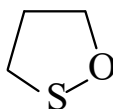




>>Entry Name: 1,2-Oxathiolane, 9CI



Related CAS Registry Numbers(s): 5684-29-7

Molecular Formula: C₃H₆OS

Molecular Weight: 90.146

Accurate Mass: 90.013935

Percentage Composition: C 39.97%; H 6.71%; O 17.75%; S 35.57%

Physical Description: Unstable, waxy solid

>>Derivative: S-Oxide, (±)

Synonym(s): 1,2-Oxathiolane-1,1-dioxide. 1,3-Propanesulfine

CAS Registry Number: 24308-28-9

Molecular Formula: C₃H₆O₂S

Molecular Weight: 106.145

Accurate Mass: 106.00885

Percentage Composition: C 33.95%; H 5.70%; O 30.15%; S 30.21%

Physical Description: Liq.

Boiling Point: Bp_{0.2} 48-49°

>>Derivative: S,S-Dioxide

Synonym(s): 1,2-Oxathiolane 2,2-dioxide, 9CI. 1,3-Propane sultone. 3-Hydroxy-1-propanesulfonic acid γ-sultone

CAS Registry Number: 1120-71-4

Molecular Formula: C₃H₆O₃S

Molecular Weight: 122.145

Accurate Mass: 122.003765

Percentage Composition: C 29.50%; H 4.95%; O 39.30%; S 26.25%

Physical Description: Prisms

Melting Point: Mp 31°

Boiling Point: Bp₁₄ 155-157°. Bp₁ 96°

Hazard & Toxicity: Suspected human brain carcinogen. Skin irritant. LD₅₀ (rat, scu) 135 mg/kg. Exp. carcinogen and teratogen

Aldrich: 29125-0

Fluka: 81815

Sigma: P8643

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 899D, (ir)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1444C, (nmr)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 834D, (ir)
Smith, C.W. *et al.*, *J.A.C.S.*, 1953, **75**, 748, (dioxide, synth)
Helberger, J.H., *Annalen*, 1954, **588**, 71, (dioxide, synth)
Fischer, R.F., *Ind. Eng. Chem.*, 1964, **56**, 41, (rev)
Scott, R.B. *et al.*, *J.O.C.*, 1966, **31**, 1999, (ir)
IARC Monog., 1974, **4**, 253; Suppl., **7**, 70, (rev, tox)
Kausch, M. *et al.*, *Org. Magn. Reson.*, 1977, **9**, 208, (pmr, cmr)
Davis, A.P. *et al.*, *Chem. Comm.*, 1981, 742, (synth, ir, uv, ms, pmr, cmr)
Carlsen, L. *et al.*, *Chem. Comm.*, 1981, 743, (synth, ms)
Doi, J.T. *et al.*, *J.O.C.*, 1985, **50**, 5716, (oxide, synth, ir, pmr)
King, J.F. *et al.*, *Tet. Lett.*, 1989, **30**, 2763, (oxide, synth)
Hazards in the Chemical Laboratory, 3rd edn., (ed. Bretherick, L.), Royal Society of Chemistry, 1981, 458
Luxon, S.G., *Hazards in the Chemical Laboratory, 5th edn.*, Royal Society of Chemistry, 1992, 1060
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, PML400