L-Valine, N-(2-thienylcarbonyl)-, methyl ester

Inchi: InChI=1S/C11H15NO3S/c1-7(2)9(11(14)15-3)12-10(13)8-5-4-6-16-8/h4-7,9H,1-3H3,(H,1
InchiKey: QQRCUPKKZCTUFI-UHFFFAOYSA-N
Formula: C11H15NO3S
SMILES: COC(=O)C(NC(=O)c1cccs1)C(C)C
Mol. weight [g/mol]: 241.31

Physical Properties

Property code	Value	Unit	Source
hvap	80.44	kJ/mol	Cheméo Relay (1.0)
ie	8.69	eV	Cheméo Relay (1.0)
logp	1.675		Crippen Method
mcvol	181.730	ml/mol	McGowan Method
rinpol	1767.00		NIST Webbook
rinpol	1767.00		NIST Webbook
tb	570.14	K	Cheméo Relay (1.0)
tf	383.31	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299595&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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