>>**Entry Name: Phenylthiourea,** 9CI

CAS Registry Number: 103-85-5

$PhNHCSNH_2$

Molecular Formula: $C_7H_8N_2S$
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, $CHCl_3$)
Physical Description: Needles (H_2O)
Melting Point: Mp 154°
Hazard & Toxicity: LD_{50} (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: $C_9H_{10}N_2OS$
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: $C_9H_{10}N_2OS$
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: $C_{14}H_{12}N_2OS$
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: $C_{14}H_{12}N_2OS$
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