

Isonipecotic acid, N-methoxycarbonyl-, hexyl ester

Inchi:	InChI=1S/C14H25NO4/c1-3-4-5-6-11-19-13(16)12-7-9-15(10-8-12)14(17)18-2/h12H,3-11
InchiKey:	WJBNPQUJFZJECE-UHFFFAOYSA-N
Formula:	C14H25NO4
SMILES:	CCCCCOC(=O)C1CCN(C(=O)OC)CC1
Mol. weight [g/mol]:	271.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Crippen Method
logp	2.588		Crippen Method
mcvol	222.120	ml/mol	McGowan Method
rinsol	2008.00		NIST Webbook
rinsol	2008.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322022&Units=SI
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

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/123-106-7/Isonipecotic-acid-N-methoxycarbonyl-hexyl-ester.pdf>

Generated by Cheméo on 2024-04-29 07:22:38.476416127 +0000 UTC m=+16664607.396993442.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.