



>>Entry Name: 4-Mercaptobenzoic acid

CAS Registry Number: 1074-36-8

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%

Use/Importance: Photographic fixer

Physical Description: Yellow powder

Melting Point: Mp 219°

pKa Value: pK_{a2} 5.9 (25°) pK_a 5.56 (48.9% EtOH)

Other Data: Dec. at 250°

Aldrich: 45144-4

>>Derivative: Me ester

CAS Registry Number: 6302-65-4

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%

Melting Point: Mp 45-47°. Mp 50°

Boiling Point: Bp_{11} 139-140°

pKa Value: pK_{a1} 5.33 (25°)

>>Derivative: Nitrile

Synonym(s): 4-Mercaptobenzonitrile, 9CI. 4-Cyanobenzenethiol

CAS Registry Number: 36801-01-1

Molecular Formula: C_7H_5NS

Molecular Weight: 135.189

Accurate Mass: 135.014269

Percentage Composition: C 62.19%; H 3.73%; N 10.36%; S 23.72%

Physical Description: Solid

>>Derivative: S-Me

>>Derivative: S-Et

Synonym(s): 4-(Ethylthio)benzoic acid

CAS Registry Number: 13205-49-7

Molecular Formula: $C_9H_{10}O_2S$

Molecular Weight: 182.243

Accurate Mass: 182.04015

Percentage Composition: C 59.32%; H 5.53%; O 17.56%; S 17.60%

Physical Description: Cryst. (AcOH aq.)

Melting Point: Mp 145-147°

References:

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

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Bramley, D. *et al.*, *J.C.S.*, 1942, 376

Gilman, H. *et al.*, *J.A.C.S.*, 1949, **71**, 4062

Krishnamurthy, S. *et al.*, *J.O.C.*, 1989, **54**, 4458, (nitrile)

Tickner, A.N. *et al.*, *Synth. Commun.*, 1995, **25**, 2497, (Me ester)