

Isonipecotic acid, N-methoxycarbonyl-, ethyl ester

Inchi:	InChI=1S/C10H17NO4/c1-3-15-9(12)8-4-6-11(7-5-8)10(13)14-2/h8H,3-7H2,1-2H3
InchiKey:	TWULIESUCDGN SQ-UHFFFAOYSA-N
Formula:	C10H17NO4
SMILES:	CCOC(=O)C1CCN(C(=O)OC)CC1
Mol. weight [g/mol]:	215.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.93		Crippen Method
logp	1.028		Crippen Method
mcvol	165.760	ml/mol	McGowan Method
rmpol	1599.00		NIST Webbook
rmpol	1599.00		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=U322016&Units=SI

Legend

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

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