

# Ecgonine ethyl ester

<b>Inchi:</b>	InChI=1S/C11H19NO3/c1-3-15-11(14)10-8-5-4-7(12(8)2)6-9(10)13/h7-10,13H,3-6H2,1-2
<b>InchiKey:</b>	ABDMBNAKYBUEEX-UHFFFAOYSA-N
<b>Formula:</b>	C11H19NO3
<b>SMILES:</b>	CCOC(=O)C1C(O)CC2CCC1N2C
<b>Mol. weight [g/mol]:</b>	213.27
<b>CAS:</b>	70939-97-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.01		Crippen Method
logp	0.393		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
rinpol	1576.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C70939978&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C70939978&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

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

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