



>>Entry Name: 3-Mercaptobenzoic acid

CAS Registry Number: 4869-59-4

Molecular Formula: $C_7H_6O_2S$

Molecular Weight: 154.189

Accurate Mass: 154.00885

Percentage Composition: C 54.53%; H 3.92%; O 20.75%; S 20.80%

Physical Description: Plates or needles (EtOH aq.)

Melting Point: Mp 148°

pKa Value: pK_{a2} 6.32 (20°) pK_a 5.42 (48.9% EtOH)

Aldrich: 45143-6

>>Derivative: Me ester

CAS Registry Number: 72886-42-1

Molecular Formula: $C_8H_8O_2S$

Molecular Weight: 168.216

Accurate Mass: 168.0245

Percentage Composition: C 57.12%; H 4.79%; O 19.02%; S 19.06%

Physical Description: Oil

Boiling Point: Bp_{11} 135-136°

>>Derivative: S-Ac

Molecular Formula: $C_9H_8O_3S$

Molecular Weight: 196.226

Accurate Mass: 196.019415

Percentage Composition: C 55.09%; H 4.11%; O 24.46%; S 16.34%

Physical Description: Cryst. (C_6H_6 /hexane)

Melting Point: Mp 152-153°

>>Derivative: S-Me

References:

CRC Atlas of Spectral Data and Physical Constants, 1973, b1054, (ir)

Smiles, S. *et al.*, *J.C.S.*, 1921, **119**, 1797

Schwarzenbach, G. *et al.*, *Helv. Chim. Acta*, 1939, **22**, 360

Org. Synth., *Coll. Vol.*, 4, 1963, 695, (synth)

Danehy, J.P. *et al.*, *J. Chem. Eng. Data*, 1968, **13**, 386