

Isonipecotic acid, N-methoxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C14H25NO4/c1-11(2)5-4-10-19-13(16)12-6-8-15(9-7-12)14(17)18-3/h11-12H,4
InchiKey: IFGBKWADV D GIPS-UHFFFAOYSA-N
Formula: C14H25NO4
SMILES: COC(=O)N1CCC(C(=O)OCCCC(C)C)CC1
Mol. weight [g/mol]: 271.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	2.444		Crippen Method
mcvol	222.120	ml/mol	McGowan Method
rinpol	1969.00		NIST Webbook
rinpol	1969.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U322021&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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