l-Phenylalanine, N-(2-thienylcarbonyl)-, methyl ester

Inchi: InChI=1S/C15H15NO3S/c1-19-15(18)12(10-11-6-3-2-4-7-11)16-14(17)13-8-5-9-20-13/h2

InchiKey: LIWKGUIEIXQWPB-UHFFFAOYSA-N

Formula: C15H15NO3S

SMILES: COC(=O)C(Cc1ccccc1)NC(=O)c1cccs1

Mol. weight [g/mol]: 289.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	2.262		Crippen Method
mcvol	214.330	ml/mol	McGowan Method
rinpol	2241.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299598&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices