

d-Proline, N-ethoxycarbonyl-, ethyl ester

Inchi:	InChI=1S/C10H17NO4/c1-3-14-9(12)8-6-5-7-11(8)10(13)15-4-2/h8H,3-7H2,1-2H3
InchiKey:	GQDLZFPIOGXLCK-UHFFFAOYSA-N
Formula:	C10H17NO4
SMILES:	CCOC(=O)C1CCCN1C(=O)OCC
Mol. weight [g/mol]:	215.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.29		Crippen Method
logp	1.170		Crippen Method
mcvol	165.760	ml/mol	McGowan Method
rinpol	1516.00		NIST Webbook
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Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320834&Units=SI

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/61-698-0/d-Proline-N-ethoxycarbonyl-ethyl-ester.pdf>

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