2-Thiopheneacetamide, N-propyl-

Inchi: InChI=1S/C9H13NOS/c1-2-5-10-9(11)7-8-4-3-6-12-8/h3-4,6H,2,5,7H2,1H3,(H,10,11)
InchiKey: FLKSMORHGNGHBO-UHFFFAOYSA-N
Formula: C9H13NOS
SMILES: CCCN=C(O)Cc1cccs1
Mol. weight [g/mol]: 183.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.27		Crippen Method
logp	2.657		Crippen Method
mcvol	146.110	ml/mol	McGowan Method
rinpol	1622.00		NIST Webbook
rinpol	1622.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407004&Units=SI

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.