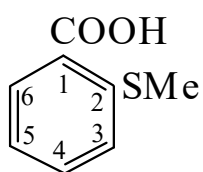




>>Entry Name: 2-(Methylthio)benzoic acid, 9CI

Synonym(s): 2-Methylmercaptobenzoic acid. S-(Methylthio)salicylic acid



CAS Registry Number: 3724-10-5

Related CAS Registry Numbers(s): 22912-54-5 23190-06-9

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 (H₂O or EtOH aq.)

Melting Point: Mp 169°

>>Derivative: Me ester

CAS Registry Number: 3704-28-7

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%

Physical Description: Cryst. (petrol)

Melting Point: Mp 66-67°

Aldrich: 45240-8

>>Derivative: Et ester

CAS Registry Number: 1442-00-8

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: Bp_{0.2} 129°

>>Derivative: Chloride

CAS Registry Number: 1442-03-1

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%

Physical Description: Cryst. (dioxan)

Melting Point: Mp 75°

>>Derivative: Nitrile

Synonym(s): 1-Cyano-2-methylthiobenzene

CAS Registry Number: 6609-54-7

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%

Melting Point: Mp 40-41°

>>Derivative: S-Oxide, (±)-

Synonym(s): 2-(Methylsulfinyl)benzoic acid, 9CI

CAS Registry Number: 33963-55-2

Molecular Formula: C₈H₈O₃S

Molecular Weight: 184.215

Accurate Mass: 184.019415

Percentage Composition: C 52.16%; H 4.38%; O 26.06%; S 17.41%

Other Data: No phys. props. reported