



>>Entry Name: 5-Methyl-2-thiophenecarboxylic acid

CAS Registry Number: 1918-79-2

Molecular Formula: C₆H₆O₂S

Molecular Weight: 142.178

Accurate Mass: 142.00885

Percentage Composition: C 50.69%; H 4.25%; O 22.51%; S 22.55%

Physical Description: Needles (H₂O)

Melting Point: Mp 135-137°

pKa Value: pK_{a1} 3.7 (25°)

Other Data: Steam-volatile

Aldrich: M8442-9

Fluka: 69390

>>Derivative: Me ester

CAS Registry Number: 19432-69-0

Molecular Formula: C₇H₈O₂S

Molecular Weight: 156.205

Accurate Mass: 156.0245

Percentage Composition: C 53.82%; H 5.16%; O 20.49%; S 20.53%

Boiling Point: Bp₁₆ 102°. Bp₅ 84°

>>Derivative: Et ester, 1,1-dioxide

CAS Registry Number: 158875-35-5

Molecular Formula: C₈H₁₀O₄S

Molecular Weight: 202.231

Accurate Mass: 202.02998

Percentage Composition: C 47.51%; H 4.98%; O 31.65%; S 15.86%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 140°

References:

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Gronowitz, S. *et al.*, *CA*, 1962, **57**, 3000, (*pmr*)

Behringer, H. *et al.*, *Chem. Ber.*, 1966, **99**, 3309, (*synth*)

Nguyen, D.T. *et al.*, *Z. Chem.*, 1973, **13**, 57, (*synth*)

Knight, D.W. *et al.*, *J.C.S. Perkin I*, 1983, 791, (*synth*)

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