

Propionylecgonine methyl ester

Other names:	Methyl 8-methyl-3-(propionyloxy)-8-azabicyclo[3.2.1]octane-2-carboxylate, [1R-(exo,exo)]-Methyl ecgonine, propanoate
Inchi:	8-Azabicyclo(3.2.1)octane-2-carboxylic acid, 8-methyl-3-(1-oxopropoxy)-, methyl ester, [1R-(exo,exo)]
InchiKey:	UXYJUSKBVTLXNE-UHFFFAOYSA-N
Formula:	C13H21NO4
SMILES:	CCC(=O)OC1CC2CCC(C1C(=O)OC)N2C
Mol. weight [g/mol]:	255.31
CAS:	203320-37-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.44		Crippen Method
logp	0.964		Crippen Method
mcvol	197.170	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C203320370&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/115-217-3/Propionylecgonine-methyl-ester.pdf>

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