Captopril di-methyl derivative

Other names:	L-Proline,1-[2-methyl-3-(methylthio)-1-oxopropyl]-, methyl ester, (S)- Captopril, dimethyl
Inchi:	InChI=1S/C11H19NO3S/c1-8(7-16-3)10(13)12-6-4-5-9(12)11(14)15-2/h8-9H,4-7H2,1-3H
InchiKey:	QIDHYXZIKNWIKJ-UHFFFAOYSA-N
Formula:	C11H19NO3S
SMILES:	COC(=O)C1CCCN1C(=O)C(C)CSC
Mol. weight [g/mol]:	245.34
CAS:	97293-62-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.28		Crippen Method
logp	1.149		Crippen Method
mcvol	190.330	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97293624&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.