

Isonipecotic acid, N-methoxycarbonyl-, butyl ester

Inchi:	InChI=1S/C12H21NO4/c1-3-4-9-17-11(14)10-5-7-13(8-6-10)12(15)16-2/h10H,3-9H2,1-2H
InchiKey:	PMQPLWYMKRTYCR-UHFFFAOYSA-N
Formula:	C12H21NO4
SMILES:	CCCCOC(=O)C1CCN(C(=O)OC)CC1
Mol. weight [g/mol]:	243.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.77		Crippen Method
logp	1.808		Crippen Method
mcvol	193.940	ml/mol	McGowan Method
rinpola	1804.00		NIST Webbook
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Sources

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=U322019&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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