

Acetamide, 2-(2-thiophenyl)-N-ethyl-N-propyl-

Inchi:	InChI=1S/C11H17NOS/c1-3-7-12(4-2)11(13)9-10-6-5-8-14-10/h5-6,8H,3-4,7,9H2,1-2H3
InchiKey:	UKDJPVNMVXXEOD-UHFFFAOYSA-N
Formula:	C11H17NOS
SMILES:	CCCN(CC)C(=O)Cc1cccs1
Mol. weight [g/mol]:	211.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.47		Crippen Method
logp	2.549		Crippen Method
mcvol	174.290	ml/mol	McGowan Method
rmpol	1887.00		NIST Webbook
rmpol	1887.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U415407&Units=SI

Legend

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

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