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

Inchi: InChI=1S/C11H15NO3S2/c1-15-11(14)8(5-7-16-2)12-10(13)9-4-3-6-17-9/h3-4,6,8H,5,7H

InchiKey: YUOSMZKMASOXEA-UHFFFAOYSA-N

Formula: C11H15NO3S2

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

Mol. weight [g/mol]: 273.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	1.773		Crippen Method
mcvol	198.080	ml/mol	McGowan Method
rinpol	2129.00		NIST Webbook
rinpol	2129.00		NIST Webbook

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=U299597&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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