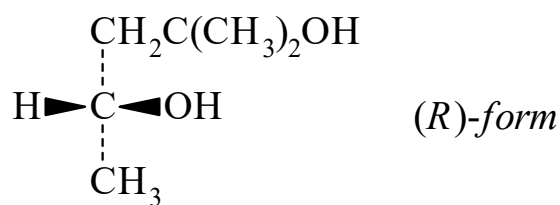




>>Entry Name: 2-Methyl-2,4-pentanediol, 9CI

Synonym(s): Hexylene glycol



CAS Registry Number: 107-41-5

Molecular Formula: C₆H₁₄O₂

Molecular Weight: 118.175

Accurate Mass: 118.09938

Percentage Composition: C 60.98%; H 11.94%; O 27.08%

Biological Source: Constit. of *Ligularia veitchiana* and *Santolina rosmarinifolia*

Hazard & Toxicity: Fl. p. 93° (oc). OES: long-term 25 ppm; short-term 25 ppm. Eye, skin and respiratory tract irritant

Aldrich: 11210-0

Fluka: 68342

Sigma: M9671

>>Variant: (R)-form

CAS Registry Number: 99210-90-9

Molecular Formula: C₆H₁₄O₂

Molecular Weight: 118.175

Accurate Mass: 118.09938

Percentage Composition: C 60.98%; H 11.94%; O 27.08%

Boiling Point: Bp₆ 108-110°

Optical Rotation: [α]_D²⁵ -14.7 (neat) (87% ee)

Aldrich: 25284-0

Fluka: 68336

Sigma: M3767

>>Variant: (S)-form

CAS Registry Number: 99210-91-0

Molecular Formula: C₆H₁₄O₂

Molecular Weight: 118.175

Accurate Mass: 118.09938

Percentage Composition: C 60.98%; H 11.94%; O 27.08%

Boiling Point: Bp₆ 87-90°

Optical Rotation: [α]_D²⁵ +15 (c, 1 in EtOH) (92% ee)

>>Variant: (±)-form

CAS Registry Number: 99113-75-4

Molecular Formula: C₆H₁₄O₂

Molecular Weight: 118.175

Accurate Mass: 118.09938

Percentage Composition: C 60.98%; H 11.94%; O 27.08%

Use/Importance: Reagent for characterisation of aldehydes as the cyclic acetals. Used as 20% soln. in 4-methyl-2-pentanone for extraction separation of boron, low acute toxicity

Physical Description: Liq.

Melting Point: Mp -40°

Boiling Point: Bp 198°

Solubility: Sol. H₂O, 4-methyl-2-pentanone, EtOH

Refractive Index: n_D²⁰ 1.4276

>>Derivative: Di-Ac