Sarcosine, N-(2-thienylcarbonyl)-, isobutyl ester

Inchi: InChI=1S/C12H17NO3S/c1-9(2)8-16-11(14)7-13(3)12(15)10-5-4-6-17-10/h4-6,9H,7-8H2,

InchiKey: LNIXBQAZRSFNTG-UHFFFAOYSA-N

Formula: C12H17NO3S

SMILES: CC(C)COC(=O)CN(C)C(=O)c1cccs1

Mol. weight [g/mol]: 255.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.09		Crippen Method
logp	2.019		Crippen Method
mcvol	195.820	ml/mol	McGowan Method
rinpol	1992.00		NIST Webbook
rinpol	1992.00		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=U321463&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

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