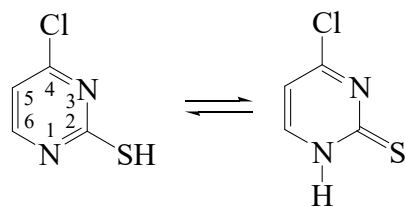




>>Entry Name: 4-Chloro-2-mercaptopyrimidine

Synonym(s): 4-Chloro-2(1*H*)-pyrimidinethione. 4-Chloro-2-pyrimidinethiol



CAS Registry Number: 63096-74-2

Molecular Formula: C₄H₃ClN₂S

Molecular Weight: 146.6

Accurate Mass: 145.970545

Percentage Composition: C 32.77%; H 2.06%; Cl 24.18%; N 19.11%; S 21.87%

>>Variant: *SH*-form

Molecular Formula: C₄H₃ClN₂S

Molecular Weight: 146.6

Accurate Mass: 145.970545

Percentage Composition: C 32.77%; H 2.06%; Cl 24.18%; N 19.11%; S 21.87%

>>Derivative: *S*-Me

Synonym(s): 4-Chloro-2-(methylthio)pyrimidine

CAS Registry Number: 49844-90-8

Molecular Formula: C₅H₅ClN₂S

Molecular Weight: 160.627

Accurate Mass: 159.986195

Percentage Composition: C 37.39%; H 3.14%; Cl 22.07%; N 17.44%; S 19.96%

Physical Description: Oil

Melting Point: Mp -2°

Boiling Point: Bp₃₆ 139-140°. Bp₁₈ 122°

Density: d 1.38

Refractive Index: n_D²⁰ 1.6000

Aldrich: 14528-9

>>Derivative: *S*-Benzyl

CAS Registry Number: 78494-41-4

Molecular Formula: C₁₁H₉ClN₂S

Molecular Weight: 236.724

Accurate Mass: 236.017495

Percentage Composition: C 55.81%; H 3.83%; Cl 14.98%; N 11.83%; S 13.55%

Physical Description: Cryst. (heptane)

Melting Point: Mp 49-50°

References:

Matsukawa, T. *et al.*, *Yakugaku Zasshi*, 1949, **69**, 491-493; *CA*, **44**, 3456d, (*S*-Me)

Koppel, H.C. *et al.*, *J.O.C.*, 1962, **27**, 181-185, (*S*-benzyl)

Katritzky, A.R. *et al.*, *J.C.S. Perkin 2*, 1989, 1499-1506, (*S*-Me)