



Boiling Point: Bp 88°

Other Data: Unstable >78°

Hazard & Toxicity: Lachrymator

>>Derivative: Amide

Synonym(s): Benzenecarbothioamide, 9Cl. Thiobenzamide

CAS Registry Number: 2227-79-4

Molecular Formula: C₇H₇NS

Molecular Weight: 137.205

Accurate Mass: 137.029919

Percentage Composition: C 61.28%; H 5.14%; N 10.21%; S 23.37%

Melting Point: Mp 116-117°

Aldrich: 14822-9

Fluka: 88491

>>Derivative: Hydrazide

CAS Registry Number: 20605-40-7

Molecular Formula: C₇H₈N₂S

Molecular Weight: 152.22

Accurate Mass: 152.040818

Percentage Composition: C 55.23%; H 5.30%; N 18.40%; S 21.07%

Use/Importance: Used as 0.01-0.02M soln. in EtOH for extraction-photometric detn. of Os ($\lambda_{\max}$ 385 nm, ϵ 13700), Re ($\lambda_{\max}$ 520 nm, ϵ 12400), Ru ($\lambda_{\max}$ 520 nm, ϵ 12000)

Physical Description: Cryst. (Et₂O/petrol)

Melting Point: Mp 68-70°

Solubility: Sol. H₂O, common org. solvs.

>>Derivative: Dimethylamide

Molecular Formula: C₉H₁₁NS

Molecular Weight: 165.259

Accurate Mass: 165.061219

Percentage Composition: C 65.41%; H 6.71%; N 8.48%; S 19.40%

Melting Point: Mp 67-68°

>>Derivative: Anilide

Synonym(s): *N*-Phenylbenzenecarbothioamide, 9Cl. Thiobenzanilide, 8Cl

CAS Registry Number: 636-04-4

Molecular Formula: C₁₃H₁₁NS

Molecular Weight: 213.303

Accurate Mass: 213.061219

Percentage Composition: C 73.20%; H 5.20%; N 6.57%; S 15.03%

Melting Point: Mp 101-103°

>>Variant: *SH*-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: *S*-Me ester

CAS Registry Number: 5925-68-8

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: Bp 210-212°

Rare Chemicals Library: S91805-9