



>>Entry Name: 3-Methyl-2-thiophenecarboxylic acid

CAS Registry Number: 23806-24-8

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 or EtOH aq.)

Melting Point: Mp 147°

Solubility: Sol. hot H₂O

Aldrich: 24820-7

>>Derivative: Me ester

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: Bp 116-117.5°

>>Derivative: Et ester

CAS Registry Number: 14300-64-2

Molecular Formula: C₈H₁₀O₂S

Molecular Weight: 170.232

Accurate Mass: 170.04015

Percentage Composition: C 56.45%; H 5.92%; O 18.80%; S 18.84%

Boiling Point: Bp₁₂ 108-109°

>>Derivative: Chloride

CAS Registry Number: 61341-26-2

Molecular Formula: C₆H₅ClOS

Molecular Weight: 160.624

Accurate Mass: 159.974962

Percentage Composition: C 44.87%; H 3.14%; Cl 22.07%; O 9.96%; S 19.96%

Boiling Point: Bp 218-220°

>>Derivative: Nitrile

Synonym(s): 2-Cyano-3-methylthiophene

CAS Registry Number: 55406-13-8

Molecular Formula: C₆H₅NS

Molecular Weight: 123.178

Accurate Mass: 123.014269

Percentage Composition: C 58.51%; H 4.09%; N 11.37%; S 26.03%

Physical Description: Liq.

Boiling Point: Bp₁₂ 84-88°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 60A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 601B, (*ir*)

Linstead, R.P. *et al.*, *J.C.S.*, 1937, 911, (*synth*)

Ger. Pat., 1960, 1 092 929; *CA*, **57**, 5895, (*deriv*)

Tilak, B.D. *et al.*, *Tet. Lett.*, 1964, 1609, (*synth*)

Tilak, B.D. *et al.*, *Indian J. Chem.*, 1969, **7**, 9, (*synth*)

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