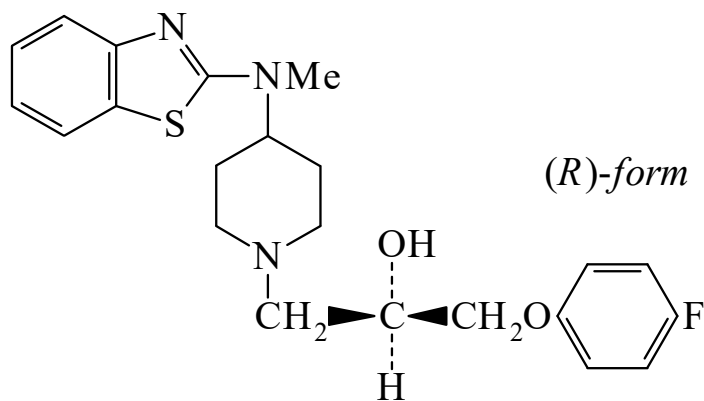




>>Entry Name: Sabeluzole, BAN, INN, USAN

Synonym(s): 4-(2-Benzothiazolylmethylamino)- α -[(4-fluorophenoxy)methyl]-1-piperidineethanol, 9CI. R 58735



CAS Registry Number: 104592-54-3

Related CAS Registry Numbers(s): 104153-38-0 104592-63-4

Molecular Formula: C₂₂H₂₆FN₃O₂S

Molecular Weight: 415.531

Accurate Mass: 415.172975

Percentage Composition: C 63.59%; H 6.31%; F 4.57%; N 10.11%; O 7.70%; S 7.72%

Use/Importance: Calcium channel antagonist. Antiepileptic, antihypoxic agent. Memory enhancer (nootropic)

Experimental Log P Data: Log P 4.61 (exp)

Calculated Log P Data: Log P 4.37 (calc)

Other Data: Enantiomers show similar activity

>>Variant: (*R*)-form

Synonym(s): R 84439

CAS Registry Number: 104607-84-3

Molecular Formula: C₂₂H₂₆FN₃O₂S

Molecular Weight: 415.531

Accurate Mass: 415.172975

Percentage Composition: C 63.59%; H 6.31%; F 4.57%; N 10.11%; O 7.70%; S 7.72%

Optical Rotation: $[\alpha]_D^{20} -1.64$ (c, 1 in MeOH)

>>Variant: (*S*)-form

Synonym(s): R 84440

CAS Registry Number: 104712-64-3

Molecular Formula: C₂₂H₂₆FN₃O₂S

Molecular Weight: 415.531

Accurate Mass: 415.172975

Percentage Composition: C 63.59%; H 6.31%; F 4.57%; N 10.11%; O 7.70%; S 7.72%

Optical Rotation: $[\alpha]_D^{20} +1.64$ (c, 1 in MeOH)

>>Variant: ($\pm$)-form

CAS Registry Number: 104383-17-7

Molecular Formula: C₂₂H₂₆FN₃O₂S

Molecular Weight: 415.531

Accurate Mass: 415.172975

Percentage Composition: C 63.59%; H 6.31%; F 4.57%; N 10.11%; O 7.70%; S 7.72%

>>Derivative: Hydrochloride

Melting Point: Mp 168-178°

>>Derivative: Fumarate (2:1)

CAS Registry Number: 104592-55-4

Melting Point: Mp 169.5°

References: