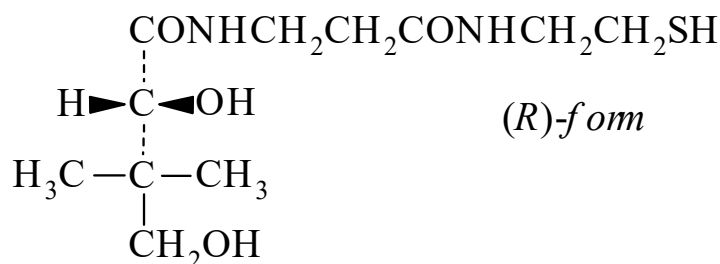




>>Entry Name: Pantetheine

Synonym(s): 2,4-Dihydroxy-N-[3-[(2-mercaptoethyl)amino]-3-oxopropyl]-3,3-dimethylbutanamide, 9CI. *Lactobacillus bulgaricus* Factor



CAS Registry Number: 496-65-1

Related CAS Registry Numbers(s): 55512-69-1

Molecular Formula: C₁₁H₂₂N₂O₄S

Molecular Weight: 278.372

Accurate Mass: 278.130028

Percentage Composition: C 47.46%; H 7.97%; N 10.06%; O 22.99%; S 11.52%

>>Variant: (R)-form

Synonym(s): D-form

CAS Registry Number: 1971-08-0

Molecular Formula: C₁₁H₂₂N₂O₄S

Molecular Weight: 278.372

Accurate Mass: 278.130028

Percentage Composition: C 47.46%; H 7.97%; N 10.06%; O 22.99%; S 11.52%

Biological Source: Growth factor for *Lactobacillus bulgaricus*. Prod. by many microorganisms. High concns. found in yeast. Component of Coenzyme A [CBW68-G](#)

Physical Description: Resin

Optical Rotation: $[\alpha]_{\text{D}}^{20} +12.9$ (H₂O)

>>Derivative: S-Ac

Molecular Formula: C₁₃H₂₄N₂O₅S

Molecular Weight: 320.409

Accurate Mass: 320.140593

Percentage Composition: C 48.73%; H 7.55%; N 8.74%; O 24.97%; S 10.01%

Optical Rotation: $[\alpha]_{\text{D}}^{26} +40$

>>Derivative: S-Benzoyl

Molecular Formula: C₁₈H₂₆N₂O₅S

Molecular Weight: 382.48

Accurate Mass: 382.156243

Percentage Composition: C 56.53%; H 6.85%; N 7.32%; O 20.92%; S 8.38%

Melting Point: Mp 116°

Optical Rotation: $[\alpha]_{\text{D}}^{26} +31$

>>Derivative: Disulfide

>>Derivative: 4'-Phosphate

Synonym(s): 4'-Phosphopantetheine

CAS Registry Number: 2226-71-3

Extra CAS Registry Numbers(s): 13147-30-3

Molecular Formula: C₁₁H₂₃N₂O₇PS

Molecular Weight: 358.352

Accurate Mass: 358.09636

Percentage Composition: C 36.87%; H 6.47%; N 7.82%; O 31.25%; P 8.64%; S 8.95%

Source/Synthesis: Obt. by acid or enzymic hydrol. of Coenzyme A [CBW68-G](#)

Use/Importance: Cofactor for acetyl-CoA synthetase

Optical Rotation: $[\alpha]_{\text{D}}^{23} +13.6$ (c, 1 in H₂O)

References: