L-Proline, N-(cyclopropylcarbonyl)-, heptyl ester

Inchi: InChI=1S/C16H27NO3/c1-2-3-4-5-6-12-20-16(19)14-8-7-11-17(14)15(18)13-9-10-13/h13

InchiKey: HNAFEXUZZVIFPC-UHFFFAOYSA-N

Formula: C16H27NO3

SMILES: CCCCCCCOC(=O)C1CCCN1C(=O)C1CC1

Mol. weight [g/mol]: 281.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	2.901		Crippen Method
mcvol	233.570	ml/mol	McGowan Method
rinpol	2186.00		NIST Webbook
rinpol	2186.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346314&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.