d-Proline, N-isobutoxycarbonyl-, propyl ester

Inchi: InChI=1S/C13H23NO4/c1-4-8-17-12(15)11-6-5-7-14(11)13(16)18-9-10(2)3/h10-11H,4-9H
InchiKey: VIODCHWXEZNDDQ-UHFFFAOYSA-N
Formula: C13H23NO4
SMILES: CCCOC(=O)C1CCCN1C(=O)OCC(C)C
Mol. weight [g/mol]: 257.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	2.197		Crippen Method
mcvol	208.030	ml/mol	McGowan Method
rinpol	1692.00		NIST Webbook
rinpol	1692.00		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=U320802&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.