Pseudoecgonine methyl ester

Inchi:	InChI=1S/C10H17NO3/c1-11-7-3-4-10(11,9(13)14-2)6-8(12)5-7/h7-8,12H,3-6H2,1-2H3
InchiKey:	XTSCVMBKKFMLQC-UHFFFAOYSA-N
Formula:	C10H17NO3
SMILES:	COC(=O)C12CCC(CC(O)C1)N2C
Mol. weight [g/mol]:	199.25
CAS:	99189-88-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.83		Crippen Method
logp	0.147		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
rinpol	1526.10		NIST Webbook
rinpol	1526.10		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C99189885&Units=SI

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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https://www.chemeo.com/cid/94-253-7/Pseudoecgonine-methyl-ester.pdf

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