

d-Proline, N-isobutoxycarbonyl-, isohexyl ester

Inchi:	InChI=1S/C16H29NO4/c1-12(2)7-6-10-20-15(18)14-8-5-9-17(14)16(19)21-11-13(3)4/h12
InchiKey:	MFIKNLBJGUNPFK-UHFFFAOYSA-N
Formula:	C16H29NO4
SMILES:	CC(C)CCCOC(=O)C1CCCN1C(=O)OCC(C)C
Mol. weight [g/mol]:	299.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.32		Crippen Method
logp	3.223		Crippen Method
mcvol	250.300	ml/mol	McGowan Method
rinpol	1889.00		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=U320805&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/123-737-7/d-Proline-N-isobutoxycarbonyl-isohexyl-ester.pdf>

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