



>>Entry Name: 3-(Methylthio)benzoic acid, 9CI

CAS Registry Number: 825-99-0

Molecular Formula: C₈H₈O₂S

Molecular Weight: 168.216

Accurate Mass: 168.0245

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

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 126-127°

Rare Chemicals Library: S92582-9

>>Derivative: Me ester

CAS Registry Number: 90721-40-7

Molecular Formula: C₉H₁₀O₂S

Molecular Weight: 182.243

Accurate Mass: 182.04015

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

Boiling Point: Bp_{0.001} 83°

>>Derivative: Et ester

CAS Registry Number: 1442-02-0

Molecular Formula: C₁₀H₁₂O₂S

Molecular Weight: 196.27

Accurate Mass: 196.0558

Percentage Composition: C 61.20%; H 6.16%; O 16.30%; S 16.34%

Boiling Point: Bp₆ 148°. Bp_{0.8} 121°

>>Derivative: Chloride

CAS Registry Number: 770-04-7

Molecular Formula: C₈H₇ClOS

Molecular Weight: 186.661

Accurate Mass: 185.990612

Percentage Composition: C 51.48%; H 3.78%; Cl 18.99%; O 8.57%; S 17.18%

Boiling Point: Bp₅ 125-130°

>>Derivative: Nitrile

Synonym(s): 1-Cyano-3-methylmercaptobenzene. 3-Cyanophenyl methyl sulfide

CAS Registry Number: 65052-48-4

Molecular Formula: C₈H₇NS

Molecular Weight: 149.216

Accurate Mass: 149.029919

Percentage Composition: C 64.40%; H 4.73%; N 9.39%; S 21.49%

Physical Description: Needles

Melting Point: Mp 40°

References:

Zincke, T. *et al.*, *Ber.*, 1913, **46**, 773, (*synth, derivs*)

Smiles, S. *et al.*, *J.C.S.*, 1921, **119**, 1792, (*synth*)

Baker, J.W. *et al.*, *J.C.S.*, 1952, 2831, (*synth, deriv*)

Seidlova, V. *et al.*, *Cesk. Farm.*, 1965, **14**, 75, (*synth, deriv*)