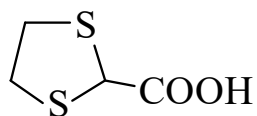




>>Entry Name: 1,3-Dithiolane-2-carboxylic acid, 9CI



Related CAS Registry Numbers(s): 5616-65-9

Molecular Formula: C₄H₆O₂S₂

Molecular Weight: 150.222

Accurate Mass: 149.98092

Percentage Composition: C 31.98%; H 4.03%; O 21.30%; S 42.69%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 91-92°

Boiling Point: Bp₂ 96-96.4°

pKa Value: pK_a 4.46 (50% EtOH aq.)

>>Derivative: Et ester

Synonym(s): Ethyl glyoxylate ethylene thioacetal

CAS Registry Number: 20461-99-8

Molecular Formula: C₆H₁₀O₂S₂

Molecular Weight: 178.276

Accurate Mass: 178.01222

Percentage Composition: C 40.42%; H 5.65%; O 17.95%; S 35.97%

Use/Importance: Forms carbonyl anion equivalent with strong bases

Boiling Point: Bp₂ 96-96.4°

Aldrich: 22630-0

Fluka: 43798

>>Derivative: Et ester, S¹,S¹,S³,S³-tetraoxide

Molecular Formula: C₆H₁₀O₆S₂

Molecular Weight: 242.273

Accurate Mass: 241.99188

Percentage Composition: C 29.75%; H 4.16%; O 39.62%; S 26.47%

Melting Point: Mp 90-91°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 676B, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1094B, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 739C, (*ir*)

Breslow, R. *et al.*, *J.A.C.S.*, 1961, **83**, 4100-4101, (*Et ester, oxide, synth*)

Minamida, I. *et al.*, *Tetrahedron*, 1968, **24**, 5293-5309, (*synth*)

Herrmann, J.L. *et al.*, *Tet. Lett.*, 1973, 2599-2602, (*synth, use*)

Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1975, **5**, 304, (*synth, use*)

Lissel, M., *Annalen*, 1982, 1589-1601, (*Et ester, synth, ir, pmr, ms*)