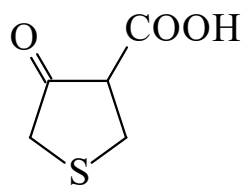




>>Entry Name: Tetrahydro-4-oxo-3-thiophenecarboxylic acid, 9CI



CAS Registry Number: 126856-34-6

Related CAS Registry Numbers(s): 78647-31-1 99328-39-9

Molecular Formula: C₅H₆O₃S

Molecular Weight: 146.167

Accurate Mass: 146.003765

Percentage Composition: C 41.09%; H 4.14%; O 32.84%; S 21.94%

>>Variant: (±)-form

CAS Registry Number: 161404-78-0

Molecular Formula: C₅H₆O₃S

Molecular Weight: 146.167

Accurate Mass: 146.003765

Percentage Composition: C 41.09%; H 4.14%; O 32.84%; S 21.94%

>>Derivative: Me ester

CAS Registry Number: 99328-39-9

Extra CAS Registry Numbers(s): 2689-68-1

Molecular Formula: C₆H₈O₃S

Molecular Weight: 160.193

Accurate Mass: 160.019415

Percentage Composition: C 44.99%; H 5.03%; O 29.96%; S 20.02%

Physical Description: Cubes (petrol)

Melting Point: Mp 36-38°

>>Derivative: Et ester

CAS Registry Number: 78647-31-1

Molecular Formula: C₇H₁₀O₃S

Molecular Weight: 174.22

Accurate Mass: 174.035065

Percentage Composition: C 48.26%; H 5.79%; O 27.55%; S 18.41%

Physical Description: Liq.

Boiling Point: Bp₉ 116-117°

References:

Woodward, R.B. *et al.*, *J.A.C.S.*, 1946, **68**, 2229-2235, (*Me ester*)

Duus, F. *et al.*, *Tetrahedron*, 1981, **37**, 2633-2640, (*Et ester*)

Tomé, A.C. *et al.*, *Tetrahedron*, 1996, **52**, 1723-1734, (*Me ester, synth, pmr*)

White, L.A. *et al.*, *Tetrahedron*, 1996, **52**, 3117-3134, (*Me ester, use*)