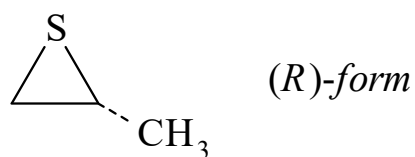




>>Entry Name: 2-Methylthiiran, 9CI

Synonym(s): Propylene sulfide. 1,2-Epithiopropene



CAS Registry Number: 1072-43-1

Molecular Formula: C<sub>3</sub>H<sub>6</sub>S

Molecular Weight: 74.146

Accurate Mass: 74.01902

Percentage Composition: C 48.60%; H 8.16%; S 43.25%

Hazard & Toxicity: LD<sub>50</sub> (rat, orl) 254 mg/kg

Aldrich: P5320-9

Fluka: 82330

>>Variant: (R)-form

CAS Registry Number: 17406-93-8

Molecular Formula: C<sub>3</sub>H<sub>6</sub>S

Molecular Weight: 74.146

Accurate Mass: 74.01902

Percentage Composition: C 48.60%; H 8.16%; S 43.25%

Optical Rotation:  $[\alpha]_{\text{D}}^{25} +32.6$  (neat)

>>Variant: (S)-form

CAS Registry Number: 16606-54-5

Molecular Formula: C<sub>3</sub>H<sub>6</sub>S

Molecular Weight: 74.146

Accurate Mass: 74.01902

Percentage Composition: C 48.60%; H 8.16%; S 43.25%

Boiling Point: Bp 74°

Optical Rotation:  $[\alpha]_{\text{D}}^{25} -50.2$  (neat)

>>Variant: (±)-form

Molecular Formula: C<sub>3</sub>H<sub>6</sub>S

Molecular Weight: 74.146

Accurate Mass: 74.01902

Percentage Composition: C 48.60%; H 8.16%; S 43.25%

Physical Description: Liq.

Boiling Point: Bp 75-77°

Solubility: Insol. H<sub>2</sub>O

Density:  $d_4^{18}$  0.946

Refractive Index:  $n_{\text{D}}^{19}$  1.4730

#### References:

*Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **1**, 433B, (nmr)

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 270A, (ir)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 354D, (ir)

Bordwell, F.G. *et al.*, *J.A.C.S.*, 1953, **75**, 4959, (synth)

*Adv. Chem. Ser.*, 1955, **15**, 438, (*props*)

Bordwell, F.G. *et al.*, *J.O.C.*, 1958, **23**, 636, (synth)

Durden, J.A. *et al.*, *J.O.C.*, 1961, **26**, 836, (synth)

Hall, L.D. *et al.*, *J.C.S.*, 1963, 5306, (synth)

Spassky, N. *et al.*, *J. Polym. Sci., Polym. Symp.*, 1975, **52**, 327, (synth)

Bucciarelli, M. *et al.*, *Tetrahedron*, 1977, **33**, 999, (synth)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, PNL750