2-Thiophenecarboxamide, N-propyl-N-(2-thiophenecarbonyl)-

Inchi: InChI=1S/C13H13NO2S2/c1-2-7-14(12(15)10-5-3-8-17-10)13(16)11-6-4-9-18-11/h3-6,8-9

InchiKey: IZMYLFLEHKALSX-UHFFFAOYSA-N

Formula: C13H13NO2S2

SMILES: CCCN(C(=O)c1cccs1)C(=O)c1cccs1

Mol. weight [g/mol]: 279.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	3.502		Crippen Method
mcvol	200.930	ml/mol	McGowan Method
rinpol	2173.00		NIST Webbook
rinpol	2173.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U407038&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.