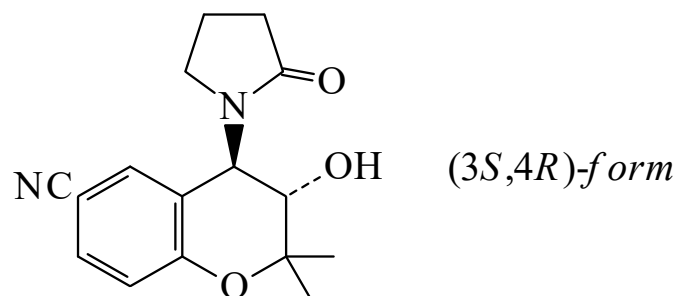




>>Entry Name: Cromakalim, BAN, INN

Synonym(s): 3,4-Dihydro-3-hydroxy-2,2-dimethyl-4-(2-oxo-1-pyrrolidinyl)-2H-1-benzopyran-6-carbonitrile, 9Cl. BRL 34915



CAS Registry Number: 86776-67-2

Related CAS Registry Numbers(s): 94535-51-0 99095-58-6 148811-93-2 150871-62-8

Molecular Formula: C₁₆H₁₈N₂O₃

Molecular Weight: 286.33

Accurate Mass: 286.131743

Percentage Composition: C 67.12%; H 6.34%; N 9.78%; O 16.76%

Biological Use/Importance: Potent vasodilator functioning by hyperpolarisation of vascular smooth muscle membranes and opening of K channels. Antihypertensive agent. Antiasthmatic. Smooth muscle relaxant

Calculated Log P Data: Log P 1.11 (uncertain value) (calc)

Other Data: (3*R*,4*R*)-Form is more pharmacol. active than (3*R*,4*S*)-form

>>Variant: (3*S*,4*R*)-form

Synonym(s): Levromakalim, BAN, INN, USAN. Lemakalim. BRL 38227

CAS Registry Number: 94535-50-9

Molecular Formula: C₁₆H₁₈N₂O₃

Molecular Weight: 286.33

Accurate Mass: 286.131743

Percentage Composition: C 67.12%; H 6.34%; N 9.78%; O 16.76%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 242-244°

Optical Rotation: $[\alpha]_D^{26} -52.2$ (c, 1 in CHCl₃)

Other Data: Most pharmacol. active isomer

>>Variant: (3*S*,4*S*)-form

CAS Registry Number: 148811-94-3

Molecular Formula: C₁₆H₁₈N₂O₃

Molecular Weight: 286.33

Accurate Mass: 286.131743

Percentage Composition: C 67.12%; H 6.34%; N 9.78%; O 16.76%

Optical Rotation: $[\alpha]_D^{20} -84.1$ (c, 1.18 in EtOH)

>>Variant: (3*RS*,4*RS*)-form

Synonym(s): (±)-*cis*-form

CAS Registry Number: 103774-92-1

Molecular Formula: C₁₆H₁₈N₂O₃

Molecular Weight: 286.33

Accurate Mass: 286.131743

Percentage Composition: C 67.12%; H 6.34%; N 9.78%; O 16.76%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 207-208°

>>Variant: (3*SR*,4*RS*)-form

Synonym(s): (±)-*trans*-form

CAS Registry Number: 94470-67-4

Molecular Formula: C₁₆H₁₈N₂O₃

Molecular Weight: 286.33

Accurate Mass: 286.131743

Percentage Composition: C 67.12%; H 6.34%; N 9.78%; O 16.76%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 230-231°

Sigma: C1055