2-Thiopheneacetamide, N-hexyl-

Inchi: InChI=1S/C12H19NOS/c1-2-3-4-5-8-13-12(14)10-11-7-6-9-15-11/h6-7,9H,2-5,8,10H2,1H
InchiKey: INAPEAREYPRSNR-UHFFFAOYSA-N
Formula: C12H19NOS
SMILES: CCCCCCN=C(O)Cc1cccs1
Mol. weight [g/mol]: 225.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	3.827		Crippen Method
mcvol	188.380	ml/mol	McGowan Method
rinpol	1910.00		NIST Webbook
rinpol	1910.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407010&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.