

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

Inchi:	InChI=1S/C18H31NOS/c1-3-5-6-7-8-9-10-11-14-19(4-2)18(20)16-17-13-12-15-21-17/h12
InchiKey:	BCLGQJQCQCVSIB-UHFFFAOYSA-N
Formula:	C18H31NOS
SMILES:	CCCCCCCCCN(CC)C(=O)Cc1cccs1
Mol. weight [g/mol]:	309.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	5.280		Crippen Method
mcvol	272.920	ml/mol	McGowan Method
rinpol	1638.00		NIST Webbook
rinpol	1638.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415418&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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