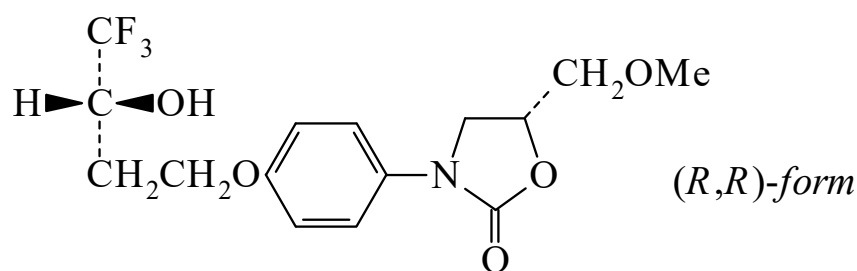




>>Entry Name: Befloxatone, INN

Synonym(s): 5-(Methoxymethyl)-3-[4-(4,4,4-trifluoro-3-hydroxybutoxy)phenyl]-2-oxazolidinone, 9CI



Related CAS Registry Numbers(s): 135968-58-0 135968-59-1 135968-67-1 135968-70-6

Molecular Formula: C₁₅H₁₈F₃NO₅

Molecular Weight: 349.306

Accurate Mass: 349.113708

Percentage Composition: C 51.58%; H 5.19%; F 16.32%; N 4.01%; O 22.90%

Use/Importance: Monoamine oxidase inhibitor. Potential antidepressant

Calculated Log P Data: Log P 1.06 (uncertain value) (calc)

>>Variant: (3*R*,5*R*)-form

Synonym(s): MD 370503

CAS Registry Number: 134564-82-2

Molecular Formula: C₁₅H₁₈F₃NO₅

Molecular Weight: 349.306

Accurate Mass: 349.113708

Percentage Composition: C 51.58%; H 5.19%; F 16.32%; N 4.01%; O 22.90%

Physical Description: Cryst. (EtOH/diisopropyl ether)

Melting Point: Mp 101°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -11.5$ (c, 1 in CH₂Cl₂)

Other Data: Pharmacol. active isomer

>>Variant: (3*R*,5*S*)-form

Synonym(s): MD 230151

CAS Registry Number: 135859-17-5

Molecular Formula: C₁₅H₁₈F₃NO₅

Molecular Weight: 349.306

Accurate Mass: 349.113708

Percentage Composition: C 51.58%; H 5.19%; F 16.32%; N 4.01%; O 22.90%

Melting Point: Mp 123°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +59.2$ (c, 1 in CH₂Cl₂)

>>Variant: (3*S*,5*R*)-form

Synonym(s): MD 370504

CAS Registry Number: 135859-19-7

Molecular Formula: C₁₅H₁₈F₃NO₅

Molecular Weight: 349.306

Accurate Mass: 349.113708

Percentage Composition: C 51.58%; H 5.19%; F 16.32%; N 4.01%; O 22.90%

Melting Point: Mp 121°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -59.7$ (c, 1 in CH₂Cl₂)

>>Variant: (3*S*,5*S*)-form

Synonym(s): MD 230154

CAS Registry Number: 135859-18-6

Molecular Formula: C₁₅H₁₈F₃NO₅

Molecular Weight: 349.306

Accurate Mass: 349.113708

Percentage Composition: C 51.58%; H 5.19%; F 16.32%; N 4.01%; O 22.90%

Melting Point: Mp 100°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +9.9$ (c, 1 in CH₂Cl₂)

References: