

Isonipecotic acid, N-methoxycarbonyl-, heptyl ester

Inchi:	InChI=1S/C15H27NO4/c1-3-4-5-6-7-12-20-14(17)13-8-10-16(11-9-13)15(18)19-2/h13H,3
InchiKey:	WOROCYGBWGMQDW-UHFFFAOYSA-N
Formula:	C15H27NO4
SMILES:	CCCCCCCOC(=O)C1CCN(C(=O)OC)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
rinpola	2109.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322023&Units=SI
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

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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