

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

Inchi:	InChI=1S/C13H17NO3S/c1-2-8-17-13(16)10-5-3-7-14(10)12(15)11-6-4-9-18-11/h4,6,9-1
InchiKey:	JWKMRNHBWLNPNPNC-UHFFFAOYSA-N
Formula:	C13H17NO3S
SMILES:	CCCOC(=O)C1CCCN1C(=O)c1cccs1
Mol. weight [g/mol]:	267.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	2.306		Crippen Method
mcvol	199.050	ml/mol	McGowan Method
rinpol	2199.00		NIST Webbook
rinpol	2199.00		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=U346368&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

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<https://www.chemeo.com/cid/120-375-2/L-Proline-N-thiophen-2-carbonyl-propyl-ester.pdf>

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