d-Proline, N-isobutoxycarbonyl-, heptadecyl ester

Inchi: InChI=1S/C27H51NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-31-26(29)25-20-1
InchiKey: UZYQJWIBERCEDT-UHFFFAOYSA-N
Formula: C27H51NO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCC(C)C
Mol. weight [g/mol]: 453.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.16		Crippen Method
logp	7.658		Crippen Method
mcvol	405.290	ml/mol	McGowan Method
rinpol	2970.00		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=U320816&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

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