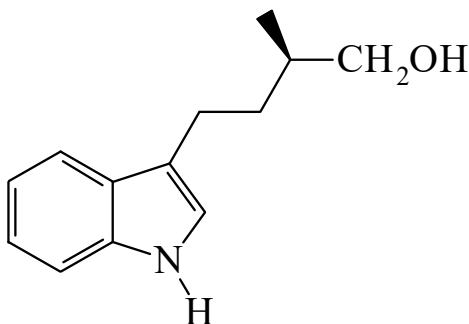




>>Entry Name: 2-Methyl-4-(3-indolyl)-1-butanol

Synonym(s): β -Methyl-1*H*-indole-3-butanol, 9Cl. **Paniculidine C**. Paniculol



Related CAS Registry Numbers(s): 120786-74-5 129172-71-0

Molecular Formula: C₁₃H₁₇NO

Molecular Weight: 203.283

Accurate Mass: 203.131014

Percentage Composition: C 76.81%; H 8.43%; N 6.89%; O 7.87%

>>Variant: (*R*)-form

CAS Registry Number: 97399-95-6

Molecular Formula: C₁₃H₁₇NO

Molecular Weight: 203.283

Accurate Mass: 203.131014

Percentage Composition: C 76.81%; H 8.43%; N 6.89%; O 7.87%

Biological Source: Alkaloid from the root bark of *Murraya paniculata* (Rutaceae)

Physical Description: Oil

Optical Rotation: $[\alpha]_{\text{D}}^{20} +45$ (c, 0.035 in CHCl₃)

>>Derivative: *N*-Methoxy

Synonym(s): 1-Methoxy- β -methyl-1*H*-indole-3-butanol, 9Cl. **Paniculidine B**

CAS Registry Number: 97399-94-5

Molecular Formula: C₁₄H₁₉NO₂

Molecular Weight: 233.31

Accurate Mass: 233.141579

Percentage Composition: C 72.07%; H 8.21%; N 6.00%; O 13.72%

Biological Source: Alkaloid from root bark of *Murraya paniculata* (Rutaceae)

Physical Description: Oil

Optical Rotation: $[\alpha]_{\text{D}}^{20} +21$ (c, 0.025 in CHCl₃)

>>Derivative: Carboxylic acid, Me ester

Synonym(s): **Paniculidine A**

CAS Registry Number: 97399-93-4

Molecular Formula: C₁₄H₁₇NO₂

Molecular Weight: 231.294

Accurate Mass: 231.125929

Percentage Composition: C 72.70%; H 7.41%; N 6.06%; O 13.83%

Biological Source: Alkaloid from root bark of *Murraya paniculata* (Rutaceae)

Physical Description: Oil

Optical Rotation: $[\alpha]_{\text{D}}^{24} -31.9$ (c, 0.1 in CHCl₃)

References:

- Kinoshita, T. *et al.*, *Chem. Pharm. Bull.*, 1985, **33**, 1770, (*uv, ir, pmr, cmr, ms, struct, synth*)
Somei, M. *et al.*, *Chem. Pharm. Bull.*, 1985, **33**, 5147, (*synth*)
Cheskis, B.A. *et al.*, *J.C.S. Perkin I*, 1989, 1353
Kinoshita, T. *et al.*, *Phytochemistry*, 1989, **28**, 147, (*isol, uv, ir, pmr, cmr, ms, struct*)
Boumendjel, A. *et al.*, *Bull. Soc. Chim. Fr.*, 1990, 645, (*synth, Paniculidine A*)
Ito, C. *et al.*, *J.C.S. Perkin I*, 1990, 2047, (*isol, pmr*)
Cheskis, B.A. *et al.*, *Zh. Org. Khim.*, 1990, **26**, 425, (*synth*)