



>>Entry Name: 3-Pyridazinethiol, 9CI

Synonym(s): 3(2*H*)-Pyridazinethione, 9CI. 3-Mercaptopyridazine

CAS Registry Number: 28544-77-6

Extra CAS Registry Numbers(s): 10443-98-8 134035-32-8

Molecular Formula: C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>S

Molecular Weight: 112.155

Accurate Mass: 112.009518

Percentage Composition: C 42.84%; H 3.59%; N 24.98%; S 28.59%

Physical Description: Yellow needles (EtOH or C<sub>6</sub>H<sub>6</sub>)

Melting Point: Mp 170°

>>Variant: *SH*-form

Molecular Formula: C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>S

Molecular Weight: 112.155

Accurate Mass: 112.009518

Percentage Composition: C 42.84%; H 3.59%; N 24.98%; S 28.59%

>>Derivative: *S*-Me

Synonym(s): 3-Methylthiopyridazine, 9CI

CAS Registry Number: 21948-71-0

Molecular Formula: C<sub>5</sub>H<sub>6</sub>N<sub>2</sub>S

Molecular Weight: 126.182

Accurate Mass: 126.025168

Percentage Composition: C 47.59%; H 4.79%; N 22.20%; S 25.41%

Physical Description: Pale yellow solid

Melting Point: Mp 39-40°

#### References:

Duffin, G.F. *et al.*, *J.C.S.*, 1959, 3789-3799, (*synth*, *S*-Me)

Carlisle, C.H. *et al.*, *Acta Cryst.*, 1966, **21**, 249-253, (*cryst struct*)

De Lannoy, J. *et al.*, *Bull. Soc. Chim. Belg.*, 1970, **79**, 329-336, (*synth*)

Nowak, M.J. *et al.*, *J. Phys. Chem.*, 1991, **95**, 2404-2411, (*ir*)