



>>Entry Name: 3,4-Thiophenedicarboxylic acid, 9CI

CAS Registry Number: 4282-29-5

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: Needles

Melting Point: Mp 230-231°

pKa Value: pK_{a1} 2.81; pK_{a2} 6.93

>>Derivative: Di-Me ester

CAS Registry Number: 4282-35-3

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: Prisms

Melting Point: Mp 59-60°

>>Derivative: Di-Et ester

CAS Registry Number: 53229-47-3

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%

Boiling Point: Bp_{1.8} 132°

>>Derivative: Dinitrile

Synonym(s): 3,4-Dicyanothiophene

CAS Registry Number: 18853-32-2

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: Solid by subl.

Melting Point: Mp 167-168°

>>Derivative: Anhydride

Synonym(s): 1*H*,3*H*-Thieno[3,4-*c*]furan-1,3-dione, 9CI

CAS Registry Number: 6007-85-8

Molecular Formula: C₆H₂O₃S

Molecular Weight: 154.146

Accurate Mass: 153.972465

Percentage Composition: C 46.75%; H 1.31%; O 31.14%; S 20.80%

Physical Description: Needles

Melting Point: Mp 145-146°

>>Derivative: Imide

Synonym(s): 4*H*-Thieno[3,4-*c*]pyrrole-4,6(5*H*)-dione

Molecular Formula: C₆H₃NO₂S

Molecular Weight: 153.161

Accurate Mass: 152.988449

Percentage Composition: C 47.05%; H 1.97%; N 9.15%; O 20.89%; S 20.94%

Physical Description: Needles

Melting Point: Mp 293-294°

References:

Sicé, J., *J.O.C.*, 1954, **19**, 70-73, (*synth, anhydride, imide*)

Tserng, K.-Y. *et al.*, *J.O.C.*, 1975, **40**, 172-175, (*synth*)

Crayston, J.A. *et al.*, *J.C.S. Perkin 2*, 1993, 1589-1595, (*synth, pmr, cmr*)