

# Acetamide, 2-(2-thiophenyl)-N-ethyl-N-pentyl-

<b>Inchi:</b>	InChI=1S/C13H21NOS/c1-3-5-6-9-14(4-2)13(15)11-12-8-7-10-16-12/h7-8,10H,3-6,9,11H
<b>InchiKey:</b>	YGROEPIBMDTOCO-UHFFFAOYSA-N
<b>Formula:</b>	C13H21NOS
<b>SMILES:</b>	CCCCCN(CC)C(=O)Cc1cccs1
<b>Mol. weight [g/mol]:</b>	239.38

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	3.329		Crippen Method
mcvol	202.470	ml/mol	McGowan Method
rinpol	2044.00		NIST Webbook
rinpol	2044.00		NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U415411&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415411&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

## Legend

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

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