



>>Entry Name: 4-Methyl-5-thiazolecarboxylic acid

CAS Registry Number: 20485-41-0

Molecular Formula: C₅H₅NO₂S

Molecular Weight: 143.166

Accurate Mass: 143.004099

Percentage Composition: C 41.95%; H 3.52%; N 9.78%; O 22.35%; S 22.40%

Use/Importance: Has antiviral, chemotherapeutic and fungicidal activity

Physical Description: Prisms (H₂O)

Boiling Point: Subl. 250°

Solubility: Mod. sol. hot H₂O, sol. EtOH, spar. sol. C₆H₆, petrol

Calculated Log P Data: Log P 1.2 (calc)

>>Derivative: Me ester

CAS Registry Number: 81569-44-0

Molecular Formula: C₆H₇NO₂S

Molecular Weight: 157.193

Accurate Mass: 157.019749

Percentage Composition: C 45.85%; H 4.49%; N 8.91%; O 20.36%; S 20.40%

Physical Description: Prisms (petrol)

Melting Point: Mp 74-75°

>>Derivative: Et ester

CAS Registry Number: 20582-55-2

Molecular Formula: C₇H₉NO₂S

Molecular Weight: 171.22

Accurate Mass: 171.035399

Percentage Composition: C 49.10%; H 5.30%; N 8.18%; O 18.69%; S 18.73%

Physical Description: Prisms

Melting Point: Mp 27-28°

Boiling Point: Bp 215-220°

Other Data: Steam-volatile

References:

Kuehle, A.E., *J.A.C.S.*, 1935, **57**, 1887, (*uv*)

Tomlinson, M.L., *J.C.S.*, 1935, 1030, (*synth*)

Jones, E.R.H. *et al.*, *J.C.S.*, 1946, 87, (*synth*)

Campaigne, E. *et al.*, *J. Med. Chem.*, 1959, **1**, 577, (*use*)

Abdel-Lateef, M. *et al.*, *Acta Phytopathol. Acad. Sci. Hung.*, 1973, **8**, 269, (*use*)

Krieg, B. *et al.*, *Annalen*, 1981, **4**, 623, (*nmr*)

Barton, A. *et al.*, *J.C.S. Perkin I*, 1982, **1**, 159, (*ir*)