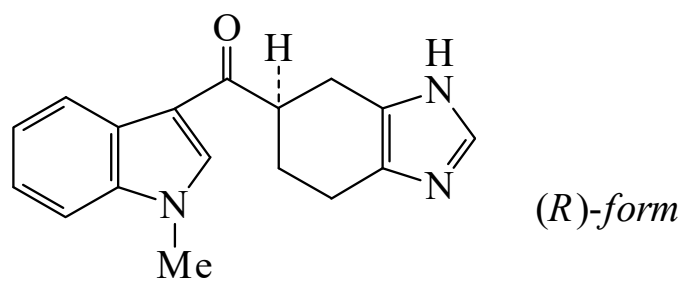




>>Entry Name: Ramosetron, INN

Synonym(s): (1-Methyl-1*H*-indol-3-yl)(4,5,6,7-tetrahydro-1*H*-benzimidazol-5-yl)methanone. Nausea. YM 060



CAS Registry Number: 132036-39-6

Related CAS Registry Numbers(s): 132036-89-6 132907-67-6 137887-27-5 138665-45-9 138680-81-6

Molecular Formula: C₁₇H₁₇N₃O

Molecular Weight: 279.341

Accurate Mass: 279.137162

Percentage Composition: C 73.10%; H 6.13%; N 15.04%; O 5.73%

Use/Importance: 5-Hydroxytryptamine (5HT₃) receptor antagonist. Potential antiemetic agent

Development Status: Launched 1996 (Japan) (Yamanouchi)

Calculated Log P Data: Log P 1.98 (calc)

>>Variant: (*R*)-form

CAS Registry Number: 132036-88-5

Molecular Formula: C₁₇H₁₇N₃O

Molecular Weight: 279.341

Accurate Mass: 279.137162

Percentage Composition: C 73.10%; H 6.13%; N 15.04%; O 5.73%

Physical Description: Foam

Optical Rotation: $[\alpha]_{\text{D}}^{20} -16.5$ (c, 1.13 in MeOH)

>>Derivative: Hydrochloride

Synonym(s): YM 060

CAS Registry Number: 132907-72-3

Hazard & Toxicity: LD₅₀ (rat, ivn) 151 mg/kg. Exp. reprod. effects

>>Variant: (*S*)-form

CAS Registry Number: 132036-90-9

Molecular Formula: C₁₇H₁₇N₃O

Molecular Weight: 279.341

Accurate Mass: 279.137162

Percentage Composition: C 73.10%; H 6.13%; N 15.04%; O 5.73%

Physical Description: Foam

Optical Rotation: $[\alpha]_{\text{D}}^{20} +28.3$ (c, 1.14 in MeOH)

>>Variant: (±)-form

Molecular Formula: C₁₇H₁₇N₃O

Molecular Weight: 279.341

Accurate Mass: 279.137162

Percentage Composition: C 73.10%; H 6.13%; N 15.04%; O 5.73%

Physical Description: Cryst.

Melting Point: Mp 139-141°

>>Derivative: Fumarate

Physical Description: Cryst. (EtOAc/MeOH)

Melting Point: Mp 97-102°

>>Derivative: Fumarate (2:1)

Melting Point: Mp 224-225°

References: