

Ecgonine

Other names:	1«alpha»H,5«alpha»H-Tropane-2«beta»-carboxylic acid, 3«beta»-hydroxy-1Â«alphaÂ»H,5Â«alphaÂ»H-Tropane-2Â«betaÂ»-carboxylic acid, 3Â«betaÂ»-hydroxy-3«beta»-Hydroxy-2«beta»-tropanecarboxylic acid 3Â«betaÂ»-Hydroxy-2Â«betaÂ»-tropanecarboxylic acid 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-hydroxy-8-methyl-, (2-endo,3-exo)- 8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-hydroxy-8-methyl-, [1R-(exo,exo)]- Ekgonin L-ecgonine [1R*-(Exo,exo)]-3-hydroxy-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylic acid
Inchi:	InChI=1S/C9H15NO3/c1-10-5-2-3-6(10)8(9(12)13)7(11)4-5/h5-8,11H,2-4H2,1H3,(H,12,13)
InchiKey:	PHMBVCPLDPDESM-RLXKETGRSA-N
Formula:	C9H15NO3
SMILES:	CN1C2CCC1C(C(=O)O)C(O)C2
Mol. weight [g/mol]:	185.22
CAS:	481-37-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.02		Aqueous Solubility Prediction Method
logp	-0.085		Crippen Method
mcvol	139.240	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=C481378&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx

Legend

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

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