



>>Entry Name: Benzenecarbothioic acid, 9Cl

Synonym(s): Thiobenzoic acid, 8Cl. Monothiobenzoic acid

CAS Registry Number: 98-91-9

PhCOSH<< >>PhC(S)OH

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%

Use/Importance: Used for extraction-separation of Co, Cu, Fe, Ni, Pd

Physical Description: Yellow oil cryst. on chilling in ice

Melting Point: Mp 15-18°. Mp 24°

pKa Value: pK_a 2.66 (H₂O)

Hazard & Toxicity: LD₅₀ (rat, ipr) 350 mg/kg

Aldrich: T2820-7

Fluka: 88500

Sigma: T2890

>>Variant: OH-form

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%

>>Derivative: O-Me ester

CAS Registry Number: 5873-86-9

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: Yellow liq.

Boiling Point: Bp₁₀ 110-112°

pKa Value: pK_a 12.8

>>Derivative: O-Et ester

CAS Registry Number: 936-61-8

Molecular Formula: C₉H₁₀OS

Molecular Weight: 166.243

Accurate Mass: 166.045235

Percentage Composition: C 65.02%; H 6.06%; O 9.62%; S 19.29%

Physical Description: Yellow liq.

Boiling Point: Bp 240°. Bp₁₁ 112-120°

>>Derivative: O-Ph ester

CAS Registry Number: 16911-57-2

Molecular Formula: C₁₃H₁₀OS

Molecular Weight: 214.287

Accurate Mass: 214.045235

Percentage Composition: C 72.87%; H 4.70%; O 7.47%; S 14.96%

Physical Description: Yellow prisms

Melting Point: Mp 32°