

Isonipecotic acid, n-butoxycarbonyl-, butyl ester

Inchi:	InChI=1S/C15H27NO4/c1-3-5-11-19-14(17)13-7-9-16(10-8-13)15(18)20-12-6-4-2/h13H,3
InchiKey:	WKLOYJBELNGJNJ-UHFFFAOYSA-N
Formula:	C15H27NO4
SMILES:	CCCCOC(=O)C1CCN(C(=O)OCCCC)CC1
Mol. weight [g/mol]:	285.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.03		Crippen Method
logp	2.978		Crippen Method
mcvol	236.210	ml/mol	McGowan Method
rinpol	2085.00		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=U322048&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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