



>>Entry Name: 3-Thienylpropanedioic acid, 9CI

Synonym(s): 3-Thienylmalonic acid

CAS Registry Number: 21080-92-2

Molecular Formula: C₇H₆O₄S

Molecular Weight: 186.188

Accurate Mass: 185.99868

Percentage Composition: C 45.16%; H 3.25%; O 34.37%; S 17.22%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 139-140°

Aldrich: 21531-7

Fluka: 88435

>>Derivative: Di-Et ester

CAS Registry Number: 37784-67-1

Molecular Formula: C₁₁H₁₄O₄S

Molecular Weight: 242.295

Accurate Mass: 242.06128

Percentage Composition: C 54.53%; H 5.82%; O 26.41%; S 13.23%

Boiling Point: Bp₄ 141-147°

Density: d₄²⁰ 1.14

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 61A, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 602A, (ir)

Campaigne, E. *et al.*, *J.A.C.S.*, 1955, **77**, 5425

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Clayton, P.J. *et al.*, *Chem. Comm.*, 1979, 500