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
log10ws	-2.40		Crippen Method
logp	1.675		Crippen Method
mcvol	181.730	ml/mol	McGowan Method
rinpol	1767.00		NIST Webbook
rinpol	1767.00		NIST Webbook

Sources

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=U299595&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:
https://www.chemeo.com/cid/123-041-9/l-Valine-N-2-thienylcarbonyl-methyl-ester.pdf
Generated by Cheméo on 2024-05-01 11:00:37.317957681 +0000 UTC m=+16850486.238534997.

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