

Captopril

Other names:	(-)-Captopril (2S)-1-(3-Mercapto-2-methylpropionyl)-L-proline 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 1-Pyrrolidinecarboxylic acid, 1-(D-3-mercapto-2-methyl-1-propionyl)-, L-(S,S)- 1-[(2S)-3-mercapto-2-methyl-1-oxopropyl]-L-proline Acediur Aceplus Acepress Acepril Alopresin Capoten Captolane Captopryl Captoril Cesplon D-2-Methyl-3-mercaptopropanoyl-L-proline D-3-Mercapto-2-methylpropanoyl-L-proline Dilabar Garranil Hipertil L-Proline, 1-(3-mercapto-2-methyl-1-oxopropyl)-, (S)- L-Proline, 1-[(2S)-3-mercapto-2-methyl-1-oxopropyl]- Lopirin Lopril SA 333 SQ 14,225 SQ 14225 Tensobon Tensoprel l-Captopril
Inchi:	InChI=1S/C9H15NO3S/c1-6(5-14)8(11)10-4-2-3-7(10)9(12)13/h6-7,14H,2-5H2,1H3,(H,1
InchiKey:	FAKRSMQSSFJEIM-NKWVEPMBSA-N
Formula:	C9H15NO3S
SMILES:	CC(CS)C(=O)N1CCCC1C(=O)O
Mol. weight [g/mol]:	217.28
CAS:	62571-86-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.87		Crippen Method
logp	0.628		Crippen Method
mcvol	162.150	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.38	kJ/mol	379.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62571862&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Captopril in 2-Propanol, Acetone, Acetonitrile, Methyl Acetate, Ethyl Acetate, and Butyl Acetate:	https://www.doi.org/10.1021/je900401z
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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