%; S 21.79%

Use/Importance: Substrate of 5-oxoprolinase; useful in enzyme studies and functions in an intracellular delivery system for L-cysteine

Physical Description: Cubes (H₂O)

Melting Point: Mp 173-174° (171-173° dec.)

Optical Rotation: [α]_D -59.4 (c, 2 in H₂O)

Solubility: Insol. C₆H₆, EtOAc

pKa Value: pK_a 3.32 (22°)

Aldrich: 30202-3

Fluka: 75951

Sigma: O6254

>>Derivative: Dicyclohexylamine salt

Physical Description: Needles (EtOH/petrol)

Melting Point: Mp 199 dec.°

>>Derivative: S-Benzylisothiuronium salt

Physical Description: Needles (H₂O)

Melting Point: Mp 131.5 dec.°

>>Derivative: Et ester

CAS Registry Number: 98155-24-9

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: Oil

Optical Rotation: [α]_D²⁰ -42 (c, 2 in CHCl₃)

Aldrich: 38095-4

>>Derivative: N-Ac

Molecular Formula: C₆H₇NO₄S

Molecular Weight: 189.192

Accurate Mass: 189.009579

Percentage Composition: C 38.09%; H 3.73%; N 7.40%; O 33.83%; S 16.95%

Physical Description: Cryst. (EtOAc/petrol)

Melting Point: Mp 152-154°

Optical Rotation: [α]_D -136.4 (c, 1.8 in Me₂CO aq.)