



>>Entry Name: 4-Mercaptobenzaldehyde, 9CI

Synonym(s): 4-Formylbenzenethiol

CAS Registry Number: 91358-96-2

Molecular Formula: C₇H₆OS

Molecular Weight: 138.19

Accurate Mass: 138.013935

Percentage Composition: C 60.84%; H 4.38%; O 11.58%; S 23.20%

Physical Description: Oil

>>Derivative: Phenylhydrazone

Melting Point: Mp 137°

>>Derivative: S-Me

Synonym(s): 4-(Methylthio)benzaldehyde

CAS Registry Number: 3446-89-7

Molecular Formula: C₈H₈OS

Molecular Weight: 152.217

Accurate Mass: 152.029585

Percentage Composition: C 63.13%; H 5.30%; O 10.51%; S 21.07%

Physical Description: Pale yellow oil

Boiling Point: Bp 273°. Bp₁ 101-103°

Aldrich: 22277-1

Fluka: 69327

>>Derivative: S-Me, oxime

CAS Registry Number: 93033-60-4

Molecular Formula: C₈H₉NOS

Molecular Weight: 167.231

Accurate Mass: 167.040484

Percentage Composition: C 57.46%; H 5.42%; N 8.38%; O 9.57%; S 19.17%

Melting Point: Mp 110°

>>Derivative: S-Me, 4-nitrophenylhydrazone

Physical Description: Orange needles

Melting Point: Mp 183°

>>Derivative: S-Me, S-oxide

Synonym(s): 4-(Methylsulfinyl)benzaldehyde, 9CI

CAS Registry Number: 37794-15-3

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%

Melting Point: Mp 92-93°

>>Derivative: S-Me, S,S-dioxide

Synonym(s): 4-(Methylsulfonyl)benzaldehyde

CAS Registry Number: 5398-77-6

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%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 158-159°

>>Derivative: S-Me, S,S-dioxide, thiosemicarbazone

Use/Importance: Formerly used as antitubercular drug

Melting Point: Mp 245-247°