

Isonipecotic acid, N-ethoxycarbonyl-, ethyl ester

Inchi:	InChI=1S/C11H19NO4/c1-3-15-10(13)9-5-7-12(8-6-9)11(14)16-4-2/h9H,3-8H2,1-2H3
InchiKey:	HTGQADRJVAFPPH-UHFFFAOYSA-N
Formula:	C11H19NO4
SMILES:	CCOC(=O)C1CCN(C(=O)OCC)CC1
Mol. weight [g/mol]:	229.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.35		Crippen Method
logp	1.418		Crippen Method
mcvol	179.850	ml/mol	McGowan Method
rinpola	1670.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322001&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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