2-Thiophenecarboxamide, N-octyl-

Inchi: InChI=1S/C13H21NOS/c1-2-3-4-5-6-7-10-14-13(15)12-9-8-11-16-12/h8-9,11H,2-7,10H2,
InchiKey: ZHACVTMITDAMOI-UHFFFAOYSA-N
Formula: C13H21NOS
SMILES: CCCCCCCCNC(=O)c1cccs1
Mol. weight [g/mol]: 239.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.50		Crippen Method
logp	3.838		Crippen Method
mcvol	202.470	ml/mol	McGowan Method
rinpol	2106.00		NIST Webbook
rinpol	2106.00		NIST Webbook

Sources

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=U407030&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.