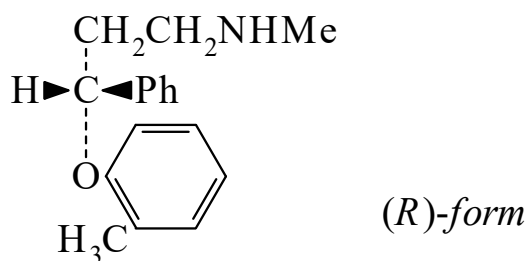




>>Entry Name: Tomoxetine, INN

Synonym(s): *N*-Methyl- γ -(2-methylphenoxy)benzenepropanamine, 9Cl. *N*-Methyl-3-phenoxy-3-phenyl-1-propylamine



CAS Registry Number: 63940-51-2

Related CAS Registry Numbers(s): 82857-39-4 105314-53-2

Molecular Formula: C₁₇H₂₁NO

Molecular Weight: 255.359

Accurate Mass: 255.162314

Percentage Composition: C 79.96%; H 8.29%; N 5.49%; O 6.27%

Use/Importance: Noradrenaline reuptake inhibitor; antidepressant

Calculated Log P Data: Log P 3.42 (uncertain value) (calc)

>>Variant: (*R*)-form

CAS Registry Number: 83015-26-3

Molecular Formula: C₁₇H₂₁NO

Molecular Weight: 255.359

Accurate Mass: 255.162314

Percentage Composition: C 79.96%; H 8.29%; N 5.49%; O 6.27%

Other Data: Pharmacol. active isomer

>>Derivative: Hydrochloride

Synonym(s): Tomoxetine hydrochloride, USAN. LY 139603

CAS Registry Number: 82248-59-7

Physical Description: Cryst. (CH₂Cl₂/EtOAc)

Melting Point: Mp 165-167°

Optical Rotation: [α]_D²⁵ -37.6 (c, 1 in MeOH)

>>Variant: ($\pm$)-form

CAS Registry Number: 105314-52-1

Molecular Formula: C₁₇H₂₁NO

Molecular Weight: 255.359

Accurate Mass: 255.162314

Percentage Composition: C 79.96%; H 8.29%; N 5.49%; O 6.27%

>>Derivative: Hydrochloride

Synonym(s): LY 135252

CAS Registry Number: 82857-40-7

Physical Description: Cryst. (CH₂Cl₂/EtOAc)

Melting Point: Mp 132-135°

References:

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