

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]:	271.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	2.444		Crippen Method
mcvol	222.120	ml/mol	McGowan Method
rinpol	1939.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U322076&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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