

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

Inchi: InChI=1S/C16H27NOS/c1-3-5-6-7-8-9-12-17(4-2)16(18)14-15-11-10-13-19-15/h10-11,13
InchiKey: GEKBBRNKIXJAOJ-UHFFFAOYSA-N
Formula: C16H27NOS
SMILES: CCCCCCCN(CC)C(=O)Cc1cccs1
Mol. weight [g/mol]: 281.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.56		Crippen Method
logp	4.500		Crippen Method
mcvol	244.740	ml/mol	McGowan Method
rmpol	2410.00		NIST Webbook
rmpol	2410.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U415416&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
rmpol: Non-polar retention indices

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