



>>Entry Name: **2,2'-Dithiobisacetic acid**, 9CI

Synonym(s): Dithiodiacetic acid, 8CI. Dithiodiglycollic acid. Disulfidoacetic acid

CAS Registry Number: 505-73-7

HOOCCH₂SSCH₂COOH

Molecular Formula: C₄H₆O₄S₂

Molecular Weight: 182.221

Accurate Mass: 181.97075

Percentage Composition: C 26.37%; H 3.32%; O 35.12%; S 35.19%

Physical Description: Leaflets (C₆H₆/EtOAc)

Melting Point: Mp 108-109°

Solubility: Sol. H₂O, EtOH, Et₂O

pKa Value: pK_{a1} 3.19; pK_{a2} 4.28 (25°, H₂O)

Sigma: D5392

>>Derivative: Mono-Et ester

CAS Registry Number: 1665-63-0

Molecular Formula: C₆H₁₀O₄S₂

Molecular Weight: 210.275

Accurate Mass: 210.00205

Percentage Composition: C 34.27%; H 4.79%; O 30.44%; S 30.50%

Physical Description: Oil

Other Data: Suscept. to rearr. to diacid and diester

>>Derivative: Di-Me ester

CAS Registry Number: 1665-64-1

Molecular Formula: C₆H₁₀O₄S₂

Molecular Weight: 210.275

Accurate Mass: 210.00205

Percentage Composition: C 34.27%; H 4.79%; O 30.44%; S 30.50%

Physical Description: Liq.

Boiling Point: Bp₁₆ 154°

Density: d₄²⁶ 1.29

>>Derivative: Diamide

CAS Registry Number: 64057-55-2

Molecular Formula: C₄H₈N₂O₂S₂

Molecular Weight: 180.251

Accurate Mass: 180.002718

Percentage Composition: C 26.65%; H 4.47%; N 15.54%; O 17.75%; S 35.58%

Melting Point: Mp 157°

References:

Stoner, G.G. *et al.*, *J.A.C.S.*, 1941, **63**, 987, (*synth*)

Owen, T.C. *et al.*, *J.O.C.*, 1973, **38**, 937, (*synth, pmr*)

Eberlein, G.A. *et al.*, *J.A.C.S.*, 1984, **106**, 3309, (*deriv, synth, pmr*)

Nash, C.P. *et al.*, *J.A.C.S.*, 1985, **107**, 7194, (*struct*)