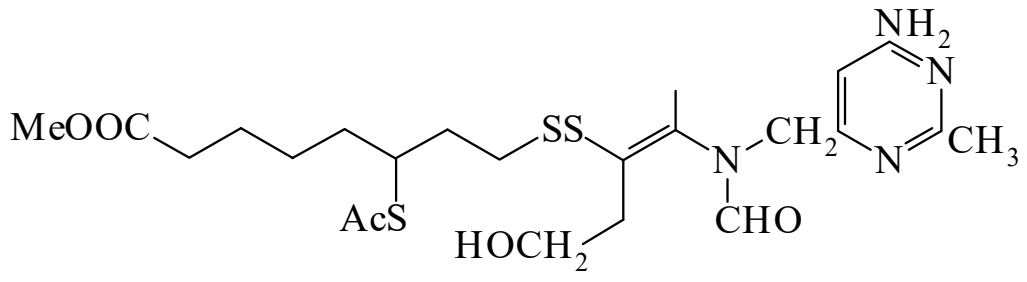
>>**Entry Name: Octotiamine,** INN, JAN

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: $C_{23}H_{36}N_4O_5S_3$
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 B_1 source). Analgesic
Physical Description: Solid with sl. bitter taste
Melting Point: Mp 106-109°
Other Data: Used mainly as hydrochloride
Hazard & Toxicity: LD_{50} (mus, orl) 2590 mg/kg. LD_{50} (mus, ipr) 522 mg/kg

>>**Derivative:** Hydrochloride

CAS Registry Number: 4270-10-4
Physical Description: Cryst. (EtOH/Et_2O)
Melting Point: Mp 134-135°

References:

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