

d-Proline, N-ethoxycarbonyl-, octyl ester

Inchi:	InChI=1S/C16H29NO4/c1-3-5-6-7-8-9-13-21-15(18)14-11-10-12-17(14)16(19)20-4-2/h14
InchiKey:	AFUJGVPDEKDTQZ-UHFFFAOYSA-N
Formula:	C16H29NO4
SMILES:	CCCCCCCCOC(=O)C1CCCN1C(=O)OCC
Mol. weight [g/mol]:	299.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	3.511		Crippen Method
mcvol	250.300	ml/mol	McGowan Method
rinpol	2010.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320839&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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<https://www.chemeo.com/cid/33-401-9/d-Proline-N-ethoxycarbonyl-octyl-ester.pdf>

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