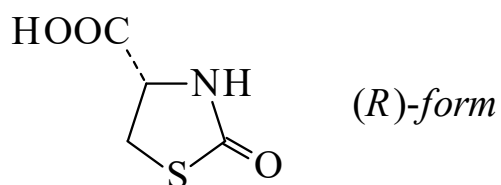




>>Entry Name: 2-Oxo-4-thiazolidinecarboxylic acid, 9CI



**CAS Registry Number:** 19750-45-9

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

**Molecular Formula:** C<sub>4</sub>H<sub>5</sub>NO<sub>3</sub>S

**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:** C<sub>4</sub>H<sub>5</sub>NO<sub>3</sub>S

**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 (H<sub>2</sub>O)

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

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub> -59.4 (c, 2 in H<sub>2</sub>O)

**Solubility:** Insol. C<sub>6</sub>H<sub>6</sub>, EtOAc

**pKa Value:** pK<sub>a</sub> 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 (H<sub>2</sub>O)

**Melting Point:** Mp 131.5 dec.°

>>Derivative: Et ester

**CAS Registry Number:** 98155-24-9

**Molecular Formula:** C<sub>6</sub>H<sub>9</sub>NO<sub>3</sub>S

**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:** [ $\alpha$ ]<sub>D</sub><sup>20</sup> -42 (c, 2 in CHCl<sub>3</sub>)

**Aldrich:** 38095-4

>>Derivative: N-Ac

**Molecular Formula:** C<sub>6</sub>H<sub>7</sub>NO<sub>4</sub>S

**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:** [ $\alpha$ ]<sub>D</sub> -136.4 (c, 1.8 in Me<sub>2</sub>CO aq.)