



Synonym(s): *N*-Methyl-*N'*-phenylthiourea, 9Cl

CAS Registry Number: 2724-69-8

Molecular Formula: C₈H₁₀N₂S

Molecular Weight: 166.246

Accurate Mass: 166.056468

Percentage Composition: C 57.80%; H 6.06%; N 16.85%; S 19.29%

Physical Description: Needles

Melting Point: Mp 113°

Rare Chemicals Library: S61518-8

>> **Derivative:** 3-*N*-Me, 1-*N*-hydroxy

Synonym(s): *N*-Hydroxy-*N'*-methyl-*N*-phenylthiourea, 9Cl

CAS Registry Number: 26118-56-9

Molecular Formula: C₈H₁₀N₂OS

Molecular Weight: 182.246

Accurate Mass: 182.051383

Percentage Composition: C 52.72%; H 5.53%; N 15.37%; O 8.78%; S 17.59%

Use/Importance: Used for photometric and gravimetric detn. of Cu ($\lambda_{\max}$ 430 nm, ϵ 24600); extraction-photometric detn. of Ni ($\lambda_{\max}$ 440 nm, ϵ 27200)

pKa Value: pK_a 11.53

>> **Derivative:** 3-*N*-Di-Me

Synonym(s): *N,N*-Dimethyl-*N'*-phenylthiourea, 9Cl. Fenthuron

CAS Registry Number: 705-62-4

Molecular Formula: C₉H₁₂N₂S

Molecular Weight: 180.273

Accurate Mass: 180.072118

Percentage Composition: C 59.96%; H 6.71%; N 15.54%; S 17.79%

Physical Description: Prisms (EtOH)

Melting Point: Mp 134-135°

Rare Chemicals Library: S34730-2

>> **Derivative:** 3-*N*-Et

CAS Registry Number: 3955-58-6

Molecular Formula: C₉H₁₂N₂S

Molecular Weight: 180.273

Accurate Mass: 180.072118

Percentage Composition: C 59.96%; H 6.71%; N 15.54%; S 17.79%

Melting Point: Mp 134-136°

References:

- Aldrich Library of FT-IR Spectra*, 1st edn., 1985, **2**, 415D, (*ir*)
- Schiff, H., *Annalen*, 1868, **148**, 338
- Pollock, E.N., *Anal. Chim. Acta*, 1969, **47**, 367, (*detn, Re, synth*)
- Sharma, C. *et al.*, *Fresenius' Z. Anal. Chem.*, 1969, **248**, 34, (*deriv, detn, Cu*)
- Jackson, F.H. *et al.*, *J.C.S.(C)*, 1969, 268, (*synth*)
- Loev, B. *et al.*, *J. Med. Chem.*, 1972, **15**, 1024, (*synth, use*)
- Mathur, S.P. *et al.*, *CA*, 1973, **78**, 48739k; 1975, **83**, 141428w; 172199b; 1976, **85**, 48739k, (*deriv, detn, Cu, Ni*)
- Joshua, C.P. *et al.*, *Chem. Ind. (London)*, 1974, 750, (*synth*)
- Patil, S.P. *et al.*, *Mikrochim. Acta*, 1974, 853, (*detn, Pd*)
- Kaválek, J. *et al.*, *Coll. Czech. Chem. Comm.*, 1985, **50**, 766, (*synth, pmr, cmr, derivs*)
- Vest, P. *et al.*, *Fresenius' Z. Anal. Chem.*, 1989, **335**, 759, (*detn, Pd*)
- Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, MOA500; PGN250