



>>Entry Name: 4-Pyridinecarbothioamide, 9Cl

Synonym(s): Thioisonicotinamide, 8Cl. 4-Thiocarbamoylpyridine

CAS Registry Number: 2196-13-6

Molecular Formula: C₆H₆N₂S

Molecular Weight: 138.193

Accurate Mass: 138.025168

Percentage Composition: C 52.15%; H 4.38%; N 20.27%; S 23.20%

Physical Description: Cryst. (Et₂O/MeOH)

Melting Point: Mp 202-203°

pKa Value: pK_a 11.58 (25°,H₂O)

>>Derivative: Hydrochloride

Melting Point: Mp 231-232°

>>Derivative: N-Oxide

Molecular Formula: C₆H₆N₂OS

Molecular Weight: 154.192

Accurate Mass: 154.020083

Percentage Composition: C 46.74%; H 3.92%; N 18.17%; O 10.38%; S 20.80%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 205-206°

>>Derivative: S-Oxide

CAS Registry Number: 91808-27-4

Molecular Formula: C₆H₆N₂OS

Molecular Weight: 154.192

Accurate Mass: 154.020083

Percentage Composition: C 46.74%; H 3.92%; N 18.17%; O 10.38%; S 20.80%

Physical Description: Cryst. (Py)

Melting Point: Mp 177-179°

References:

Gardner, T.S. *et al.*, *J.O.C.*, 1954, **19**, 753-757; 1957, **22**, 984-986, (*synth, N-oxide*)

Walter, W. *et al.*, *Chem. Ber.*, 1960, **93**, 1511-1517, (*S-oxide*)

Colleter, J.C. *et al.*, *Bull. Soc. Chim. Fr.*, 1967, 3463-3469, (*cryst struct*)

Pin, P.-Y. *et al.*, *Synthesis*, 1992, 1219-1220, (*synth, ir, pmr, ms*)

Gauthier, J.Y. *et al.*, *Phosphorus, Sulfur, Silicon, Relat. Elem.*, 1994, **95/96**, 325-326, (*synth*)