d-Proline, n-propoxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C15H27NO4/c1-4-10-20-15(18)16-9-5-8-13(16)14(17)19-11-6-7-12(2)3/h12-13
InchiKey: FWDCYYQSMKKCED-UHFFFAOYSA-N
Formula: C15H27NO4
SMILES: CCCOC(=O)N1CCCC1C(=O)OCCCC(C)C
Mol. weight [g/mol]: 285.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Crippen Method
logp	2.977		Crippen Method
mcvol	236.210	ml/mol	McGowan Method
rinpol	1852.00		NIST Webbook
rinpol	1852.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320822&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

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