

L-Proline, N-(cyclohexanecarbonyl)-, isobutyl ester

Inchi:	InChI=1S/C16H27NO3/c1-12(2)11-20-16(19)14-9-6-10-17(14)15(18)13-7-4-3-5-8-13/h12
InchiKey:	NPAJIUMYWALDEX-UHFFFAOYSA-N
Formula:	C16H27NO3
SMILES:	CC(C)COC(=O)C1CCCN1C(=O)C1CCCCC1
Mol. weight [g/mol]:	281.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.15		Crippen Method
logp	2.757		Crippen Method
mcvol	233.570	ml/mol	McGowan Method
rinpol	2132.00		NIST Webbook
rinpol	2132.00		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=U346178&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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