

Ecgonidine, methyl ester

Other names:	2-Tropidinecarboxylic acid, methyl ester Methyl ecgonidine Anhydroecgonine methyl ester
Inchi:	InChI=1S/C10H15NO2/c1-11-7-3-5-8(10(12)13-2)9(11)6-4-7/h5,7,9H,3-4,6H2,1-2H3
InchiKey:	MPSNEAHFGOEKBI-UHFFFAOYSA-N
Formula:	C10H15NO2
SMILES:	<chem>COC(=O)C1=CCC2CCC1N2C</chem>
Mol. weight [g/mol]:	181.23
CAS:	127379-24-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.31		Crippen Method
logp	0.952		Crippen Method
mcvol	143.160	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C127379242&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/90-955-2/Ecgonidine-methyl-ester.pdf>

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