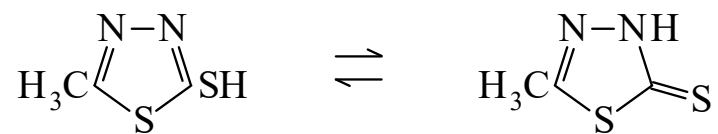




>>Entry Name: 2-Mercapto-5-methyl-1,3,4-thiadiazole

Synonym(s): 5-Methyl-1,3,4-thiadiazole-2-thiol, 8Cl. 5-Methyl-1,3,4-thiadiazole-2(3*H*)-thione, 9Cl. 2-Methyl-1,3,4-thiadiazolin-5-thione



CAS Registry Number: 29490-19-5

Molecular Formula: C₃H₄N₂S₂

Molecular Weight: 132.21

Accurate Mass: 131.981588

Percentage Composition: C 27.25%; H 3.05%; N 21.19%; S 48.51%

Use/Importance: Photofixing agent. Intermediate in prepn. of semisynthetic cephalosporin antibiotics

Physical Description: Rods (EtOH)

Melting Point: Mp 186-187°

Aldrich: 18857-3

>>Variant: *NH*-form

Molecular Formula: C₃H₄N₂S₂

Molecular Weight: 132.21

Accurate Mass: 131.981588

Percentage Composition: C 27.25%; H 3.05%; N 21.19%; S 48.51%

>>Derivative: *N*-Formyl

Molecular Formula: C₄H₄N₂OS₂

Molecular Weight: 160.22

Accurate Mass: 159.976503

Percentage Composition: C 29.99%; H 2.52%; N 17.48%; O 9.99%; S 40.03%

Use/Importance: Selective formylating reagent under mild conditions

Physical Description: Yellow cryst.

Melting Point: Mp 95-96°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 117C, (*nmr*)

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 1236D, (*ir*)

Sandström, J. *et al.*, *Acta Chem. Scand.*, 1966, **20**, 57, (*synth, uv*)

Ger. Pat., 1970, 1 963 295; *CA*, **73**, 72091, (*use*)

U.K. Pat., 1975, 1 383 292; *CA*, **83**, 43340s, (*synth*)

Yazawa, H. *et al.*, *Tet. Lett.*, 1985, **26**, 3703, (*deriv, synth, ir, pmr, uv, use*)