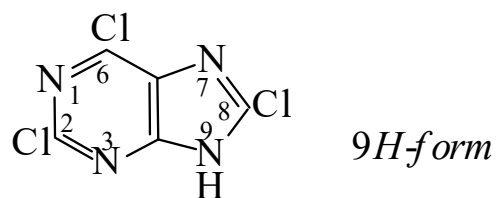




>>Entry Name: 2,6,8-Trichloropurine



CAS Registry Number: 2562-52-9

Molecular Formula: C₅HCl₃N₄

Molecular Weight: 223.448

Accurate Mass: 221.926677

Percentage Composition: C 26.88%; H 0.45%; Cl 47.60%; N 25.07%

Physical Description: Cryst.

Melting Point: Mp 185 dec.°

>>Variant: 7H-form

Molecular Formula: C₅HCl₃N₄

Molecular Weight: 223.448

Accurate Mass: 221.926677

Percentage Composition: C 26.88%; H 0.45%; Cl 47.60%; N 25.07%

>>Derivative: 7-Me

Molecular Formula: C₆H₃Cl₃N₄

Molecular Weight: 237.475

Accurate Mass: 235.942327

Percentage Composition: C 30.35%; H 1.27%; Cl 44.79%; N 23.59%

Physical Description: Needles (EtOH)

Melting Point: Mp 159-161°

>>Variant: 9H-form

Molecular Formula: C₅HCl₃N₄

Molecular Weight: 223.448

Accurate Mass: 221.926677

Percentage Composition: C 26.88%; H 0.45%; Cl 47.60%; N 25.07%

>>Derivative: 9-Me

Molecular Formula: C₆H₃Cl₃N₄

Molecular Weight: 237.475

Accurate Mass: 235.942327

Percentage Composition: C 30.35%; H 1.27%; Cl 44.79%; N 23.59%

Physical Description: Needles (EtOH)

Melting Point: Mp 176-176.5°

References:

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Xu, K. *et al.*, *J.A.C.S.*, 1994, **116**, 105, (*cryst struct, 9-Me*)