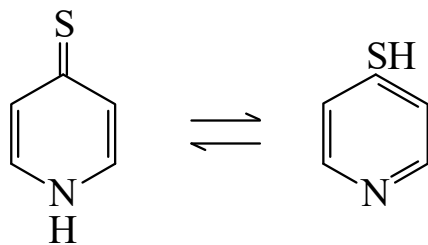




>>Entry Name: 4-Pyridinethiol

Synonym(s): 4(1*H*)-Pyridinethione, 9Cl. 4-Thiopyridone. 4-Mercaptopyridine



Molecular Formula: C₅H₅NS

Molecular Weight: 111.167

Accurate Mass: 111.014269

Percentage Composition: C 54.02%; H 4.53%; N 12.60%; S 28.84%

pKa Value: p*K*_{a1} 1.43; p*K*_{a2} 8.86 (20°, H₂SO₄ aq.)

>>Derivative: 1-Hydroxy

CAS Registry Number: 101084-70-2

Molecular Formula: C₅H₅NOS

Molecular Weight: 127.167

Accurate Mass: 127.009184

Percentage Composition: C 47.23%; H 3.96%; N 11.01%; O 12.58%; S 25.22%

Use/Importance: Efficient photochemical source of OH radicals

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 140 dec.°

Hazard & Toxicity: Cytotoxic by photochemical activation

>>Variant: Thioxo-form

CAS Registry Number: 19829-29-9

Molecular Formula: C₅H₅NS

Molecular Weight: 111.167

Accurate Mass: 111.014269

Percentage Composition: C 54.02%; H 4.53%; N 12.60%; S 28.84%

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 177°. Mp 186°

Solubility: Sol. H₂O

Hazard & Toxicity: LD₅₀ (mus, ipr) 150 mg/kg

>>Derivative: *N*-Me

CAS Registry Number: 6887-59-8

Molecular Formula: C₆H₇NS

Molecular Weight: 125.194

Accurate Mass: 125.029919

Percentage Composition: C 57.56%; H 5.64%; N 11.19%; S 25.61%

Physical Description: Yellow plates (EtOH)

Melting Point: Mp 161-163°

>>Variant: *SH*-form

CAS Registry Number: 4556-23-4

Molecular Formula: C₅H₅NS

Molecular Weight: 111.167

Accurate Mass: 111.014269

Percentage Composition: C 54.02%; H 4.53%; N 12.60%; S 28.84%

Aldrich: 14820-2