Acetamide, N-(4-methoxyphenyl)-2-(2-thienyl)-

Inchi: InChI=1S/C13H13NO2S/c1-16-11-6-4-10(5-7-11)14-13(15)9-12-3-2-8-17-12/h2-8H,9H2,1
InchiKey: ZKDDGJXJRDSOSK-UHFFFAOYSA-N
Formula: C13H13NO2S
SMILES: COc1ccc(NC(=O)Cc2cccs2)cc1
Mol. weight [g/mol]: 247.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	2.938		Crippen Method
mcvol	184.580	ml/mol	McGowan Method
rinpol	2234.00		NIST Webbook
rinpol	2234.00		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=U306904&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.