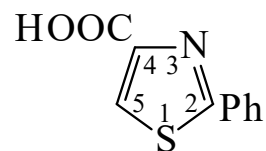




>>Entry Name: 2-Phenyl-4-thiazolecarboxylic acid, 9CI, 8CI



CAS Registry Number: 7113-10-2

Molecular Formula: C₁₀H₇NO₂S

Molecular Weight: 205.237

Accurate Mass: 205.019749

Percentage Composition: C 58.52%; H 3.44%; N 6.82%; O 15.59%; S 15.62%

Physical Description: Cryst. (EtOH aq. or xylene)

Melting Point: Mp 175-176°

pKa Value: pK_a 3.62 (H₂O)

>>Derivative: Me ester

Molecular Formula: C₁₁H₉NO₂S

Molecular Weight: 219.264

Accurate Mass: 219.035399

Percentage Composition: C 60.26%; H 4.14%; N 6.39%; O 14.59%; S 14.62%

Physical Description: Prisms (C₆H₆/petrol)

Melting Point: Mp 77-78°

>>Derivative: Et ester

CAS Registry Number: 59937-01-8

Molecular Formula: C₁₂H₁₁NO₂S

Molecular Weight: 233.29

Accurate Mass: 233.051049

Percentage Composition: C 61.78%; H 4.75%; N 6.00%; O 13.72%; S 13.75%

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 48-49°

>>Derivative: Amide

Molecular Formula: C₁₀H₈N₂O

Molecular Weight: 172.186

Accurate Mass: 172.063663

Percentage Composition: C 69.76%; H 4.68%; N 16.27%; O 9.29%

Physical Description: Needles (C₆H₆)

Melting Point: Mp 143-144°

>>Derivative: Nitrile

Synonym(s): 4-Cyano-2-phenylthiazole

Molecular Formula: C₁₀H₆N₂S

Molecular Weight: 186.237

Accurate Mass: 186.025168

Percentage Composition: C 64.49%; H 3.25%; N 15.04%; S 17.22%

Physical Description: Solid

Melting Point: Mp 95-96°

Boiling Point: Subl._{1.5} 130°

References:

- Huntress, E.H. *et al.*, *J.A.C.S.*, 1943, **65**, 1667; 2167, (*synth*)
Erlenmeyer, H. *et al.*, *Helv. Chim. Acta*, 1944, **27**, 1432, (*synth*)
Mijovic, M.P.V. *et al.*, *J.C.S.*, 1961, 3381, (*ir*)
Hall, G.E. *et al.*, *J.C.S.(C)*, 1966, 1357, (*synth*, *Me ester*, *Et ester*, *amide*, *nitrile*)
Benko, A. *et al.*, *Chem. Ber.*, 1967, **100**, 2178, (*synth*, *pKa*)
Simiti, I. *et al.*, *Bull. Soc. Chim. Fr.*, 1968, 3862, (*synth*)
Riordan, J.M. *et al.*, *J. Med. Chem.*, 1983, **26**, 884, (*Et ester*, *ir*, *pmr*)
Demian, H. *et al.*, *Org. Mass Spectrom.*, 1984, **19**, 196, (*ms*)
Kim, H.S. *et al.*, *J. Het. Chem.*, 1995, **32**, 937, (*Et ester*, *pmr*, *cmr*, *ir*, *ms*)