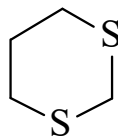




>>Entry Name: 1,3-Dithiane, 9CI

ENTRY UNDER REVIEW

Synonym(s): *m*-Dithiane, 8CI. 1,3-Dithiacyclohexane



CAS Registry Number: 505-23-7

Related CAS Registry Numbers(s): 63865-78-1

Type of Compound Code(s): WI1600 VA2950 WA4700

Molecular Formula: C₄H₈S₂

Molecular Weight: 120.239

Accurate Mass: 120.00674

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

Biological Source: Constit. of garlic and other *Allium* spp.

Use/Importance: Used in synth. as a formyl anion equivalent

Physical Description: Cryst. (MeOH)

Melting Point: Mp 54°

Other Data: Sublimes

Aldrich: 15787-2

Fluka: 43745

>>Derivative: *S*-Oxide (*R*-)

CAS Registry Number: 63865-79-2

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%

Physical Description: Pale yellow cryst. (CH₂Cl₂)

Melting Point: Mp 106-107°

Optical Rotation: [α]_D²⁰ +208.6 (c, 1.05 in EtOH) (90% ee)

>>Derivative: *S*-Oxide (±)

CAS Registry Number: 16452-25-8

Extra CAS Registry Numbers(s): 16487-10-8

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 87-88°

>>Derivative: *S*¹,*S*¹-Dioxide

CAS Registry Number: 55337-75-2

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%

Physical Description: Cryst. (CHCl₃/Et₂O)

Melting Point: Mp 139-140°

>>Derivative: *cis*-*S*¹,*S*³-Dioxide

CAS Registry Number: 55337-76-3

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%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 239-240° (215-216°)