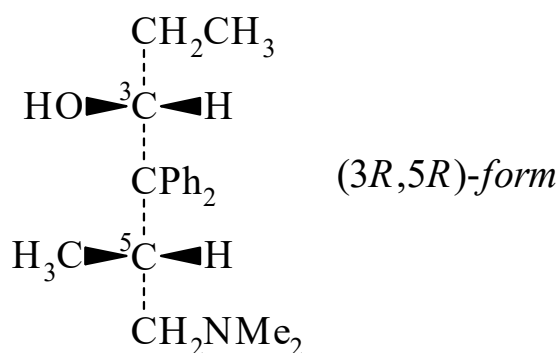




>>Entry Name: Isomethadol

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: $C_{21}H_{29}NO$

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: (3R,5R)-form

Synonym(s): (-)- β -form

CAS Registry Number: 26532-77-4

Molecular Formula: $C_{21}H_{29}NO$

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: $[\alpha]_D^{20} -13.8$ (c, 1.09 in EtOH)

>>Derivative: Hydrochloride

CAS Registry Number: 49570-66-3

Melting Point: Mp 241-243°

Optical Rotation: $[\alpha]_D^{20} -13.5$ (c, 1.56 in H_2O)

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

Synonym(s): (-)- α -form

CAS Registry Number: 14347-92-3

Molecular Formula: $C_{21}H_{29}NO$

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: $[\alpha]_D^{20} -19.7$ (c, 1.43 in EtOH)

Other Data: Shows little analgesic activity

>>Derivative: Hydrochloride

Physical Description: Rectangular plates + $\frac{1}{2}$ H_2O (Me_2CO)

Melting Point: Mp 202-204°

Optical Rotation: $[\alpha]_D^{20} -9.6$ (c, 2.93 in H_2O)

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

Synonym(s): (+)- α -form

CAS Registry Number: 26533-05-1

Molecular Formula: $C_{21}H_{29}NO$

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: $[\alpha]$