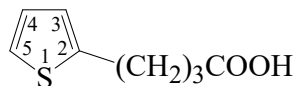




>>Entry Name: 2-Thiophenebutanoic acid, 9CI

Synonym(s): 4-(2-Thienyl)butanoic acid



CAS Registry Number: 4653-11-6

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%

Physical Description: Liq.

Melting Point: Mp 13.5-15°

Boiling Point: Bp₁₄ 170-172°

>>Derivative: Me ester

CAS Registry Number: 20828-66-4

Molecular Formula: C₉H₁₂O₂S

Molecular Weight: 184.259

Accurate Mass: 184.0558

Percentage Composition: C 58.67%; H 6.56%; O 17.37%; S 17.40%

Boiling Point: Bp₇ 116-116.5°

>>Derivative: Et ester

CAS Registry Number: 91950-17-3

Molecular Formula: C₁₀H₁₄O₂S

Molecular Weight: 198.285

Accurate Mass: 198.07145

Percentage Composition: C 60.57%; H 7.12%; O 16.14%; S 16.17%

Boiling Point: Bp₂₀ 164-165°

>>Derivative: Amide

CAS Registry Number: 4653-12-7

Molecular Formula: C₈H₁₁NOS

Molecular Weight: 169.247

Accurate Mass: 169.056134

Percentage Composition: C 56.77%; H 6.55%; N 8.28%; O 9.45%; S 18.95%

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 83-84°

References:

Fieser, L.F. *et al.*, *J.A.C.S.*, 1938, **57**, 1611-1616, (*synth*)

Cagniant, P. *et al.*, *Bull. Soc. Chim. Fr.*, 1953, 62-69, (*synth*)

Padwa, A. *et al.*, *J.O.C.*, 1994, **59**, 7072-7084, (*synth*, *ir*, *pmr*, *cmr*)

Kellogg, R.M. *et al.*, *Chem. Eur. J.*, 1999, **5**, 937-950, (*synth*, *pmr*, *cmr*)