

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

Inchi:	InChI=1S/C12H19NOS/c1-3-5-8-13(4-2)12(14)10-11-7-6-9-15-11/h6-7,9H,3-5,8,10H2,1-2
InchiKey:	XQYHCOZWOUKJII-UHFFFAOYSA-N
Formula:	C12H19NOS
SMILES:	CCCCN(CC)C(=O)Cc1cccs1
Mol. weight [g/mol]:	225.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	2.939		Crippen Method
mcvol	188.380	ml/mol	McGowan Method
rinsol	1986.00		NIST Webbook
rinsol	1986.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415409&Units=SI
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

Legend

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

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