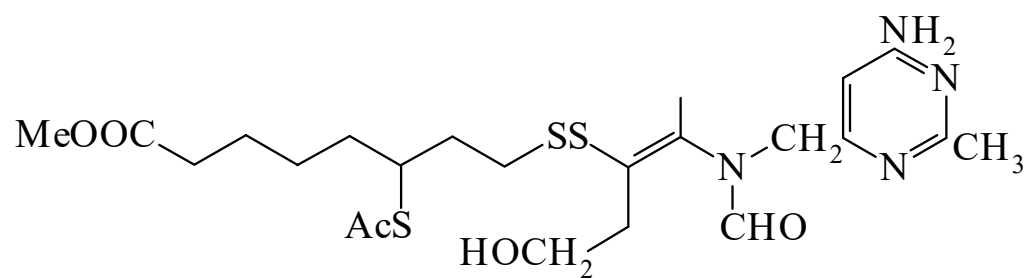




>>Entry Name: Octotiamine, INN, JAN

Synonym(s): Methyl 6-(acetylthio)-8-[[2-[[[(4-amino-2-methyl-5-pyrimidinyl)methyl]formylamino]-1-(2-hydroxyethyl)-1-propenyl]dithio]octanoic acid, 9Cl. Methyl 8-[[2-[N-[(4-amino-2-methyl-5-pyrimidinyl)methyl]formamido]-1-(2-hydroxyethyl)propenyl]dithio]-6-mercaptooctanoate S-acetate, 8Cl. Gerostop. Neuvitan. TATD. Thioctothiamine



CAS Registry Number: 137-86-0

Related CAS Registry Numbers(s): 1181-74-4 139369-65-6

Molecular Formula: C₂₃H₃₆N₄O₅S₃

Molecular Weight: 544.759

Accurate Mass: 544.184781

Percentage Composition: C 50.71%; H 6.66%; N 10.28%; O 14.68%; S 17.66%

Use/Importance: Long-acting oral thiamine analogue (vitamin B₁ source). Analgesic

Physical Description: Solid with sl. bitter taste

Melting Point: Mp 106-109°

Other Data: Used mainly as hydrochloride

Hazard & Toxicity: LD₅₀ (mus, orl) 2590 mg/kg. LD₅₀ (mus, ipr) 522 mg/kg

>>Derivative: Hydrochloride

CAS Registry Number: 4270-10-4

Physical Description: Cryst. (EtOH/Et₂O)

Melting Point: Mp 134-135°

References:

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Nose, Y. *et al.*, *Arzneim.-Forsch.*, 1964, **14**, 439, (*metab*)

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Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., *Van Nostrand Reinhold*, 1992, GEK200