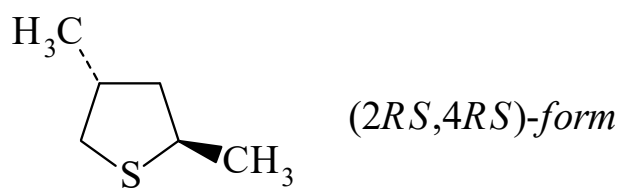




>>Entry Name: Tetrahydro-2,4-dimethylthiophene, 9Cl, 8Cl

Synonym(s): 2,4-Dimethylthiolane



CAS Registry Number: 4740-02-7

Related CAS Registry Numbers(s): 5161-79-5

Molecular Formula: C₆H₁₂S

Molecular Weight: 116.227

Accurate Mass: 116.06597

Percentage Composition: C 62.00%; H 10.41%; S 27.59%

Boiling Point: Bp 147-148°

Other Data: Stereochem. not detd.

>>Derivative: S,S-Dioxide

Synonym(s): 2,4-Dimethylsulfolane

CAS Registry Number: 1003-78-7

Molecular Formula: C₆H₁₂O₂S

Molecular Weight: 148.226

Accurate Mass: 148.0558

Percentage Composition: C 48.62%; H 8.16%; O 21.59%; S 21.63%

Use/Importance: Solvent

Physical Description: Liq.

Melting Point: Mp -3°

Boiling Point: Bp 280°. Bp₅ 123°

Density: d₄²⁰ 1.14

Other Data: Stereochem. not detd.

Hazard & Toxicity: LD₅₀ (mus, orl) 140 mg/kg

Aldrich: D18640-6

Fluka: 41630

>>Variant: (1*RS*,3*RS*)-form

Synonym(s): (±)-*trans*-form

CAS Registry Number: 5161-80-8

Molecular Formula: C₆H₁₂S

Molecular Weight: 116.227

Accurate Mass: 116.06597

Percentage Composition: C 62.00%; H 10.41%; S 27.59%

Boiling Point: Bp 149-151°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1422B, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 883B, (*ir*)

U.S. Pat., 1948, 2 451 298; *CA*, **43**, 1065, (*synth*)

U.S. Pat., 1949, 2 471 077; *CA*, **43**, 7512e, (*synth*)

Yurev, Y.K. *et al.*, *Zh. Obshch. Khim.*, 1952, **22**, 513, (*synth*)

Feairheller, E.R. *et al.*, *Spectrochim. Acta A*, 1964, **20**, 1099, (*ir*)

Barbarella, G. *et al.*, *Org. Magn. Reson.*, 1980, **13**, 282, (*synth, cmr*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, DUD400, (*dioxide*)