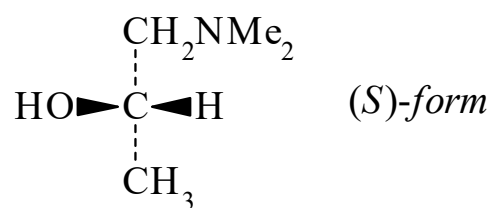




>>Entry Name: 1-Dimethylamino-2-propanol, 9CI

Synonym(s): Dimepranol, INN



CAS Registry Number: 108-16-7

Related CAS Registry Numbers(s): 53636-17-2

Type of Compound Code(s): XA2400

Molecular Formula: C₅H₁₃NO

Molecular Weight: 103.164

Accurate Mass: 103.099714

Percentage Composition: C 58.21%; H 12.70%; N 13.58%; O 15.51%

Use/Importance: Antiviral agent

Calculated Log P Data: Log P -0.27 (calc)

Hazard & Toxicity: Skin and severe eye irritant. LD₅₀ (rat, orl) 1890 mg/kg

Aldrich: 47022-8

Fluka: 39300

>>Variant: (S)-form

Synonym(s): L-form

CAS Registry Number: 53636-15-0

Molecular Formula: C₅H₁₃NO

Molecular Weight: 103.164

Accurate Mass: 103.099714

Percentage Composition: C 58.21%; H 12.70%; N 13.58%; O 15.51%

Boiling Point: Bp 118-122°

Optical Rotation: [α]_D²⁵ +23.22 (c, 0.9 in EtOH)

Aldrich: 46202-0

>>Derivative: Methiodide

Melting Point: Mp 174-175°

Optical Rotation: [α]_D²⁴ +27.27 (c, 2.2 in EtOH aq.)

>>Derivative: O-Ac

Molecular Formula: C₇H₁₅NO₂

Molecular Weight: 145.201

Accurate Mass: 145.110279

Percentage Composition: C 57.90%; H 10.41%; N 9.65%; O 22.04%

Melting Point: Mp 177.5-178.5° (as methiodide)

Optical Rotation: [α]_D²² +27 (c, 2 in EtOH aq.) (methiodide)

>>Variant: (±)-form

CAS Registry Number: 53657-16-2

Molecular Formula: C₅H₁₃NO

Molecular Weight: 103.164

Accurate Mass: 103.099714

Percentage Composition: C 58.21%; H 12.70%; N 13.58%; O 15.51%

Boiling Point: Bp 124-125°

Hazard & Toxicity: Fl. p. 27°

>>Derivative: Picrate

Melting Point: Mp 72°

References: