Pipecolic acid, N-isobutoxycarbonyl-, pentyl ester

Inchi: InChI=1S/C16H29NO4/c1-4-5-8-11-20-15(18)14-9-6-7-10-17(14)16(19)21-12-13(2)3/h13
InchiKey: NNWLJJSKTYXEFM-UHFFFAOYSA-N
Formula: C16H29NO4
SMILES: CCCCCOC(=O)C1CCCCN1C(=O)OCC(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	2005.00		NIST Webbook
rinpol	2005.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U393019&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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