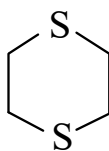




>>Entry Name: 1,4-Dithiane, 9CI

ENTRY UNDER REVIEW

Synonym(s): *p*-Dithiane, 8CI. Tetrahydro-1,4-dithiin



CAS Registry Number: 505-29-3

Related CAS Registry Numbers(s): 10348-97-7 57983-04-7

Type of Compound Code(s): PA2300

Molecular Formula: C₄H₈S₂

Molecular Weight: 120.239

Accurate Mass: 120.00674

Percentage Composition: C 39.96%; H 6.71%; S 53.34%

Use/Importance: Gives colour reaction with HgCl₂

Physical Description: Monoclinic prisms

Melting Point: Mp 112-113°

Boiling Point: Bp 199-200°

Solubility: Sol. EtOH, Et₂O, Me₂CO, AcOH; spar. sol. H₂O

Other Data: Subl. at r.t., volatile in steam and EtOH

Aldrich: D21770-0

>>Derivative: S-Oxide

Molecular Formula: C₄H₈OS₂

Molecular Weight: 136.239

Accurate Mass: 136.001655

Percentage Composition: C 35.26%; H 5.92%; O 11.74%; S 47.07%

Melting Point: Mp 125.5-127°

>>Derivative: S¹,S¹-Dioxide

Molecular Formula: C₄H₈O₂S₂

Molecular Weight: 152.238

Accurate Mass: 151.99657

Percentage Composition: C 31.56%; H 5.30%; O 21.02%; S 42.13%

Melting Point: Mp 200°

>>Derivative: *trans*-S¹,S⁴-Dioxide

CAS Registry Number: 10348-98-8

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 261-262 dec.°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 435C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 271D, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 357A, (*ir*)

Org. Synth., Coll. Vol., 4, 1963, 396, (*synth*)

Hunter, G. *et al.*, *J.C.S. Perkin 2*, 1978, 712, (*pmr*)

Sandell, E.A. *et al.*, *Photometric Determination of Traces of Metals*, Wiley, New York, 1978, (*use*)

Juaristi, E. *et al.*, *Tetrahedron*, 1984, **40**, 1477, (*S*-oxide, *synth*, *cmr*)

Fujihara, H. *et al.*, *Bull. Chem. Soc. Jpn.*, 1987, **60**, 4451, (*S*-oxide, *synth*, *ir*, *pmr*)

Fujihara, H. *et al.*, *J.O.C.*, 1987, **52**, 4254, (*sulfoxide*, *synth*, *ir*)

Clennan, E.J. *et al.*, *J.A.C.S.*, 1992, **114**, 3021, (*dioxide*, *synth*, *pmr*)