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]: 289.36

Physical Properties

Property code	Value	Unit	Source
hvap	102.49	kJ/mol	Cheméo Relay (1.0)
ie	8.69	eV	Cheméo Relay (1.0)
log10ws	-3.35		Cheméo Relay (1.0)
logp	2.262		Crippen Method
mcvol	214.330	ml/mol	McGowan Method
rinpol	2241.00		NIST Webbook
tb	634.26	K	Cheméo Relay (1.0)
tf	367.03	K	Cheméo Relay (1.0)

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

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

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

Legend

hvap: Enthalpy of vaporization at standard conditions

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point