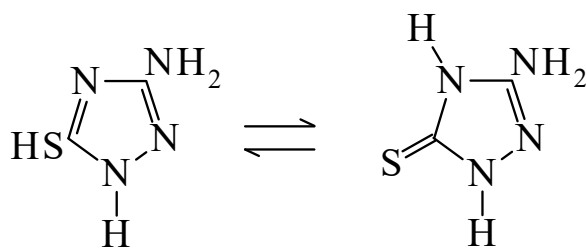




>>Entry Name: 3-Amino-5-mercapto-1*H*-1,2,4-triazole

Synonym(s): 3-Amino-1*H*-1,2,4-triazol-5-thiol, 9CI. 3-Amino-1,4-dihydro-1,2,4-triazole-4-thione



CAS Registry Number: 16691-43-3

Related CAS Registry Numbers(s): 97292-31-4 118025-46-0 118025-48-2 118025-49-3

Molecular Formula: C₂H₄N₄S

Molecular Weight: 116.146

Accurate Mass: 116.015666

Percentage Composition: C 20.68%; H 3.47%; N 48.24%; S 27.61%

General Statement: Tautomerism possible

Physical Description: Opaque prisms (EtOH aq.)

Melting Point: Mp 300-302 dec.°

Solubility: Sol. hot H₂O; insol. Et₂O, C₆H₆, Me₂CO

Aldrich: 14026-0

Fluka: 8383

>>Variant: *SH*-form

Molecular Formula: C₂H₄N₄S

Molecular Weight: 116.146

Accurate Mass: 116.015666

Percentage Composition: C 20.68%; H 3.47%; N 48.24%; S 27.61%

>>Derivative: *S*-Me

CAS Registry Number: 45534-08-5

Molecular Formula: C₃H₆N₄S

Molecular Weight: 130.173

Accurate Mass: 130.031316

Percentage Composition: C 27.68%; H 4.65%; N 43.04%; S 24.63%

Physical Description: Cryst. (MeCN)

Melting Point: Mp 139-140° (136-137°)

Aldrich: 19068-3

References:

Arndt, F. *et al.*, *Ber.*, 1927, **54**, 2089, (*synth*)

Godfrey, L.E.A. *et al.*, *J.C.S.*, 1960, 3437, (*synth, uv*)

Heitke, B.T. *et al.*, *Can. J. Chem.*, 1974, **52**, 2861, (*S*-Me, *ms*)

Heitke, B.T. *et al.*, *J.O.C.*, 1974, **39**, 1522, (*S*-Me, *synth, uv, ir, pmr*)

Reiter, J. *et al.*, *J. Het. Chem.*, 1982, **19**, 1157, (*S*-Me, *synth, ir, uv*)

Reiter, J. *et al.*, *Monatsh. Chem.*, 1988, **119**, 341, (*tautom*)

Orendt, A.H. *et al.*, *Magn. Reson. Chem.*, 1989, **27**, 1, (*S*-Me, *N-15 nmr, tautom*)