



Formula: C<sub>9</sub>H<sub>15</sub>NO<sub>3</sub>S

MW: 217.29

CAS: 62571-86-2

MDL NUMBER: MFCD00599437

IUPAC: (2S)-1-((2S)-2-methyl-3-sulfanylpropanoyl)pyrrolidine-2-carboxylic acid

Smiles: C(O)([C@H]1N(CCC1)C([C@@H](CS)C)=O)=O

Captopril 98%

THERAPEUTIC CATEGORY: Antihypertensive

ACCEPTORS: 3

DONORS: 1

ROTATION BONDS: 5

N+O: 4

Chiral Centers: 2

LogP: 2.06

LogS: -3.37

LIPINSKI: 4

Synonyms:

1-((2s)-3-mercapto-2-methylpropionyl)-l-proline;1-(3-mercapto-2-methyl-1-oxopropyl)-l-proline;1-(d-3-mercapto-2-methyl-1-oxopropyl)-l-proline(s,s);1-(d-3-mercapto-2-methyl-1-propionyl)-,l-(s,s)-1-pyrrolidinecarboxylicaci;3-mercapto-2-methylpropionyl-proline;acediur;aceplus;acepress

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EINECS:263-607-1

Product Categories:Active Pharmaceutical Ingredients;Inhibitors;Intermediates & Fine Chemicals;Pharmaceuticals;API's;Angiotensin;APIS Captopril

Chemical Properties: mp 104-108 C(lit.) alpha -129.5 (c=1, EtOH) refractive index -127.5 (C=1.7, EtOH) solubility H2O: 0.1 g/mL, very slightly hazy, colorless Water Solubility soluble Merck 1774 Stability:Stable. Incompatible with strong oxidizing agents.

CAS DataBase Reference: 62571-86-2(

CAS DataBase Reference: ) NIST Chemistry ReferenceCaptopril(62571-86-2) Xn,Xi Risk Statements 43-63-36/37/38-40 Safety Statements 36/37-37/39-26-36-22 WGK Germany 2 RTECS UY0550000 Hazardous Substances Data62571-86-2(Hazardous Substances Data) Captopril Captopril

Usage And Synthesis:

Chemical Properties: white crystalline powder UsageOrally active angiotensin-converting enzyme (ACE) inhibitor Captopril

