



>>Entry Name: *N,N'*-Diphenylthiourea, 9Cl

Synonym(s): Thiocarbanilide, 8Cl. *sym*-Diphenylthiourea. Nocceler C

CAS Registry Number: 102-08-9

Type of Compound Code(s): PM7250 PS7700 PA3350 PS8300
PhNHCSNHPH

Molecular Formula: C₁₃H₁₂N₂S

Molecular Weight: 228.317

Accurate Mass: 228.072118

Percentage Composition: C 68.39%; H 5.30%; N 12.27%; S 14.04%

Use/Importance: Used in extraction separation and photometric detn. of Te (ϵ 150000), Ag, Pt, Rh, Ru

Physical Description: Leaflets (EtOH)

Melting Point: Mp 154-155°

pKa Value: pK_a 2

Hazard & Toxicity: LD₅₀ (rat, orl) 50 mg/kg. Exp. reprod. and teratogenic effects

Aldrich: T2835-5

Fluka: 43350

>>Derivative: *S*-Decyl

Synonym(s): *N,N'*-Diphenylcarbamidodithioic acid decyl ester, 9Cl. *S*-(1-Decyl)-*N,N'*-diphenylisothiuronium

CAS Registry Number: 62554-27-2

Type of Compound Code(s): PS7700

Molecular Formula: C₂₃H₃₂N₂S

Molecular Weight: 368.585

Accurate Mass: 368.228618

Percentage Composition: C 74.95%; H 8.75%; N 7.60%; S 8.70%

Use/Importance: Used as 5% soln. of hydrobromide salt in 2,6-dimethyl-4-heptanone for group extraction separation of noble metals

Physical Description: Viscous liq. (as hydrobromide)

Solubility: Sol. CHCl₃, 4-methyl-2-pentanone, 2,6-dimethyl-4-heptanone, EtOH, dioxan

>>Derivative: *N*-Hydroxy

Synonym(s): *N*-Hydroxy-*N,N'*-diphenylthiourea, 9Cl. 1-Hydroxy-1,3-diphenyl-2-thiourea, 8Cl. *N*-Hydroxythiocarbanilide. *N,N'*-Diphenylthiocarbamoylhydroxamic acid

CAS Registry Number: 20577-12-2

Type of Compound Code(s): PA2350 PA1450 PA2400 PM6750 PM7250 PS7700 PS8300

Use/Importance: Used as a 0.01*M* soln. in CHCl₃ for extraction-photometric detn. of Cu, Mo; photometric detn. of Ni ($\lambda_{\max}$ 470 nm, ϵ 16000)

Physical Description: Cryst. (C₆H₆) or leaflets (EtOH)

Melting Point: Mp 108-110 dec.°

Solubility: Sol. EtOH, C₆H₆, CHCl₃, Me₂CO, AcOH, dioxan

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1475C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 418B, (*ir*)

Sadtler Standard C-13 NMR Spectra, 2968, (*cmr*)

Sadtler Standard Ultraviolet Spectra, 2170, (*uv*)

Snedker, S.J.C., *J. Soc. Chem. Ind., London*, 1925, **44**, 74T; 486, (*synth*)

Geilmann, W. *et al.*, *Fresenius' Z. Anal. Chem.*, 1957, **156**, 420, (*detn, Ru*)

Russel, B.G. *et al.*, *Talanta*, 1967, **14**, 957, (*detn, Te*)

Maklakova, V.P. *et al.*, *Zavod. Lab.*, 1968, **34**, 1049, (*detn, Mo*)

Maklakova, V.P. *et al.*, *Zh. Anal. Khim.*, 1970, **25**, 257, (*detn, Cu*)

Seryakova, I.V. *et al.*, *Zh. Anal. Khim.*, 1972, **27**, 1840, (*detn, Ag*)

Diamantatos, A. *et al.*, *Anal. Chim. Acta*, 1977, **91**, 287; **94**, 49, (*detn, Pt, Rh, Te*)

Jones, E.A. *et al.*, *Anal. Chim. Acta*, 1977, **94**, 257, (*synth, use*)

Hasan, M. *et al.*, *Indian J. Technol.*, 1978, **16**, 123; *CA*, **89**, 208603u, (*detn, Ni*)

Ramnathan, A. *et al.*, *Acta Cryst. C*, 1995, **51**, 2446, (*cryst struct*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, DWN800