

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

Inchi: InChI=1S/C12H15NO3S/c1-2-16-12(15)9-5-3-7-13(9)11(14)10-6-4-8-17-10/h4,6,8-9H,2-3
InchiKey: DBYZFIVYXHZYAU-UHFFFAOYSA-N
Formula: C12H15NO3S
SMILES: CCOC(=O)C1CCCN1C(=O)c1cccs1
Mol. weight [g/mol]: 253.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.33		Crippen Method
logp	1.916		Crippen Method
mcvol	184.960	ml/mol	McGowan Method
rinpol	2114.00		NIST Webbook
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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=U346367&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/94-091-7/L-Proline-N-thiophen-2-carbonyl-ethyl-ester.pdf>

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