



>>Entry Name: 3-Thiopheneacetic acid

Synonym(s): 3-Thienylacetic acid

CAS Registry Number: 6964-21-2

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: Cryst. (petrol)

Melting Point: Mp 79-80°

Aldrich: 22063-9

Fluka: 89017

>>Derivative: Et ester

CAS Registry Number: 37784-63-7

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: Bp₆ 107-115°

Aldrich: 25765-6

>>Derivative: Nitrile

Synonym(s): 3-(Cyanomethyl)thiophene

CAS Registry Number: 13781-53-8

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: Bp₁₆ 124-125°

Refractive Index: n_D²⁰ 1.5460

Aldrich: 21919-3

Fluka: 88972

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 60C; 63A, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 601D; 603C, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1477B; 1478B, (*ir*)

Campaigne, E. *et al.*, *J.A.C.S.*, 1948, **70**, 1555

Cagniant, P. *et al.*, *Bull. Soc. Chim. Fr.*, 1970, 308, (*nitrile*)