



>>Entry Name: *N,N'*-Bis(4-hydroxyphenyl)thiourea, 9Cl

Synonym(s): 4,4'-Dihydroxythiocarbanilide, 8Cl. 1,3-Di-*p*-hydroxyphenylthiourea



CAS Registry Number: 1473-33-2

Molecular Formula: C₁₃H₁₂N₂O₂S

Molecular Weight: 260.316

Accurate Mass: 260.061948

Percentage Composition: C 59.98%; H 4.65%; N 10.76%; O 12.29%; S 12.32%

Physical Description: Leaflets (H₂O)

Melting Point: Mp 224-225°

>>Derivative: Di-Me ether

Synonym(s): *N,N'*-Bis(4-methoxyphenyl)thiourea

CAS Registry Number: 1227-45-8

Molecular Formula: C₁₅H₁₆N₂O₂S

Molecular Weight: 288.37

Accurate Mass: 288.093248

Percentage Composition: C 62.48%; H 5.59%; N 9.71%; O 11.10%; S 11.12%

Melting Point: Mp 188-189°

Hazard & Toxicity: LD₅₀ (mus, ipr) 750 mg/kg

Rare Chemicals Library: S55646-7

>>Derivative: Di-Et ether

Synonym(s): *N,N'*-Bis(4-ethoxyphenyl)thiourea, 9Cl. **Etocarlide**, INN. Aethoksid. Athoxyd. Aethoxydum. Ethoxyd. Etoksid

CAS Registry Number: 1234-30-6

Molecular Formula: C₁₇H₂₀N₂O₂S

Molecular Weight: 316.423

Accurate Mass: 316.124548

Percentage Composition: C 64.53%; H 6.37%; N 8.85%; O 10.11%; S 10.13%

Use/Importance: Tuberculostatic

Melting Point: Mp 170-171°

Calculated Log P Data: Log P 4.22 (calc)

Hazard & Toxicity: LD₅₀ (mus, ipr) 510 mg/kg

References:

Dyson, G.M. *et al.*, *J.C.S.*, 1924, **125**, 1702, (*synth*)

Bersch, H.W. *et al.*, *Arzneim.-Forsch.*, 1955, **5**, 335, (*pharmacol*)

Lieber, E. *et al.*, *Can. J. Chem.*, 1957, **35**, 832, (*synth*)

Pohloudek-Fabini, R. *et al.*, *Arch. Pharm. (Weinheim, Ger.)*, 1965, **298**, 51, (*synth*)

Ritchie, R.K. *et al.*, *Spectrochim. Acta A*, 1970, **26**, 9, (*uv*)

Martindale, *The Extra Pharmacopoeia*, 28th/29th edn., Pharmaceutical Press, 1982, 1571