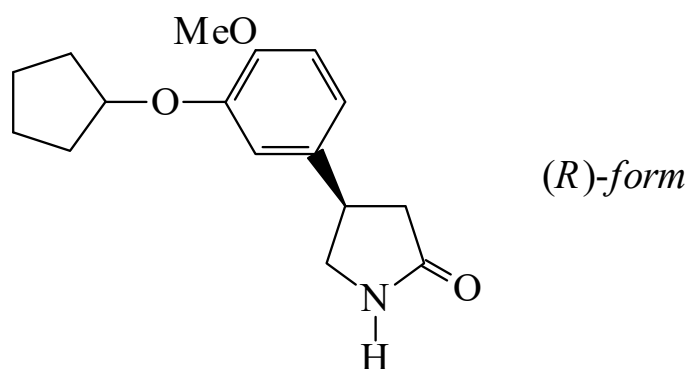




>>Entry Name: Rolipram, INN, USAN

Synonym(s): 4-[3-(Cyclopentyloxy)-4-methoxyphenyl]-2-pyrrolidinone, gcl. ZK 62711



CAS Registry Number: 61413-54-5

Molecular Formula: C₁₆H₂₁NO₃

Molecular Weight: 275.347

Accurate Mass: 275.152144

Percentage Composition: C 69.79%; H 7.69%; N 5.09%; O 17.43%

Use/Importance: Phosphodiesterase (type IV) inhibitor. Inhibited development of autoimmune encephalomyelitis in animal models. Implications for treatment of multiple sclerosis. Antiinflammatory props. Tranquilliser

Calculated Log P Data: Log P 1.21 (calc)

Sigma: R6520

>>Variant: (*R*)-form

CAS Registry Number: 85416-75-7

Molecular Formula: C₁₆H₂₁NO₃

Molecular Weight: 275.347

Accurate Mass: 275.152144

Percentage Composition: C 69.79%; H 7.69%; N 5.09%; O 17.43%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 131-133°

Optical Rotation: $[\alpha]_D^{24} -31$ (c, 0.5 in MeOH) (>99% ee)

Other Data: Pharmacol. active isomer

>>Variant: (*S*)-form

CAS Registry Number: 85416-73-5

Molecular Formula: C₁₆H₂₁NO₃

Molecular Weight: 275.347

Accurate Mass: 275.152144

Percentage Composition: C 69.79%; H 7.69%; N 5.09%; O 17.43%

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 129-131°

Optical Rotation: $[\alpha]_D^{24} +30.9$ (c, 0.5 in MeOH) (>98% ee)

>>Variant: (±)-form

CAS Registry Number: 85416-74-6

Molecular Formula: C₁₆H₂₁NO₃

Molecular Weight: 275.347

Accurate Mass: 275.152144

Percentage Composition: C 69.79%; H 7.69%; N 5.09%; O 17.43%

Physical Description: Solid

Melting Point: Mp 132°

References: