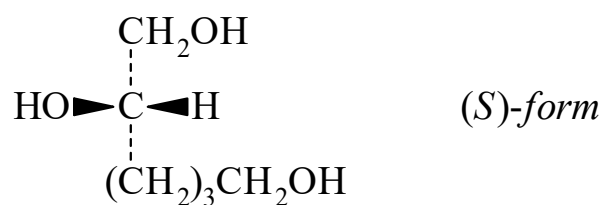




>>Entry Name: 1,2,6-Hexanetriol, 9CI

Synonym(s): 2,3,4-Trideoxyhexitol



CAS Registry Number: 106-69-4

Related CAS Registry Numbers(s): 112254-74-7 130232-56-3

Extra CAS Registry Numbers(s): 25323-24-4

Molecular Formula: C<sub>6</sub>H<sub>14</sub>O<sub>3</sub>

Molecular Weight: 134.175

Accurate Mass: 134.094295

Percentage Composition: C 53.71%; H 10.52%; O 35.77%

Use/Importance: Diuretic ointment base. Low oral toxicity

Aldrich: W50240-5

Fluka: 52900

Sigma: T1386

>>Variant: (S)-form

CAS Registry Number: 130232-56-3

Molecular Formula: C<sub>6</sub>H<sub>14</sub>O<sub>3</sub>

Molecular Weight: 134.175

Accurate Mass: 134.094295

Percentage Composition: C 53.71%; H 10.52%; O 35.77%

Use/Importance: Component of alkyd resins, inks etc.

Physical Description: Oil

Melting Point: Mp 25° (approx.)

Optical Rotation: [α]<sub>D</sub> -3.4

Density: d 1.109

Refractive Index: n<sub>D</sub><sup>20</sup> 1.4760 (approx.)

Hazard & Toxicity: LD<sub>50</sub> (rat, orl) 15500 mg/kg

>>Derivative: Tris(4-nitrobenzoyl)

Physical Description: Cryst. (EtOH/EtOAc)

Melting Point: Mp 120-121°

Optical Rotation: [α]<sub>D</sub> +8.6 (CHCl<sub>3</sub>)

>>Variant: (±)-form

CAS Registry Number: 112254-74-7

Molecular Formula: C<sub>6</sub>H<sub>14</sub>O<sub>3</sub>

Molecular Weight: 134.175

Accurate Mass: 134.094295

Percentage Composition: C 53.71%; H 10.52%; O 35.77%

Boiling Point: Bp<sub>1.5</sub> 155-159°

Solubility: Misc. H<sub>2</sub>O

Density: d<sup>20</sup> 1.03

Hazard & Toxicity: Eye and skin irritant, fl. p. 191° (oc)

>>Derivative: Tri-Ac

CAS Registry Number: 923-87-5

Molecular Formula: C<sub>12</sub>H<sub>20</sub>O<sub>6</sub>

Molecular Weight: 260.286

Accurate Mass: 260.12599

Percentage Composition: C 55.37%; H 7.74%; O 36.88%

Boiling Point: Bp<sub>2.3</sub> 157-158° (lit. gives a pressure range)

Density: d<sup>20</sup> 1.1