

Methyl ecgonine

Other names:	Ecgonine methyl ester
Inchi:	InChI=1S/C10H17NO3/c1-11-6-3-4-7(11)9(8(12)5-6)10(13)14-2/h6-9,12H,3-5H2,1-2H3
InchiKey:	QIQNNBXHAYSQRY-UHFFFAOYSA-N
Formula:	C10H17NO3
SMILES:	<chem>COC(=O)C1C(O)CC2CCC1N2C</chem>
Mol. weight [g/mol]:	199.25
CAS:	7143-09-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.59		Crippen Method
logp	0.003		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
rinpol	1504.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1439.00		NIST Webbook

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=C7143091&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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