d-Proline, n-butoxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C16H29NO4/c1-4-5-11-21-16(19)17-10-6-9-14(17)15(18)20-12-7-8-13(2)3/h13
InchiKey: XKAPDRIGPGJWFN-UHFFFAOYSA-N
Formula: C16H29NO4
SMILES: CCCCOC(=O)N1CCCC1C(=O)OCCCC(C)C
Mol. weight [g/mol]: 299.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	3.367		Crippen Method
mcvol	250.300	ml/mol	McGowan Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U321083&Units=SI

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.