



>>Entry Name: 2,5-Thiophenedicarboxylic acid, 9CI

Synonym(s): Thiophene- α,α' -dicarboxylic acid

CAS Registry Number: 4282-31-9

Molecular Formula: C₆H₄O₄S

Molecular Weight: 172.161

Accurate Mass: 171.98303

Percentage Composition: C 41.86%; H 2.34%; O 37.17%; S 18.63%

Physical Description: Cryst. powder

Melting Point: Mp 358.5-359.5° (sealed tube)

Solubility: Spar. sol. H₂O

Other Data: Subl. at 150-300°

Aldrich: 40519-1

>>Derivative: Di-Me ester

CAS Registry Number: 4282-34-2

Molecular Formula: C₈H₈O₄S

Molecular Weight: 200.215

Accurate Mass: 200.01433

Percentage Composition: C 47.99%; H 4.03%; O 31.96%; S 16.02%

Physical Description: Needles (Et₂O), prisms (EtOH)

Melting Point: Mp 151°

>>Derivative: Mono-Et ester

CAS Registry Number: 156910-49-5

Molecular Formula: C₈H₈O₄S

Molecular Weight: 200.215

Accurate Mass: 200.01433

Percentage Composition: C 47.99%; H 4.03%; O 31.96%; S 16.02%

Physical Description: Solid

Melting Point: Mp 300°

>>Derivative: Di-Et ester

CAS Registry Number: 61755-85-9

Molecular Formula: C₁₀H₁₂O₄S

Molecular Weight: 228.268

Accurate Mass: 228.04563

Percentage Composition: C 52.62%; H 5.30%; O 28.04%; S 14.05%

Physical Description: Needles (EtOH)

Melting Point: Mp 51.5°

>>Derivative: Dinitrile

Synonym(s): 2,5-Dicyanothiophene

CAS Registry Number: 18853-40-2

Molecular Formula: C₆H₂N₂S

Molecular Weight: 134.161

Accurate Mass: 133.993868

Percentage Composition: C 53.72%; H 1.50%; N 20.88%; S 23.90%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 92-92.5°

References:

Hinsberg, O., *Ber.*, 1912, **45**, 2413-2418, (*synth*)

Campaigne, E. *et al.*, *J.A.C.S.*, 1948, **70**, 3941-3942, (*synth*)

Galvez, C. *et al.*, *J. Het. Chem.*, 1986, **23**, 1103-1108, (*synth*)

Noto, R. *et al.*, *J.C.S. Perkin 2*, 1987, 689-694, (*cmr*)

Dawson, M.I. *et al.*, *J. Med. Chem.*, 1995, **38**, 3368-3383, (*mono-Et ester*)