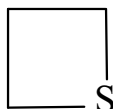




>>Entry Name: Thietane, 9CI

Synonym(s): Trimethylene sulfide, 8CI. Thiacyclobutane



CAS Registry Number: 287-27-4

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. with disagreeable odour

Melting Point: Fp -73.25°

Boiling Point: Bp<sub>752</sub> 93.8-94.2°

Density: d<sub>4</sub><sup>20</sup> 1.0228

Refractive Index: n<sub>D</sub><sup>20</sup> 1.5096

Aldrich: 18894-8

Fluka: 92458

>>Derivative: Methiodide (1:2)

Physical Description: Needles

Melting Point: Mp 98.5-99.5°

>>Derivative: S-Oxide

Synonym(s): Thietane sulfoxide. Trimethylene sulfoxide

CAS Registry Number: 13153-11-2

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

Molecular Weight: 90.146

Accurate Mass: 90.013935

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

Physical Description: Liq.

Boiling Point: Bp<sub>14</sub> 91-92°. Bp<sub>0.36</sub> 43-44°

>>Derivative: S,S-Dioxide

Synonym(s): Thietane sulfone. Trimethylene sulfone

CAS Registry Number: 5687-92-3

Molecular Formula: C<sub>3</sub>H<sub>6</sub>O<sub>2</sub>S

Molecular Weight: 106.145

Accurate Mass: 106.00885

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

Physical Description: Needles (H<sub>2</sub>O, MeOH/Et<sub>2</sub>O or Et<sub>2</sub>O/petrol)

Melting Point: Mp 75.5-76°

Solubility: Sol. H<sub>2</sub>O, EtOH; spar. sol. Et<sub>2</sub>O

Rare Chemicals Library: S62073-4

#### References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **1**, 433C, (*nmr*)  
*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 270D, (*ir*)  
*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 355D, (*ir*)  
*Sadtler Standard Proton NMR Spectra*, 19046, (*pmr*)  
*Adv. Chem. Ser.*, 1955, **15**, 520, (*props*)  
Trost, B.M. *et al.*, *J.A.C.S.*, 1971, **93**, 676, (*synth*)  
d'Annibale, A. *et al.*, *J.C.S. Perkin 2*, 1973, 1908, (*conformn*)  
Scala, A.A. *et al.*, *J. Het. Chem.*, 1978, **15**, 421, (*oxide, ms*)  
Fronza, G. *et al.*, *J. Magn. Reson.*, 1979, **36**, 343, (*oxide, pmr*)  
Nagasawa, K. *et al.*, *Chem. Pharm. Bull.*, 1982, **30**, 4189; 1985, **33**, 5048, (*synth, cmr*)  
Lancaster, M. *et al.*, *Synthesis*, 1982, 582, (*synth*)  
Chadha, V.K. *et al.*, *J. Med. Chem.*, 1983, **26**, 916, (*oxide, synth*)  
Sedergran, T.C. *et al.*, *J.O.C.*, 1984, **49**, 2408, (*dioxide*)  
Barbarella, G. *et al.*, *J.O.C.*, 1987, **52**, 3857, (*oxide, S-33 nmr*)  
Wieser, H. *et al.*, *J. Phys. Chem.*, 1988, **92**, 6528, (*ir, Raman*)  
Tokue, I. *et al.*, *J. Chem. Phys.*, 1989, **91**, 2808, (*uv*)