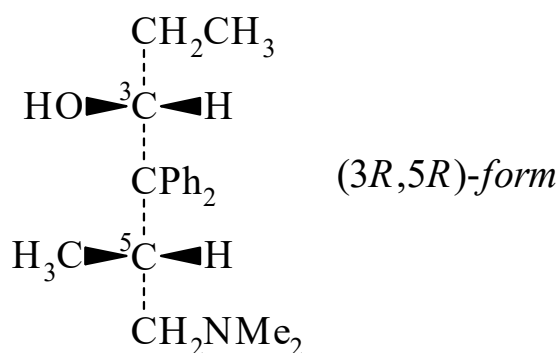




>>Entry Name: Isomethadol

Synonym(s): β -[2-(Dimethylamino)-2-methylethyl]- α -ethyl- β -phenylbenzeneethanol, 9Cl. 6-Dimethylamino-5-methyl-4,4-diphenyl-3-hexanol, 8Cl



CAS Registry Number: 25117-79-7

Molecular Formula: C₂₁H₂₉NO

Molecular Weight: 311.466

Accurate Mass: 311.224914

Percentage Composition: C 80.98%; H 9.38%; N 4.50%; O 5.14%

Use/Importance: Analgesic

Calculated Log P Data: Log P 3.45 (calc)

>>Variant: (3*R*,5*R*)-form

Synonym(s): (–)- β -form

CAS Registry Number: 26532-77-4

Molecular Formula: C₂₁H₂₉NO

Molecular Weight: 311.466

Accurate Mass: 311.224914

Percentage Composition: C 80.98%; H 9.38%; N 4.50%; O 5.14%

Melting Point: Mp 93.5-94.5°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -13.8$ (c, 1.09 in EtOH)

>>Derivative: Hydrochloride

CAS Registry Number: 49570-66-3

Melting Point: Mp 241-243°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -13.5$ (c, 1.56 in H₂O)

>>Variant: (3*R*,5*S*)-form

Synonym(s): (–)- α -form

CAS Registry Number: 14347-92-3

Molecular Formula: C₂₁H₂₉NO

Molecular Weight: 311.466

Accurate Mass: 311.224914

Percentage Composition: C 80.98%; H 9.38%; N 4.50%; O 5.14%

Physical Description: Prisms (EtOH aq.)

Melting Point: Mp 125-126°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -19.7$ (c, 1.43 in EtOH)

Other Data: Shows little analgesic activity

>>Derivative: Hydrochloride

Physical Description: Rectangular plates +½ H₂O (Me₂CO)

Melting Point: Mp 202-204°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -9.6$ (c, 2.93 in H₂O)

>>Variant: (3*S*,5*R*)-form

Synonym(s): (+)- α -form

CAS Registry Number: 26533-05-1

Molecular Formula: C₂₁H₂₉NO

Molecular Weight: 311.466

Accurate Mass: 311.224914

Percentage Composition: C 80.98%; H 9.38%; N 4.50%; O 5.14%

Melting Point: Mp 124.5-125.5°

Optical Rotation: $[\alpha]$