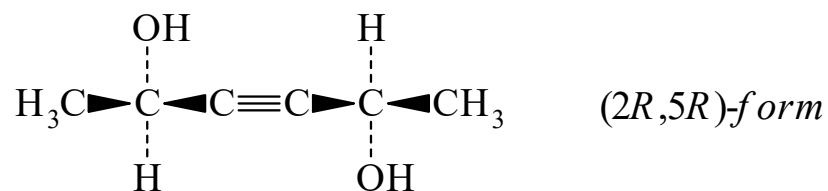




>>Entry Name: 3-Hexyne-2,5-diol



CAS Registry Number: 3031-66-1

Related CAS Registry Numbers(s): 21784-84-9 110318-64-4 110318-66-6

Molecular Formula: C₆H₁₀O₂

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Aldrich: 25039-2

Fluka: 53082

Rare Chemicals Library: S37221-8

>>Variant: (2*R*,5*R*)-form

CAS Registry Number: 152694-51-4

Molecular Formula: C₆H₁₀O₂

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Physical Description: Cryst.

Melting Point: Mp 58-60°

Optical Rotation: [α]_D²⁵+70.8 (c, 1 in CHCl₃)

>>Variant: (2*RS*,5*RS*)-form

Synonym(s): (±)-form

CAS Registry Number: 131375-88-7

Molecular Formula: C₆H₁₀O₂

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Melting Point: Mp 44-46° (42°)

Boiling Point: Bp₁₀ 125-127°

>>Derivative: Bis(4-methylbenzenesulfonyl)

CAS Registry Number: 131375-89-8

Molecular Formula: C₂₀H₂₂O₆S₂

Molecular Weight: 422.522

Percentage Composition: C 56.85%; H 5.25%; O 22.72%; S 15.18%

Physical Description: Cryst. (Et₂O)

Melting Point: Mp 110-111°

>>Variant: (2*RS*,5*SR*)-form

Synonym(s): *meso*-form

CAS Registry Number: 110318-65-5

Molecular Formula: C₆H₁₀O₂

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Physical Description: Cryst. (Et₂O/hexane)

Melting Point: Mp 71-72°

Boiling Point: Bp₂ 110-115°. Bp_{0.4} 105°