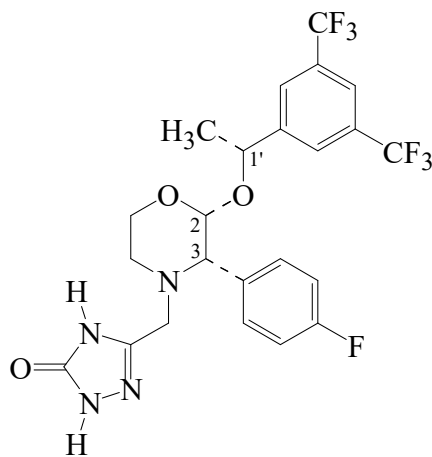




>>Entry Name: Aprepitant, INN

Synonym(s): 5-[[2-[1-[3,5-Bis(trifluoromethyl)phenyl]ethoxy]-3-(4-fluorophenyl)-4-morpholinyl]methyl]-1,2-dihydro-3H-1,2,4-triazol-3-one, 9Cl. MK 869. L 754030



Related CAS Registry Numbers(s): 170902-81-5 172822-28-5 172822-29-6

Molecular Formula: C₂₃H₂₁F₇N₄O₃

Molecular Weight: 534.433

Accurate Mass: 534.150187

Percentage Composition: C 51.69%; H 3.96%; F 24.88%; N 10.48%; O 8.98%

Biological Use/Importance: Tachykinin NK-1 receptor antagonist. Inhibits cisplatin-induced emesis. Antiemetic in chemotherapy-induced emesis. Antidepressant. Used in the treatment of psychiatric conditions

>>Variant: (1'R,2R,3S)-form

CAS Registry Number: 170729-80-3

Molecular Formula: C₂₃H₂₁F₇N₄O₃

Molecular Weight: 534.433

Accurate Mass: 534.150187

Percentage Composition: C 51.69%; H 3.96%; F 24.88%; N 10.48%; O 8.98%

Melting Point: Mp 244-245°

Optical Rotation: [α]_D +68.1 (c, 0.6 in MeOH)

References:

- Pat. Coop. Treaty (WIPO)*, 1995, *Merck*, 95 16 679; *CA*, **124**, 29769x, (*synth, isomers, pharmacol*)
Pat. Coop. Treaty (WIPO), 1995, *Merck*, 95 23 798; *CA*, **124**, 146177p, (*synth, isomers, pharmacol*)
Hale, J.J. *et al.*, *J. Med. Chem.*, 1998, **41**, 4607-4614; 2000, **43**, 1234-1241, (*synth, pharmacol*)
Kramer, M.S. *et al.*, *Science (Washington, D.C.)*, 1998, **281**, 1640-1645, (*pharmacol*)
Tattersall, F.D. *et al.*, *Neuropharmacology*, 2000, **39**, 652-663, (*pharmacol*)