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