

Isonipecotic acid, N-methoxycarbonyl-, octyl ester

Inchi:	InChI=1S/C16H29NO4/c1-3-4-5-6-7-8-13-21-15(18)14-9-11-17(12-10-14)16(19)20-2/h14
InchiKey:	ADAVEXCUDTXASJ-UHFFFAOYSA-N
Formula:	C16H29NO4
SMILES:	CCCCCCCCOC(=O)C1CCN(C(=O)OC)CC1
Mol. weight [g/mol]:	299.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	3.368		Crippen Method
mcvol	250.300	ml/mol	McGowan Method
rinsol	2204.00		NIST Webbook
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Sources

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=U322024&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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