d-Proline, N-isobutoxycarbonyl-, undecyl ester

Inchi: InChI=1S/C21H39NO4/c1-4-5-6-7-8-9-10-11-12-16-25-20(23)19-14-13-15-22(19)21(24)2
InchiKey: RSLRURFZYOCTCR-UHFFFAOYSA-N
Formula: C21H39NO4
SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCC(C)C
Mol. weight [g/mol]: 369.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.65		Crippen Method
logp	5.317		Crippen Method
mcvol	320.750	ml/mol	McGowan Method
rinpol	2361.00		NIST Webbook
rinpol	2361.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320811&Units=SI
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

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.