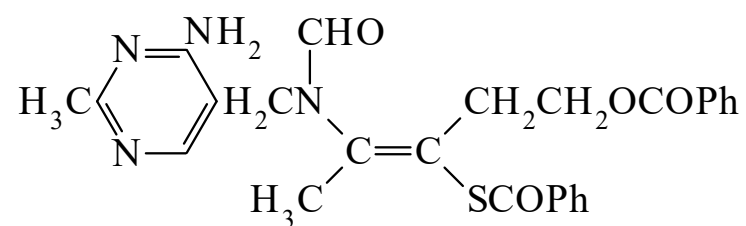




>>Entry Name: **Bentiamine**, INN

Synonym(s): *S*-[2-[[[(4-Amino-2-methyl-5-pyrimidinyl)methyl]formylamino]-1-[(2-benzoyloxyloxy)]ethyl-1-propenyl] benzenecarbothioate, 9Cl. *N*-[(Amino-2-methyl-5-pyrimidinyl)methyl]-*N*-(4-hydroxy-2-mercapto-1-methyl-1-butenyl)formamide *O,S*-dibenzoate, 8Cl. Dibenzoylthiamine. **DBT**‡



CAS Registry Number: 299-88-7

Related CAS Registry Numbers(s): 35660-60-7

Molecular Formula: C₂₆H₂₆N₄O₄S

Molecular Weight: 490.582

Accurate Mass: 490.167476

Percentage Composition: C 63.66%; H 5.34%; N 11.42%; O 13.05%; S 6.54%

Use/Importance: Topical analgesic (Vit. B₁ source)

Physical Description: Cryst. (EtOH)

Melting Point: Mp 153-154°

Hazard & Toxicity: LD₅₀ (mus, orl) 7480 mg/kg. LD₅₀ (mus, ipr) 2120 mg/kg

References:

Takamizawa, A. *et al.*, *Chem. Pharm. Bull.*, 1964, **12**, 558, (*synth*)

Asahi, Y., *Shionogi Kenkyusho Nenpo*, 1968, **27**, 58, (*nmr*)

Heywood, R. *et al.*, *Toxicol. Lett.*, 1985, **26**, 53, (*tox*)

Shin, W., *Acta Cryst. C*, 1988, **44**, 1754, (*cryst structt*)