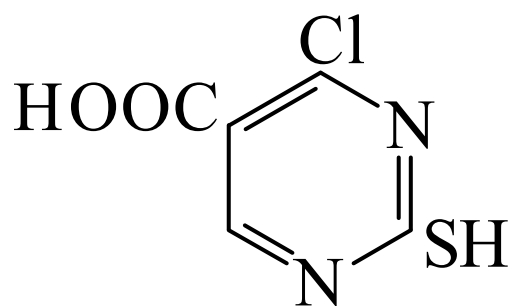




>>Entry Name: 4-Chloro-2-mercapto-5-pyrimidinecarboxylic acid, 9Cl



Molecular Formula: C₅H₃ClN₂O₂S

Molecular Weight: 190.61

Accurate Mass: 189.960375

Percentage Composition: C 31.51%; H 1.59%; Cl 18.60%; N 14.70%; O 16.79%; S 16.82%

>>Derivative: S-Me, Me ester

CAS Registry Number: 38275-39-7

Molecular Formula: C₇H₇ClN₂O₂S

Molecular Weight: 218.663

Accurate Mass: 217.991675

Percentage Composition: C 38.45%; H 3.23%; Cl 16.21%; N 12.81%; O 14.63%; S 14.66%

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 76-78°

>>Derivative: S-Me, Et ester

CAS Registry Number: 5909-24-0

Molecular Formula: C₈H₉ClN₂O₂S

Molecular Weight: 232.69

Accurate Mass: 232.007325

Percentage Composition: C 41.29%; H 3.90%; Cl 15.24%; N 12.04%; O 13.75%; S 13.78%

Physical Description: Cryst. (petrol)

Melting Point: Mp 60-63°

Hazard & Toxicity: Mild vesicant

Aldrich: 14596-3

Sigma: C0781

>>Derivative: S-Me, nitrile

Synonym(s): 4-Chloro-5-cyano-2-(methylthio)pyrimidine

CAS Registry Number: 33089-15-5

Molecular Formula: C₆H₄ClN₃S

Molecular Weight: 185.636

Accurate Mass: 184.981444

Percentage Composition: C 38.82%; H 2.17%; Cl 19.10%; N 22.64%; S 17.27%

Physical Description: Cryst. (pentane)

Melting Point: Mp 61-63°

>>Derivative: S-Me, anhydride

CAS Registry Number: 62094-69-3

Molecular Formula: C₁₂H₈Cl₂N₄O₃S₂

Molecular Weight: 391.258

Accurate Mass: 389.941485

Percentage Composition: C 36.84%; H 2.06%; Cl 18.12%; N 14.32%; O 12.27%; S 16.39%

Physical Description: Cryst. (hexane)

Melting Point: Mp 117-118°

References:

Todd, C.W. *et al.*, *J.A.C.S.*, 1943, **65**, 352, (*synth*)

Shadbolt, R.S. *et al.*, *J.C.S.(C)*, 1967, 1172, (*synth*)

Santilli, A.A. *et al.*, *J. Het. Chem.*, 1971, **8**, 445, (*nitrile*)

Budesinsky, Z. *et al.*, *Coll. Czech. Chem. Comm.*, 1972, **37**, 1721, (*synth, Me ester*)

Kimura, Y. *et al.*, *Chem. Pharm. Bull.*, 1976, **24**, 2637, (*anhydride*)