



>>Entry Name: Phenylthiourea, 9CI

CAS Registry Number: 103-85-5

PhNHCSNH₂

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 2.5% soln. in EtOH or aq. DMF for extraction-photometric detn. of Pd (λ_{max} 400 nm, ϵ 3000), Re (λ_{max} 410 nm, CHCl₃)

Physical Description: Needles (H₂O)

Melting Point: Mp 154°

Hazard & Toxicity: LD₅₀ (rat, orl) 3 mg/kg. Exp. teratogen

Aldrich: 22290-9

Fluka: 79180

Rare Chemicals Library: S62993-6

Sigma: P5272

>>Derivative: 1-*N*-Ac

Synonym(s): *N*-(Aminothioxomethyl)-*N*-phenylacetamide, 9CI. *N*-Acetyl-*N*-phenylthiourea

CAS Registry Number: 22713-55-9

Molecular Formula: C₉H₁₀N₂OS

Molecular Weight: 194.257

Accurate Mass: 194.051383

Percentage Composition: C 55.65%; H 5.19%; N 14.42%; O 8.24%; S 16.51%

Physical Description: Prisms (EtOH aq.)

Melting Point: Mp 140° (139° dec.)

>>Derivative: 3-*N*-Ac

Synonym(s): *N*-[(Phenylamino)thioxomethyl]acetamide, 9CI. *N*-Acetyl-*N'*-phenylthiourea

CAS Registry Number: 1132-44-1

Molecular Formula: C₉H₁₀N₂OS

Molecular Weight: 194.257

Accurate Mass: 194.051383

Percentage Composition: C 55.65%; H 5.19%; N 14.42%; O 8.24%; S 16.51%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 173°

Rare Chemicals Library: S78573-3

>>Derivative: 1-*N*-Benzoyl

Synonym(s): *N*-(Aminothioxomethyl)-*N*-phenylbenzamide, 9CI. *N*-Benzoyl-*N*-phenylthiourea

CAS Registry Number: 98095-85-3

Molecular Formula: C₁₄H₁₂N₂OS

Molecular Weight: 256.328

Accurate Mass: 256.067033

Percentage Composition: C 65.60%; H 4.72%; N 10.93%; O 6.24%; S 12.51%

Melting Point: Mp 133-137°

>>Derivative: 3-*N*-Benzoyl

Synonym(s): *N*-[(Phenylamino)thioxomethyl]benzamide, 9CI. *N*-Benzoyl-*N'*-phenylthiourea

CAS Registry Number: 4921-82-8

Molecular Formula: C₁₄H₁₂N₂OS

Molecular Weight: 256.328

Accurate Mass: 256.067033

Percentage Composition: C 65.60%; H 4.72%; N 10.93%; O 6.24%; S 12.51%

Use/Importance: Used as toluene soln. for extraction separation of Pd(II)

Physical Description: Cryst. (EtOH)

Melting Point: Mp 141-143°

Rare Chemicals Library: S50552-8