

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

Inchi: InChI=1S/C15H25NOS/c1-3-5-6-7-8-11-16(4-2)15(17)13-14-10-9-12-18-14/h9-10,12H,3-
InchiKey: XQCPMKXDWIANSY-UHFFFAOYSA-N
Formula: C15H25NOS
SMILES: CCCCCCN(CC)C(=O)Cc1cccs1
Mol. weight [g/mol]: 267.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.14		Crippen Method
logp	4.110		Crippen Method
mcvol	230.650	ml/mol	McGowan Method
rinpol	2302.00		NIST Webbook
rinpol	2302.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U415415&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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
rinpol: Non-polar retention indices

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