



>>Entry Name: 2-Chloro-5-thiazolecarboxylic acid, 9Cl

CAS Registry Number: 101012-12-8

Structure by analogy with 2-Chloro-4-thiazolecarboxylic acid, [BQO49-D](#)

Molecular Formula: C₄H₂ClNO₂S

Molecular Weight: 163.584

Accurate Mass: 162.949476

Percentage Composition: C 29.37%; H 1.23%; Cl 21.67%; N 8.56%; O 19.56%; S 19.60%

Melting Point: Mp 165°

>>Derivative: Et ester

CAS Registry Number: 81449-93-6

Molecular Formula: C₆H₆ClNO₂S

Molecular Weight: 191.638

Accurate Mass: 190.980776

Percentage Composition: C 37.61%; H 3.16%; Cl 18.50%; N 7.31%; O 16.70%; S 16.73%

Physical Description: Oil

>>Derivative: Chloride

Molecular Formula: C₄HCl₂NOS

Molecular Weight: 182.029

Accurate Mass: 180.915588

Percentage Composition: C 26.39%; H 0.55%; Cl 38.95%; N 7.69%; O 8.79%; S 17.62%

Physical Description: Amorph. solid

>>Derivative: Nitrile

Synonym(s): 2-Chloro-5-cyanothiazole

CAS Registry Number: 51640-36-9

Molecular Formula: C₄HCIN₂S

Molecular Weight: 144.584

Accurate Mass: 143.954895

Percentage Composition: C 33.23%; H 0.70%; Cl 24.52%; N 19.38%; S 22.18%

Melting Point: Mp 54-55°

References:

Erlenmeyer, H., *Helv. Chim. Acta*, 1944, **27**, 1432-1436, (*synth*)

Borthwick, A.D. *et al.*, *J.C.S. Perkin I*, 1973, 2769-2772, (*nitrile, synth, uv*)

Sakai, Y. *et al.*, *Heterocycles*, 1993, **36**, 565-573, (*Et ester, chloride, synth, pmr*)