

d-Proline, N-allyloxycarbonyl-, isohexyl ester

Inchi:	InChI=1S/C15H25NO4/c1-4-10-20-15(18)16-9-5-8-13(16)14(17)19-11-6-7-12(2)3/h4,12-
InchiKey:	BVIVKZJDTJHLCC-UHFFFAOYSA-N
Formula:	C15H25NO4
SMILES:	C=CCOC(=O)N1CCCC1C(=O)OCCCC(C)C
Mol. weight [g/mol]:	283.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	2.753		Crippen Method
mcvol	231.910	ml/mol	McGowan Method
rinpol	1948.00		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=U320967&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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