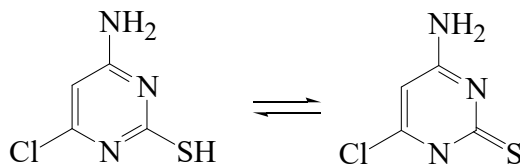




>>Entry Name: 4-Amino-6-chloro-2-mercaptopyrimidine

Synonym(s): 4-Amino-6-chloro-2(1*H*)-pyrimidinethione, 9Cl



Related CAS Registry Numbers(s): 38897-12-0 74619-77-5

Molecular Formula: C₄H₄ClN₃S

Molecular Weight: 161.614

Accurate Mass: 160.981444

Percentage Composition: C 29.73%; H 2.49%; Cl 21.94%; N 26.00%; S 19.84%

Aldrich: A4600-5

Sigma: A3273

>>Derivative: S-Me

Synonym(s): 4-Amino-6-chloro-2-(methylthio)pyrimidine. 6-Chloro-2-(methylthio)-4-pyrimidinamine, 9Cl

CAS Registry Number: 1005-38-5

Molecular Formula: C₅H₆ClN₃S

Molecular Weight: 175.641

Accurate Mass: 174.997094

Percentage Composition: C 34.19%; H 3.44%; Cl 20.18%; N 23.92%; S 18.26%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 132° (126-127°)

>>Derivative: S-Me, S-oxide

Synonym(s): 6-Chloro-2-(methylsulfinyl)-4-pyrimidinamine. 6-Amino-4-chloro-2-(methylsulfinyl)pyrimidine

CAS Registry Number: 66380-47-0

Molecular Formula: C₅H₆ClN₃OS

Molecular Weight: 191.641

Accurate Mass: 190.992009

Percentage Composition: C 31.34%; H 3.16%; Cl 18.50%; N 21.93%; O 8.35%; S 16.73%

Physical Description: Needles (MeOH)

Melting Point: Mp 255-260° (242-243°)

>>Derivative: 4-N, S-Di-Me

Molecular Formula: C₆H₈ClN₃S

Molecular Weight: 189.668

Accurate Mass: 189.012744

Percentage Composition: C 38.00%; H 4.25%; Cl 18.69%; N 22.15%; S 16.91%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 130-131°

References:

Baddiley, J., *J.C.S.*, 1944, 678, (*synth*)

Baker, B.R. *et al.*, *J.O.C.*, 1954, **19**, 631, (*synth*)

Pfleiderer, W. *et al.*, *Annalen*, 1962, **657**, 149, (*synth*)

Thompson, W.K., *J.C.S.*, 1962, 617, (*ir*)

Israel, M. *et al.*, *J. Med. Chem.*, 1964, **7**, 5, (*uv*)

Southon, I.W. *et al.*, *Chem. Ber.*, 1978, **111**, 1006, (*S-Me, S-oxide*)