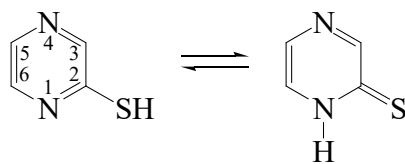




>>Entry Name: 2-Pyrazinethiol, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2(1*H*)-Pyrazinethione, 9CI. 2-Mercaptopyrazine



CAS Registry Number: 38521-06-1

Molecular Formula: C₄H₄N₂S

Molecular Weight: 112.155

Accurate Mass: 112.009518

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

Use/Importance: Shows some antithyroid activity

Physical Description: Orange solid or yellow plates

Melting Point: Mp 229 (215-218°) dec.°

pKa Value: p*K*_a 6.72 (50% EtOH aq., anion)

Other Data: Mp is not a reliable criterion of purity

>>Variant: *SH*-form

Molecular Formula: C₄H₄N₂S

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): 2-(Methylthio)pyrazine. Pyrazinyl methyl sulfide. FEMA 3231

CAS Registry Number: 21948-70-9

Molecular Formula: C₅H₆N₂S

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 cream solid

Melting Point: Mp 44-47°

Aldrich: 46767-7

Other: Oakwood 2751

>>Derivative: Disulfide

Synonym(s): Di(2-pyrazinyl)disulfide

CAS Registry Number: 98437-14-0

Molecular Formula: C₈H₆N₄S₂

Molecular Weight: 222.294

Accurate Mass: 222.003386

Percentage Composition: C 43.23%; H 2.72%; N 25.20%; S 28.85%

Melting Point: Mp 107-109°

References:

Roblin, R.O. *et al.*, *J.A.C.S.*, 1950, **72**, 4890, (*synth*)

Cheeseman, G.W.H., *J.C.S.*, 1960, 242, (*synth, uv, tautom*)

Albert, A. *et al.*, *J.C.S.*, 1962, 3129, (*synth*)

Barlin, E.B. *et al.*, *Aust. J. Chem.*, 1986, **39**, 69, (*synth*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 708

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 2386-2387