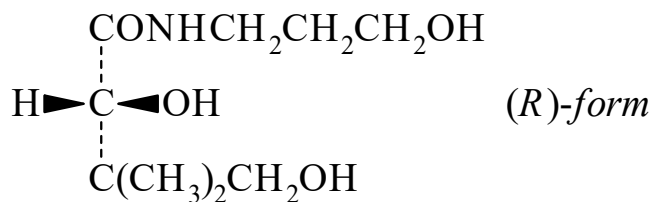




>>Entry Name: **Panthenol**, BAN, INN, USAN

Synonym(s): 2,4-Dihydroxy-*N*-(3-hydroxypropyl)-3,3-dimethylbutanamide, 9CI. Panthoderm. Pantothenyl alcohol. Pantothenol



CAS Registry Number: 62507-76-0

Related CAS Registry Numbers(s): 17307-32-3 74561-18-5

Molecular Formula: C₉H₁₉NO₄

Molecular Weight: 205.253

Accurate Mass: 205.131409

Percentage Composition: C 52.67%; H 9.33%; N 6.82%; O 31.18%

Use/Importance: Low acute mammalian toxicity. Hair tonic ingredient. Bactericide, used in cosmetics

Biological Use/Importance: Drug used in treatment of paralytic ileus and postoperative distension. Also a growth factor related to pantothenic acid

Calculated Log P Data: Log P -2.52 (calc)

>>Variant: (*R*)-form

Synonym(s): **Dexpanthenol**, BAN, INN, USAN. Pantol. Bepanthon

CAS Registry Number: 81-13-0

Molecular Formula: C₉H₁₉NO₄

Molecular Weight: 205.253

Accurate Mass: 205.131409

Percentage Composition: C 52.67%; H 9.33%; N 6.82%; O 31.18%

Physical Description: Viscous oil

Boiling Point: Bp_{0.2} 118-120°

Optical Rotation: [α]_D²⁰ +29.7 (c, 0.03 in H₂O)

Solubility: V. sol. H₂O; spar. sol. Et₂O

Density: d₂₀²⁰ 1.2

Refractive Index: n_D²⁰ 1.4970

Fluka: 76200

Rare Chemicals Library: S61643-5

Sigma: P2375

>>Derivative: 4'-Phosphate

CAS Registry Number: 25531-31-1

Molecular Formula: C₉H₂₀NO₇P

Molecular Weight: 285.233

Accurate Mass: 285.097741

Percentage Composition: C 37.90%; H 7.07%; N 4.91%; O 39.26%; P 10.86%

Optical Rotation: [α]_D²⁸ +13.5 (c, 1.0 in H₂O) (Ba salt)

>>Derivative: 3"-Phosphate

CAS Registry Number: 25531-30-0

Molecular Formula: C₉H₂₀NO₇P

Molecular Weight: 285.233

Accurate Mass: 285.097741

Percentage Composition: C 37.90%; H 7.07%; N 4.91%; O 39.26%; P 10.86%

Optical Rotation: [α]_D²² +22.6 (c, 1.0 in H₂O) (di-Li salt)

>>Derivative: Tri-Ac

Molecular Formula: C₁₅H₂₅NO₇

Molecular Weight: 331.365

Accurate Mass: 331.163104

Percentage Composition: C 54.37%; H 7.60%; N 4.23%; O 33.80%

Boiling Point: Bp_{0.000005} 130°

Optical Rotation: [α]_D²⁰ -4.65 (EtOH)