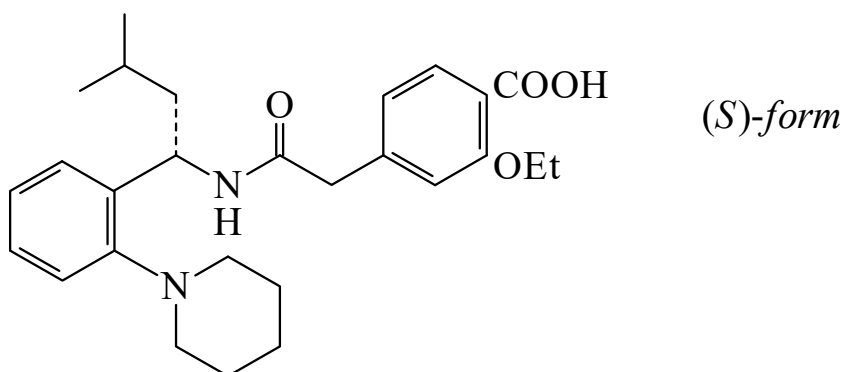




>>Entry Name: Repaglinide, BAN, INN, USAN

Synonym(s): 2-Ethoxy-4-[2-[[3-methyl-1-[2-(1-piperidiny)phenyl]butyl]amino]-2-oxoethyl]benzoic acid, 9Cl. Novonorm. Prandin. AGEE 388 ZW



Related CAS Registry Numbers(s): 108157-53-5 147770-06-7 147770-08-9 147852-25-3

Molecular Formula: C₂₇H₃₆N₂O₄

Molecular Weight: 452.592

Accurate Mass: 452.267508

Percentage Composition: C 71.65%; H 8.02%; N 6.19%; O 14.14%

Biological Use/Importance: Antihyperglycaemic agent used in the treatment of diabetes

Development Status: Approved by FDA (1997)

Calculated Log P Data: Log P 4.99 (uncertain value) (calc)

>>Variant: (R)-form

CAS Registry Number: 147852-26-4

Molecular Formula: C₂₇H₃₆N₂O₄

Molecular Weight: 452.592

Accurate Mass: 452.267508

Percentage Composition: C 71.65%; H 8.02%; N 6.19%; O 14.14%

Physical Description: Cryst. (toluene/petrol) + 0.4 H₂O

Melting Point: Mp 103-105° (as hydrate)

Optical Rotation: $[\alpha]_D^{20}$ -6.5 (c, 1 in MeOH) (99.7% ee)

>>Derivative: Et ester

Molecular Formula: C₂₉H₄₀N₂O₄

Molecular Weight: 480.646

Accurate Mass: 480.298808

Percentage Composition: C 72.47%; H 8.39%; N 5.83%; O 13.31%

Physical Description: Cryst. (petrol/Me₂CO)

Melting Point: Mp 122-124°

Optical Rotation: $[\alpha]_D^{20}$ -8.3 (c, 1 in MeOH)

>>Variant: (S)-form

CAS Registry Number: 135062-02-1

Molecular Formula: C₂₇H₃₆N₂O₄

Molecular Weight: 452.592

Accurate Mass: 452.267508

Percentage Composition: C 71.65%; H 8.02%; N 6.19%; O 14.14%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 130-131° (126-128°)

Optical Rotation: $[\alpha]_D^{20}$ +6.97 (c, 0.975 in MeOH)

Other Data: Pharmacol. active isomer

>>Variant: (±)-form

CAS Registry Number: 135969-54-9

Molecular Formula: C₂₇H₃₆N₂O₄

Molecular Weight: 452.592

Accurate Mass: 452.267508

Percentage Composition: C 71.65%; H 8.02%; N 6.19%; O 14.14%

Physical Description: Cryst.

Melting Point: Mp 90-92°