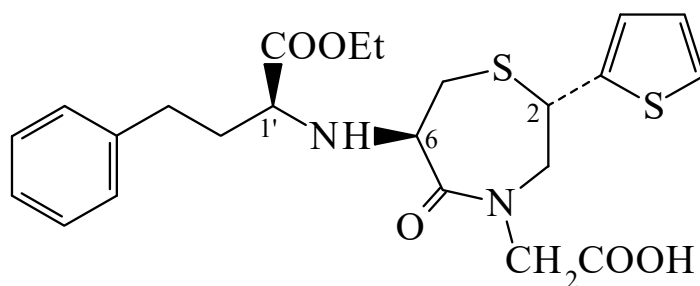




>>Entry Name: **Temocapril**, BAN, INN

Synonym(s): 6-[[1-(Ethoxycarbonyl)-3-phenylpropyl]amino]tetrahydro-5-oxo-2-(2-thienyl)-1,4-thiazepine-4(5*H*)-acetic acid. Acecol. Escol. Locapril. CS 622. RS 5142



(1'*S*,2*S*,6*R*)-form

Molecular Formula: C₂₃H₂₈N₂O₅S₂

Molecular Weight: 476.617

Accurate Mass: 476.143963

Percentage Composition: C 57.96%; H 5.92%; N 5.88%; O 16.78%; S 13.46%

Use/Importance: Angiotensin-converting enzyme inhibitor. Antihypertensive agent

Development Status: Launched 1994 (Japan)

Calculated Log P Data: Log P 2.31 (uncertain value) (calc)

>>Variant: (1'*S*,2*S*,6*R*)-form

CAS Registry Number: 111902-57-9

Molecular Formula: C₂₃H₂₈N₂O₅S₂

Molecular Weight: 476.617

Accurate Mass: 476.143963

Percentage Composition: C 57.96%; H 5.92%; N 5.88%; O 16.78%; S 13.46%

Other Data: Pharmacol. active isomer

>>Derivative: Hydrochloride

Synonym(s): **Temocapril hydrochloride**, USAN

CAS Registry Number: 110221-44-8

Physical Description: Cryst. (EtOH/EtOAc)

Melting Point: Mp 187 dec.°

Optical Rotation: [α]_D +47.7

Hazard & Toxicity: LD₅₀ (rat, orl) >5000 mg/kg. LD₅₀ (rat, ipr) 253 mg/kg. Exp. reprod. and teratogenic effects

>>Derivative: *tert*-Butyl ester

CAS Registry Number: 110221-37-9

Molecular Formula: C₂₇H₃₆N₂O₅S₂

Molecular Weight: 532.724

Accurate Mass: 532.206563

Percentage Composition: C 60.88%; H 6.81%; N 5.26%; O 15.02%; S 12.04%

Physical Description: Syrup

Optical Rotation: [α]_D +39.3

>>Derivative: Parent acid

Synonym(s): 6-[(1-Carboxy-3-phenylpropyl)amino]tetrahydro-5-oxo-2-(2-thienyl)-1,4-thiazepine-4(5*H*)-acetic acid, 9CI. **Temocaprilat**, BAN, INN

CAS Registry Number: 110221-53-9

Molecular Formula: C₂₁H₂₄N₂O₅S₂

Molecular Weight: 448.563

Accurate Mass: 448.112663

Percentage Composition: C 56.23%; H 5.39%; N 6.25%; O 17.83%; S 14.30%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 246 dec.°

Optical Rotation: [α]_D +63.4