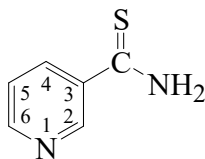




>>Entry Name: 3-Pyridinecarbothioamide, 9Cl

Synonym(s): Thionicotinamide, 8Cl. 3-Thiocarbamoylpyridine



CAS Registry Number: 4621-66-3

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 191-192°

>>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 161-164°

>>Derivative: *S*-Oxide

CAS Registry Number: 2669-11-6

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%

Melting Point: Mp 132-134°

References:

Gardner, T.S. *et al.*, *J.O.C.*, 1957, **22**, 984-986, (*N*-oxide)

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

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Cassar, L. *et al.*, *Synthesis*, 1978, 917-919, (*synth*)

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