2-Thiopheneacetamide, N-pentyl-

Inchi: InChI=1S/C11H17NOS/c1-2-3-4-7-12-11(13)9-10-6-5-8-14-10/h5-6,8H,2-4,7,9H2,1H3,(H
InchiKey: NYPYPXOKKRQDJI-UHFFFAOYSA-N
Formula: C11H17NOS
SMILES: CCCCCN=C(O)Cc1cccs1
Mol. weight [g/mol]: 211.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	3.437		Crippen Method
mcvol	174.290	ml/mol	McGowan Method
rinpol	1812.00		NIST Webbook
rinpol	1812.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407008&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.