Isonipecotic acid, N-propoxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C14H25NO4/c1-4-9-18-14(17)15-7-5-12(6-8-15)13(16)19-10-11(2)3/h11-12H,4

InchiKey: KXTCEVIFVKMRPQ-UHFFFAOYSA-N

Formula: C14H25NO4

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

Mol. weight [g/mol]: 271.36

Physical Properties

Property code	Value	Unit	Source
logp	2.444		Crippen Method
mcvol	222.120	ml/mol	McGowan Method
rinpol	1939.00		NIST Webbook

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U322076&Units=SI

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

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

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices