d-Proline, N-allyloxycarbonyl-, octyl ester

Inchi: InChI=1S/C17H29NO4/c1-3-5-6-7-8-9-14-21-16(19)15-11-10-12-18(15)17(20)22-13-4-2/h
InchiKey: FYIRHYMVLDRSEO-UHFFFAOYSA-N
Formula: C17H29NO4
SMILES: C=CCOC(=O)N1CCCC1C(=O)OCCCCCCCC
Mol. weight [g/mol]: 311.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.07		Crippen Method
logp	3.677		Crippen Method
mcvol	260.090	ml/mol	McGowan Method
rinpol	2207.00		NIST Webbook
rinpol	2207.00		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=U320968&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.