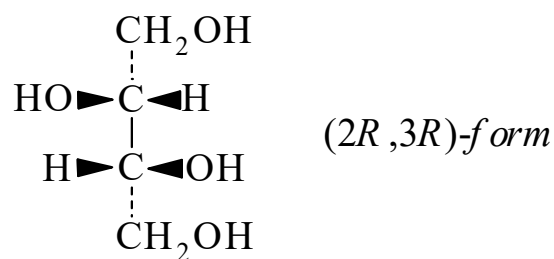




>>Entry Name: Threitol

ENTRY UNDER REVIEW

Synonym(s): (*R*,R**)-1,2,3,4-Butanetetrol, 9CI



CAS Registry Number: 7493-90-5

Related CAS Registry Numbers(s): 20638-61-3 50623-73-9 71641-34-4 102779-61-3 114924-93-5

Molecular Formula: C₄H₁₀O₄

Molecular Weight: 122.121

Accurate Mass: 122.05791

Percentage Composition: C 39.34%; H 8.25%; O 52.41%

Calculated Log P Data: Log P -3.02 (calc)

>>Variant: (2*R*,3*R*)-form

Synonym(s): D-form

CAS Registry Number: 2418-52-2

Molecular Formula: C₄H₁₀O₄

Molecular Weight: 122.121

Accurate Mass: 122.05791

Percentage Composition: C 39.34%; H 8.25%; O 52.41%

Biological Source: Found in the edible fungus *Armillaria mellea*. Constit. of bark, stem and leaf of jute (*Corchorus capsularis* and *Corchorus olitorius*), bark, stem and leaf of the pigeon pea plant (*Cajanus cajan*); also traces found in the lichen *Parmotrema cetratum*

Physical Description: Needles (EtOH)

Melting Point: Mp 72-74°. Mp 88.5-89°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +6$ (c, 2 in Me₂CO). $[\alpha]_{\text{D}}^{20} +4.6$ (c, 6 in H₂O). $[\alpha]_{\text{D}}^{20} -11.5$ (c, 5 in EtOH)

Solubility: V. sol. hot EtOH

Aldrich: 37761-9

Fluka: 89173

Sigma: T1907

>>Derivative: Tetrabenzoyl

Synonym(s): 1,2,3,4-Tetra-*O*-benzoyl-D-threitol

CAS Registry Number: 114926-25-9

Molecular Formula: C₃₂H₂₆O₈

Molecular Weight: 538.553

Accurate Mass: 538.16277

Percentage Composition: C 71.37%; H 4.87%; O 23.77%

Melting Point: Mp 97°

>>Derivative: 2,3-*O*-Isopropylidene

Synonym(s): 2,2-Dimethyl-1,3-dioxolane-4,5-dimethanol, 9CI. 2,3-*O*-Isopropylidene-D-threitol

CAS Registry Number: 73346-74-4

Molecular Formula: C₇H₁₄O₄

Molecular Weight: 162.185

Accurate Mass: 162.08921

Percentage Composition: C 51.84%; H 8.70%; O 39.46%

Physical Description: Cryst. (diisopropyl ether)

Melting Point: Mp 48-51°

Boiling Point: Bp_{0.01} 91-93°

Optical Rotation: $[\alpha]_{\text{D}}^{26} -4.8$ (c, 10.3 in CHCl₃). $[\alpha]_{\text{D}}^{26} +3.1$ (c, 10 in EtOH)

Aldrich: 24141-5

Fluka: 59535