

L-Proline, N-(thiophen-2-carbonyl)-, pentyl ester

Inchi:	InChI=1S/C15H21NO3S/c1-2-3-4-10-19-15(18)12-7-5-9-16(12)14(17)13-8-6-11-20-13/h6
InchiKey:	KTFGSMLHTNXUMU-UHFFFAOYSA-N
Formula:	C15H21NO3S
SMILES:	CCCCCOC(=O)C1CCCN1C(=O)c1cccs1
Mol. weight [g/mol]:	295.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	3.086		Crippen Method
mcvol	227.230	ml/mol	McGowan Method
rinpol	2399.00		NIST Webbook
rinpol	2399.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346371&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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