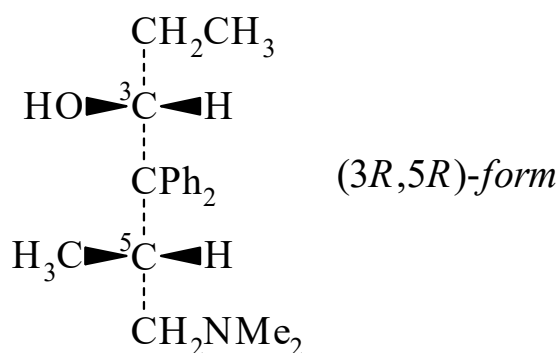




>>Entry Name: Isomethadol

Synonym(s):  $\beta$ -[2-(Dimethylamino)-2-methylethyl]- $\alpha$ -ethyl- $\beta$ -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): (-)- $\beta$ -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): (-)- $\alpha$ -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): (+)- $\alpha$ -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:  $[\alpha]$