

Isonipecotic acid, N-methoxycarbonyl-, nonyl ester

Inchi:	InChI=1S/C17H31NO4/c1-3-4-5-6-7-8-9-14-22-16(19)15-10-12-18(13-11-15)17(20)21-2/
InchiKey:	FZCIVMWGCQJGRM-UHFFFAOYSA-N
Formula:	C17H31NO4
SMILES:	CCCCCCCCCOC(=O)C1CCN(C(=O)OC)CC1
Mol. weight [g/mol]:	313.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.86		Crippen Method
logp	3.759		Crippen Method
mcvol	264.390	ml/mol	McGowan Method
rinpol	2321.00		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=U322025&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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