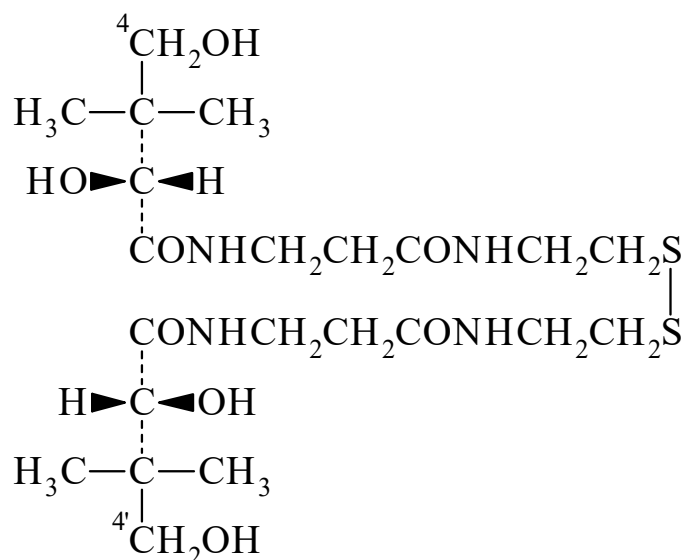




>>Entry Name: Pantethine, JAN

Synonym(s): *N,N'*-[Dithiobis[2,1-ethanediylimino(3-oxo-3,1-propanediyl)]]bis[2,4-dihydroxy-3,3-dimethylbutanamide], 9Cl. *N,N'*-[Dithiobis(ethyleneiminocarbonylethylene)]bis[2,4-dihydroxy-3,3-dimethylbutyramide], 8Cl. Bis(pantothenyl-2-aminoethyl)disulfide



CAS Registry Number: 303-05-9

Molecular Formula: C₂₂H₄₂N₄O₈S₂

Molecular Weight: 554.728

Accurate Mass: 554.244406

Percentage Composition: C 47.63%; H 7.63%; N 10.10%; O 23.07%; S 11.56%

>>Variant: (*R,R*)-form

Synonym(s): D-form. Lipodel. Pantetina. Panthecin. Pantomin. Pantosin

CAS Registry Number: 16816-67-4

Molecular Formula: C₂₂H₄₂N₄O₈S₂

Molecular Weight: 554.728

Accurate Mass: 554.244406

Percentage Composition: C 47.63%; H 7.63%; N 10.10%; O 23.07%; S 11.56%

Biological Source: Found in foods

Use/Importance: Synth. intermed. for Coenzyme A [CBW68-G](#)

Biological Use/Importance: Bacterial growth factor. Antihyperlipidaemic agent

Physical Description: Cryst. (MeOH/Me₂CO), glass (H₂O)

Optical Rotation: [α]_D²²+17.9 (c, 3.2 in H₂O)

Other Data: Hydrol. by acids

Hazard & Toxicity: LD₅₀ (mus, ipr) 4800 mg/kg. Exp. reprod. and teratogenic effects

Sigma: P2125

>>Derivative: 4,4'-Diphosphate

CAS Registry Number: 17451-69-3

Molecular Formula: C₂₂H₄₄N₄O₁₄P₂S₂

Molecular Weight: 714.687

Accurate Mass: 714.17707

Percentage Composition: C 36.97%; H 6.21%; N 7.84%; O 31.34%; P 8.67%; S 8.97%

Use/Importance: Intermediate for synth. of Coenzyme A [CBW68-G](#)

Physical Description: Powder (MeOH) (as Ba salt)

Optical Rotation: [α]_D²⁰+12.2 (c, 1 in H₂O)

References:

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Bowman, R.E. *et al.*, *J.C.S.*, 1954, 1171, (*anal, rev, bibl*)
Moffatt, J.G. *et al.*, *J.A.C.S.*, 1961, **83**, 663, (*chromatog*)
Shimizu, M. *et al.*, *Chem. Pharm. Bull.*, 1965, **13**, 180, (*synth, chromatog, ir, uv*)
Nagase, O., *Chem. Pharm. Bull.*, 1967, **15**, 648, (*phosphate, synth*)
Zhdanovich, E.S. *et al.*, *J. Gen. Chem. USSR (Engl. Transl.)*, 1967, **37**, 337, (*synth, ir*)
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