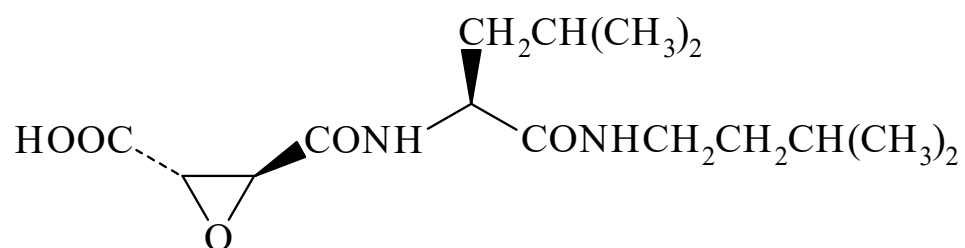




>>Entry Name: 3-[3-Methyl-1-(3-methylbutylcarbamoyl)butylcarbamoyl]-2-oxiranecarboxylic acid

Synonym(s): E-64



CAS Registry Number: 76684-89-4

Molecular Formula: C₁₅H₂₆N₂O₅

Molecular Weight: 314.381

Accurate Mass: 314.184173

Percentage Composition: C 57.31%; H 8.34%; N 8.91%; O 25.45%

Use/Importance: Potent inhibitor of cysteine proteinases, on trial (1987) against muscular dystrophy

Other Data: Stereochem. is all (S)

Hazard & Toxicity: LD₅₀ (rat, ipr) 2140 mg/kg

Sigma: E0514

>>Derivative: Et ester

Synonym(s): Aloxistatin, INN. Loxistatin. Estate. EST. Ep-453

CAS Registry Number: 88321-09-9

Molecular Formula: C₁₇H₃₀N₂O₅

Molecular Weight: 342.434

Accurate Mass: 342.215473

Percentage Composition: C 59.63%; H 8.83%; N 8.18%; O 23.36%

Use/Importance: More soluble deriv. of parent acid, showing improved absorbability

Physical Description: Fine needles (EtOH)

Melting Point: Mp 126.2°

Optical Rotation: [α]_D²⁰ +51.7 (c, 1 in EtOH)

Other Data: Diastereoisomers also prepd.

Hazard & Toxicity: LD₅₀ (rat, ipr) 2050 mg/kg. Exp. reprod. and teratogenic effects

Sigma: E8640

References:

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Ishida, T. *et al.*, *J.C.S. Perkin 2*, 1988, 851, (*cryst struct, conformn*)

Kai, M. *et al.*, *J. Chromatogr.*, 1993, **621**, 181, (*hplc*)

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