



>>Entry Name: α -Oxo-2-thiopheneacetic acid

Synonym(s): 2-Thienylglyoxylic acid. 2-Thiopheneglyoxylic acid



CAS Registry Number: 4075-59-6

Molecular Formula: C₆H₄O₃S

Molecular Weight: 156.162

Accurate Mass: 155.988115

Percentage Composition: C 46.15%; H 2.58%; O 30.74%; S 20.53%

Melting Point: Mp 58-59° (+ 1H₂O). Mp 91.5° (anhyd.)

Solubility: V. sol. H₂O

Other Data: Heat → 2-Thiophenecarboxaldehyde [BMN04-F](#)

Aldrich: 22227-5

>>Derivative: Me ester

CAS Registry Number: 26878-13-7

Molecular Formula: C₇H₆O₃S

Molecular Weight: 170.189

Accurate Mass: 170.003765

Percentage Composition: C 49.40%; H 3.55%; O 28.20%; S 18.84%

Melting Point: Mp 28.5°

>>Derivative: Me ester, oxime

Molecular Formula: C₇H₇NO₃S

Molecular Weight: 185.203

Accurate Mass: 185.014664

Percentage Composition: C 45.40%; H 3.81%; N 7.56%; O 25.92%; S 17.31%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 104-105° (softens at 97°)

>>Derivative: Et ester

CAS Registry Number: 4075-58-5

Molecular Formula: C₈H₈O₃S

Molecular Weight: 184.215

Accurate Mass: 184.019415

Percentage Composition: C 52.16%; H 4.38%; O 26.06%; S 17.41%

Physical Description: Oil

Boiling Point: Bp_{0.8} 102-110°

Rare Chemicals Library: S46221-7

Sigma: E5633

Other: Oakwood 3725

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 602D, (*ir*)

Blicke, F.F. *et al.*, *J.A.C.S.*, 1944, **66**, 1645, (*synth*)

Micetich, R.G., *Org. Prep. Proced. Int.*, 1970, **2**, 249; 1971, **3**, 167, (*esters*)