



>>Entry Name: 4-Amino-5-iodopyrimidine

Synonym(s): 5-Iodo-4-pyrimidinamine, 9CI

CAS Registry Number: 91416-96-5

Molecular Formula: C₄H₄IN₃

Molecular Weight: 221

Accurate Mass: 220.944995

Percentage Composition: C 21.74%; H 1.82%; I 57.42%; N 19.01%

Physical Description: Cryst.

Melting Point: Mp 188-189°

>>Derivative: 1-*N*-Oxide

CAS Registry Number: 91416-94-3

Molecular Formula: C₄H₄IN₃O

Molecular Weight: 237

Accurate Mass: 236.93991

Percentage Composition: C 20.27%; H 1.70%; I 53.55%; N 17.73%; O 6.75%

Physical Description: Cryst.

Melting Point: Mp 241-243.5°

>>Derivative: 4-*N*-Me

CAS Registry Number: 91416-97-6

Molecular Formula: C₅H₆IN₃

Molecular Weight: 235.027

Accurate Mass: 234.960645

Percentage Composition: C 25.55%; H 2.57%; I 54.00%; N 17.88%

Physical Description: Liq.

Boiling Point: Bp_{0.5} 55-56°

>>Derivative: 4-*N*-Me, 1-*N*-oxide

CAS Registry Number: 91416-95-4

Molecular Formula: C₅H₆IN₃O

Molecular Weight: 251.026

Accurate Mass: 250.95556

Percentage Composition: C 23.92%; H 2.41%; I 50.55%; N 16.74%; O 6.37%

Physical Description: Cryst.

Melting Point: Mp 200-201°

References:

Jovanovic, M.V., *Heterocycles*, 1984, **22**, 1195-1210, (*synth, derivs, pmr*)