Isonipecotic acid, N-methoxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C12H21NO4/c1-9(2)8-17-11(14)10-4-6-13(7-5-10)12(15)16-3/h9-10H,4-8H2,1-

InchiKey: YZNUVAVHQISUCK-UHFFFAOYSA-N

Formula: C12H21NO4

SMILES: COC(=O)N1CCC(C(=O)OCC(C)C)CC1

Mol. weight [g/mol]: 243.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.53		Crippen Method
logp	1.664		Crippen Method
mcvol	193.940	ml/mol	McGowan Method
rinpol	1762.00		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=U322018&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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