2-Thiopheneacetamide, N-heptyl-

Inchi: InChI=1S/C13H21NOS/c1-2-3-4-5-6-9-14-13(15)11-12-8-7-10-16-12/h7-8,10H,2-6,9,11H
InchiKey: IVSBQQHOYTXQPP-UHFFFAOYSA-N
Formula: C13H21NOS
SMILES: CCCCCCCNC(=O)Cc1cccs1
Mol. weight [g/mol]: 239.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	3.377		Crippen Method
mcvol	202.470	ml/mol	McGowan Method
rinpol	2020.00		NIST Webbook
rinpol	2020.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407012&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.