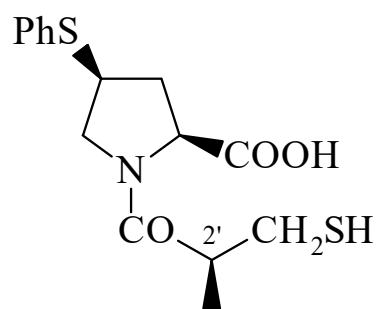




>>Entry Name: Zofenoprilat, INN

Synonym(s): 1-(3-Mercapto-2-methyl-1-oxopropyl)-4-(phenylthio)proline, 9CI. 1-(3-Mercapto-2-methylpropionyl)-4-(phenylthio)proline. SQ 26333



CAS Registry Number: 75176-37-3

Related CAS Registry Numbers(s): 113564-66-2

Molecular Formula: C₁₅H₁₉NO₃S₂

Molecular Weight: 325.452

Accurate Mass: 325.080634

Percentage Composition: C 55.36%; H 5.88%; N 4.30%; O 14.75%; S 19.71%

Metabolism: Active metabolite of Zofenopril

Biological Use/Importance: Angiotensin-converting enzyme inhibitor. Antihypertensive agent. Additional cardioprotective mechanisms

Physical Description: Oil

Optical Rotation: $[\alpha]_D -43$ (c, 1 in EtOH)

Calculated Log P Data: Log P 3.12 (calc)

Other Data: Stereochem. is (2*S*,2'*S*,4*S*)

>>Derivative: Arginine salt (1:1)

Synonym(s): Zofenoprilat arginine, USAN. SQ 26703

CAS Registry Number: 81872-09-5

Melting Point: Mp 126-128°

Optical Rotation: $[\alpha]_D -44$ (c, 1 in MeOH)

>>Derivative: S-Benzoyl

Synonym(s): Zofenopril, BAN, INN. 1-[3-(Benzoylthio)-2-methyl-1-oxopropyl]-4-(phenylthio)-L-proline, 9CI

CAS Registry Number: 81872-10-8

Molecular Formula: C₂₂H₂₃NO₄S₂

Molecular Weight: 429.56

Accurate Mass: 429.106849

Percentage Composition: C 61.51%; H 5.40%; N 3.26%; O 14.90%; S 14.93%

Metabolism: Metab. *in vivo* to parent acid

Biological Use/Importance: ACE inhibitor. Antihypertensive agent

Calculated Log P Data: Log P 4.72 (uncertain value) (calc)

>>Derivative: S-Benzoyl, Ca salt (2:1)

Synonym(s): Zofenopril calcium, USAN. Zoprace. SQ 26991

CAS Registry Number: 81938-43-4

Melting Point: Mp 235-237°

>>Derivative: S-Benzoyl, K salt

CAS Registry Number: 81938-42-3

Physical Description: Cryst. + 1.5H₂O

Melting Point: Mp 195-205°

Optical Rotation: $[\alpha]_D -14$ (c, 1 in H₂O)

References: