



>>Entry Name: 4-Chloro-6-hydroxypyrimidine

Synonym(s): 6-Chloro-4(1*H*)-pyrimidinone, 9Cl. 6-Chloro-4-pyrimidinol

CAS Registry Number: 4765-77-9

Related CAS Registry Numbers(s): 20635-32-9 79343-82-1

Molecular Formula: C<sub>4</sub>H<sub>3</sub>ClN<sub>2</sub>O

Molecular Weight: 130.533

Accurate Mass: 129.99339

Percentage Composition: C 36.81%; H 2.32%; Cl 27.16%; N 21.46%; O 12.26%

Physical Description: Needles or plates (EtOH or H<sub>2</sub>O)

Melting Point: Mp 196-197° (192-193°)

Boiling Point: Subl.<sub>0.001</sub> 110°

pKa Value: p*K*<sub>a</sub> 7.43 (20°,H<sub>2</sub>O)

>>Variant: *NH*-form

Molecular Formula: C<sub>4</sub>H<sub>3</sub>ClN<sub>2</sub>O

Molecular Weight: 130.533

Accurate Mass: 129.99339

Percentage Composition: C 36.81%; H 2.32%; Cl 27.16%; N 21.46%; O 12.26%

>>Derivative: Hydrazone

CAS Registry Number: 5767-35-1

Physical Description: Needles (H<sub>2</sub>O)

Melting Point: Mp 177 dec.°

>>Derivative: 1-*N*-Me

Molecular Formula: C<sub>5</sub>H<sub>5</sub>ClN<sub>2</sub>O

Molecular Weight: 144.56

Accurate Mass: 144.00904

Percentage Composition: C 41.54%; H 3.49%; Cl 24.52%; N 19.38%; O 11.07%

Physical Description: Solid

Melting Point: Mp 87-88°

>>Variant: *OH*-form

Molecular Formula: C<sub>4</sub>H<sub>3</sub>ClN<sub>2</sub>O

Molecular Weight: 130.533

Accurate Mass: 129.99339

Percentage Composition: C 36.81%; H 2.32%; Cl 27.16%; N 21.46%; O 12.26%

>>Derivative: Me ether

Synonym(s): 6-Chloro-4-methoxypyrimidine

Molecular Formula: C<sub>5</sub>H<sub>5</sub>ClN<sub>2</sub>O

Molecular Weight: 144.56

Accurate Mass: 144.00904

Percentage Composition: C 41.54%; H 3.49%; Cl 24.52%; N 19.38%; O 11.07%

Physical Description: Solid

Melting Point: Mp 31-32°

Boiling Point: Bp<sub>18</sub> 80°

Other Data: Sublimes

References:

Chesterfield, J. *et al.*, *J.C.S.*, 1955, 3478, (*hydrazone*)

Isbecque, D. *et al.*, *Helv. Chim. Acta*, 1959, **42**, 1317, (*synth, uv, deriv*)

Brown, D.J. *et al.*, *J.C.S.*, 1961, 1298, (*synth, derivs*)

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