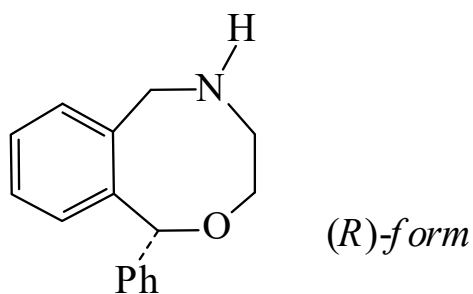




>>Entry Name: 3,4,5,6-Tetrahydro-1-phenyl-1*H*-2,5-benzoxazocine, 9CI

Synonym(s): *N*-Demethylnefopam



CAS Registry Number: 46868-19-3

Related CAS Registry Numbers(s): 53586-18-8 53648-31-0 69319-31-9 69319-32-0 108941-81-7

Molecular Formula: C₁₆H₁₇NO

Molecular Weight: 239.316

Accurate Mass: 239.131014

Percentage Composition: C 80.30%; H 7.16%; N 5.85%; O 6.69%

Source/Synthesis: Metab. of Nefopam

>>Variant: (*R*)-form

Molecular Formula: C₁₆H₁₇NO

Molecular Weight: 239.316

Accurate Mass: 239.131014

Percentage Composition: C 80.30%; H 7.16%; N 5.85%; O 6.69%

>>Derivative: *N*-Me

Molecular Formula: C₁₇H₁₉NO

Molecular Weight: 253.343

Percentage Composition: C 80.60%; H 7.56%; N 5.53%; O 6.32%

>>Derivative: *N*-Me; hydrochloride

CAS Registry Number: 53625-25-5

Physical Description: Prisms (Me₂CO)

Melting Point: Mp 108-183°

Optical Rotation: $[\alpha]_D^{27} -119$ (c, 1 in DMSO)

>>Variant: (±)-form

CAS Registry Number: 53586-17-7

Molecular Formula: C₁₆H₁₇NO

Molecular Weight: 239.316

Accurate Mass: 239.131014

Percentage Composition: C 80.30%; H 7.16%; N 5.85%; O 6.69%

>>Derivative: Hydrochloride

CAS Registry Number: 147656-98-2

Physical Description: Cryst.

Melting Point: Mp 202-203 dec.°

>>Derivative: *N*-Me

Synonym(s): Nefopam, BAN, INN. 3,4,5,6-Tetrahydro-5-methyl-1-phenyl-1*H*-2,5-benzoxazocine, 9CI. Fenazoxine

CAS Registry Number: 13669-70-0

Molecular Formula: C₁₇H₁₉NO

Molecular Weight: 253.343

Accurate Mass: 253.146664

Percentage Composition: C 80.60%; H 7.56%; N 5.53%; O 6.32%

Use/Importance: Antidepressant, muscle relaxant, analgesic

Calculated Log P Data: Log P 3.68 (calc)

Hazard & Toxicity: LD₅₀ (rat, orl) 178 mg/kg