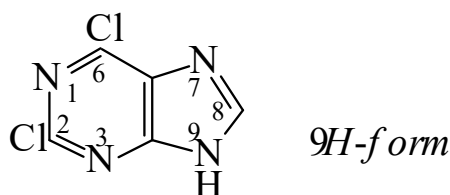




>>Entry Name: **2,6-Dichloropurine**

Synonym(s): 2,6-Dichloro-1*H*-purine, 9Cl



CAS Registry Number: 5451-40-1

Molecular Formula: C₅H₂Cl₂N₄

Molecular Weight: 189.003

Accurate Mass: 187.96565

Percentage Composition: C 31.77%; H 1.07%; Cl 37.52%; N 29.64%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 179-181°. Mp 188-190°

pKa Value: p*K*_{a1} -1.16; p*K*_{a2} 7.06 (20°)

Aldrich: D7310-3

Fluka: 36390

Sigma: D2253

>>Variant: 7*H*-form

Molecular Formula: C₅H₂Cl₂N₄

Molecular Weight: 189.003

Accurate Mass: 187.96565

Percentage Composition: C 31.77%; H 1.07%; Cl 37.52%; N 29.64%

>>Derivative: 7-Me

Molecular Formula: C₆H₄Cl₂N₄

Molecular Weight: 203.03

Accurate Mass: 201.9813

Percentage Composition: C 35.50%; H 1.99%; Cl 34.92%; N 27.60%

Physical Description: Needles (H₂O)

Melting Point: Mp 196-197°

>>Variant: 9*H*-form

Molecular Formula: C₅H₂Cl₂N₄

Molecular Weight: 189.003

Accurate Mass: 187.96565

Percentage Composition: C 31.77%; H 1.07%; Cl 37.52%; N 29.64%

>>Derivative: 9-Me

Molecular Formula: C₆H₄Cl₂N₄

Molecular Weight: 203.03

Accurate Mass: 201.9813

Percentage Composition: C 35.50%; H 1.99%; Cl 34.92%; N 27.60%

Physical Description: Needles (EtOAc)

Melting Point: Mp 152-153°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 708C, (*ir*)

Aldrich Library of NMR Spectra, 2nd edn., 1983, **2**, 583A, (*nmr*)

Montgomery, J.A., *J.A.C.S.*, 1956, **78**, 1928, (*synth*)

Beaman, A.G. *et al.*, *J. Appl. Chem.*, 1962, **12**, 432, (*synth*)

Kawashim, H. *et al.*, *Bull. Chem. Soc. Jpn.*, 1967, **40**, 639, (*synth*)

Thorpe, M.C. *et al.*, *J. Magn. Reson.*, 1974, **15**, 98, (*cmr*)