



>>Entry Name: Tetrahydro-2-thiophenecarboxylic acid, 9CI

Synonym(s): 2-Thiolanecarboxylic acid



CAS Registry Number: 19418-11-2

Related CAS Registry Numbers(s): 63521-95-9 112212-94-9 112212-95-0

Molecular Formula: C₅H₈O₂S

Molecular Weight: 132.183

Accurate Mass: 132.0245

Percentage Composition: C 45.43%; H 6.10%; O 24.21%; S 24.26%

>>Variant: (R)-form

CAS Registry Number: 17570-08-0

Molecular Formula: C₅H₈O₂S

Molecular Weight: 132.183

Accurate Mass: 132.0245

Percentage Composition: C 45.43%; H 6.10%; O 24.21%; S 24.26%

Optical Rotation: $[\alpha]_{\text{D}}^{20} -14.2$ (c, 13 in EtOH)

>>Variant: (S)-form

CAS Registry Number: 63358-63-4

Molecular Formula: C₅H₈O₂S

Molecular Weight: 132.183

Accurate Mass: 132.0245

Percentage Composition: C 45.43%; H 6.10%; O 24.21%; S 24.26%

Optical Rotation: $[\alpha]_{\text{D}} +98$ (c, 2.48 in EtOH)

pKa Value: pK_a 3.94

>>Variant: (±)-form

CAS Registry Number: 105499-35-2

Molecular Formula: C₅H₈O₂S

Molecular Weight: 132.183

Accurate Mass: 132.0245

Percentage Composition: C 45.43%; H 6.10%; O 24.21%; S 24.26%

Physical Description: Plates (H₂O)

Melting Point: Mp 51°

Boiling Point: Bp_{0.4} 110-112°

Solubility: V. sol. H₂O, EtOH; spar. sol. Et₂O

Other Data: Steam-volatile

>>Derivative: Me ester

Molecular Formula: C₆H₁₀O₂S

Molecular Weight: 146.21

Accurate Mass: 146.04015

Percentage Composition: C 49.29%; H 6.89%; O 21.89%; S 21.93%

Boiling Point: Bp 206°

>>Derivative: Et ester

CAS Registry Number: 18342-42-2

Molecular Formula: C₇H₁₂O₂S

Molecular Weight: 160.237

Accurate Mass: 160.0558

Percentage Composition: C 52.47%; H 7.55%; O 19.97%; S 20.01%

Boiling Point: Bp₁₁ 102.5-104°