

Isonipecotic acid, N-allyloxycarbonyl-, butyl ester

Inchi:	InChI=1S/C14H23NO4/c1-3-5-11-18-13(16)12-6-8-15(9-7-12)14(17)19-10-4-2/h4,12H,2-
InchiKey:	ACVLGLULFLANIZ-UHFFFAOYSA-N
Formula:	C14H23NO4
SMILES:	C=CCOC(=O)N1CCC(C(=O)OCCCC)CC1
Mol. weight [g/mol]:	269.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.46		Crippen Method
logp	2.364		Crippen Method
mcvol	217.820	ml/mol	McGowan Method
rinpola	1962.00		NIST Webbook
rinpola	1962.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U321990&Units=SI

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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