Isonipecotic acid, N-isobutoxycarbonyl-, pentyl ester

Inchi: InChI=1S/C16H29NO4/c1-4-5-6-11-20-15(18)14-7-9-17(10-8-14)16(19)21-12-13(2)3/h13

InchiKey: PCWODTPUJVUQBH-UHFFFAOYSA-N

Formula: C16H29NO4

SMILES: CCCCCOC(=O)C1CCN(C(=O)OCC(C)C)CC1

Mol. weight [g/mol]: 299.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.20		Crippen Method
logp	3.224		Crippen Method
mcvol	250.300	ml/mol	McGowan Method
rinpol	2123.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U322063&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices