

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

Inchi:	InChI=1S/C14H23NOS/c1-3-5-6-7-10-15(4-2)14(16)12-13-9-8-11-17-13/h8-9,11H,3-7,10
InchiKey:	CFIMLISVFUGWCN-UHFFFAOYSA-N
Formula:	C14H23NOS
SMILES:	CCCCCN(CC)C(=O)Cc1cccs1
Mol. weight [g/mol]:	253.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.73		Crippen Method
logp	3.719		Crippen Method
mcvol	216.560	ml/mol	McGowan Method
rinpol	2096.00		NIST Webbook
rinpol	2096.00		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=U415413&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

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