Acetamide, N-(2,5-dimethoxyphenyl)-2-(2-thienyl)-

Inchi: InChI=1S/C14H15NO3S/c1-17-10-5-6-13(18-2)12(8-10)15-14(16)9-11-4-3-7-19-11/h3-8H

InchiKey: CHNWVENRMYNFAF-UHFFFAOYSA-N

Formula: C14H15NO3S

SMILES: COc1ccc(OC)c(NC(=O)Cc2cccs2)c1

Mol. weight [g/mol]: 277.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.29		Crippen Method
logp	2.946		Crippen Method
mcvol	204.540	ml/mol	McGowan Method
rinpol	2335.00		NIST Webbook
rinpol	2335.00		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=U306906&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.