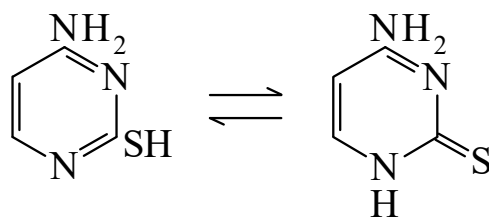




>>Entry Name: 4-Amino-2-mercaptopyrimidine

Synonym(s): 4-Amino-2(1*H*)-pyrimidinethione, 9Cl. 4-Amino-2-pyrimidinethiol, 8Cl. Thiocytosine



CAS Registry Number: 333-49-3

Related CAS Registry Numbers(s): 5807-22-7

Molecular Formula: C₄H₅N₃S

Molecular Weight: 127.17

Accurate Mass: 127.020417

Percentage Composition: C 37.78%; H 3.96%; N 33.04%; S 25.22%

General Statement: Tautomerism is possible

Physical Description: Long needles (H₂O)

Melting Point: Mp 285-290 dec.°

pKa Value: p*K*_{a1} 3.32; p*K*_{a2} 10.63 (20°, H₂O)

Aldrich: 23362-5

Fluka: 88550

Sigma: T6000

>>Variant: *NH*-form

Molecular Formula: C₄H₅N₃S

Molecular Weight: 127.17

Accurate Mass: 127.020417

Percentage Composition: C 37.78%; H 3.96%; N 33.04%; S 25.22%

>>Derivative: 1-β-D-Ribofuranosyl

Synonym(s): 2-Thiocytidine

CAS Registry Number: 13239-97-9

Molecular Formula: C₉H₁₃N₃O₄S

Molecular Weight: 259.285

Accurate Mass: 259.062677

Percentage Composition: C 41.69%; H 5.05%; N 16.21%; O 24.68%; S 12.37%

Melting Point: Mp 208-209°

References:

- Hitchings, G.H. *et al.*, *J. Biol. Chem.*, 1949, **117**, 357, (*synth*)
Russell, P.B. *et al.*, *J.A.C.S.*, 1949, **71**, 2279, (*synth*)
Brown, D.J. *et al.*, *Aust. J. Chem.*, 1965, **18**, 559, (*uv, tautom*)
Veda, T. *et al.*, *Chem. Pharm. Bull.*, 1966, **14**, 666, (*2-Thiocytidine, synth, ir, uv*)
Furberg, S. *et al.*, *Acta Cryst. B*, 1970, **26**, 1260, (*cryst struct*)
Cleve, G. *et al.*, *Chem. Ber.*, 1973, **106**, 3062, (*2-Thiocytidine, pmr, cd*)
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