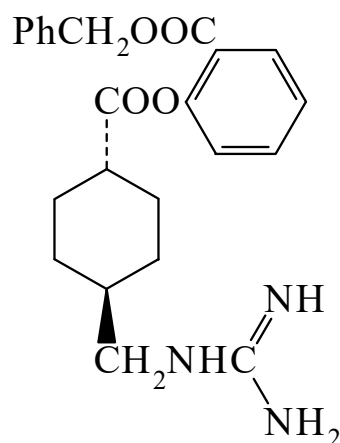




>>Entry Name: Benexate, INN

Synonym(s): Phenylmethyl 2-[[[4-[[[aminoiminomethyl]amino]methyl]cyclohexyl]carbonyl]oxy]benzoate, 9CI. Benzyl [4-(4-guanidinylmethyl)cyclohexyl] phthalate. Beguhexate



CAS Registry Number: 78718-52-2

Related CAS Registry Numbers(s): 91574-91-3 115910-12-8

Molecular Formula: C₂₃H₂₇N₃O₄

Molecular Weight: 409.484

Accurate Mass: 409.200157

Percentage Composition: C 67.46%; H 6.65%; N 10.26%; O 15.63%

Biological Use/Importance: Protease inhibitor. Antiulcerogenic. Gastric secretion inhibitor

Development Status: Launched 1987

Calculated Log P Data: Log P 3.24 (uncertain value) (calc)

Hazard & Toxicity: LD₅₀ (rat, orl) 8010 mg/kg

>>Derivative: Hydrochloride

Synonym(s): TKG 01. CM 125

CAS Registry Number: 78718-25-9

Melting Point: Mp 82-84°

>>Derivative: Hydrochloride, β-cyclodextrin clathrate compd. (1:1)

Synonym(s): Benexate hydrochloride β-cyclodextrin clathrate, JAN. Benexate. Lonmiel. Ulgut. TA 903

CAS Registry Number: 91574-91-3

Use/Importance: Antiulcerogenic

References:

Satoh, T. *et al.*, *J. Pharmacobio-Dyn.*, 1982, **5**, S-51, (*pharmacol*)

U.S. Pat., 1982, *Nippon ChemiPhar*, 4 348 410; *CA*, **95**, 114902n, (*synth*)

U.S. Pat., 1984, *Teikoku*, 4 478 995; *CA*, **99**, 22240z, (*cyclodextrin compd*)

Satoh, T. *et al.*, *Chem. Pharm. Bull.*, 1985, **33**, 647, (*synth, pharmacol*)

Martindale, The Extra Pharmacopoeia, 30th edn., *Pharmaceutical Press*, 1993, 871