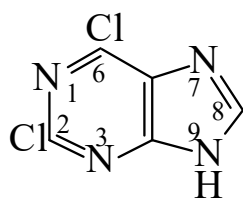




>>Entry Name: **2,6-Dichloropurine**

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



*9H-form*

CAS Registry Number: 5451-40-1

Molecular Formula: C<sub>5</sub>H<sub>2</sub>Cl<sub>2</sub>N<sub>4</sub>

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. (H<sub>2</sub>O)

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

pKa Value: pK<sub>a1</sub> -1.16; pK<sub>a2</sub> 7.06 (20°)

Aldrich: D7310-3

Fluka: 36390

Sigma: D2253

>>Variant: *7H*-form

Molecular Formula: C<sub>5</sub>H<sub>2</sub>Cl<sub>2</sub>N<sub>4</sub>

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: C<sub>6</sub>H<sub>4</sub>Cl<sub>2</sub>N<sub>4</sub>

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 (H<sub>2</sub>O)

Melting Point: Mp 196-197°

>>Variant: *9H*-form

Molecular Formula: C<sub>5</sub>H<sub>2</sub>Cl<sub>2</sub>N<sub>4</sub>

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: C<sub>6</sub>H<sub>4</sub>Cl<sub>2</sub>N<sub>4</sub>

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:

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

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