

Pilocarpine

Other names:	2(3H)-Furanone, 3-ethylidihydro-4-[(1-methyl-1H-imidazol-5-yl)methyl]-, (3S-cis)- (3S-cis)-3-Ethylidihydro-4-((1-methyl-1H-imidazol-5-yl)methyl)-2(3H)-furanone Imidazole-5-butyric acid, «alpha»-ethyl-«beta»-(hydroxymethyl)-1-methyl-, «gamma»-lactone Pilocarpin Pilocarpol Pilocarpine, (+)- (+)-Pilocarpine Pilocarpin Syncarpine Ocuser P 20 3-Ethylidihydro-4-[(1-methyl-1H-imidazol-5-yl)methyl]-2(3H)-furanone-, (3S,4R)- Ocuser Pilo
Inchi:	InChI=1S/C11H16N2O2/c1-3-10-8(6-15-11(10)14)4-9-5-12-7-13(9)2/h5,7-8,10H,3-4,6H2
InchiKey:	QCHFTSOMWOSFHM-UHFFFAOYSA-N
Formula:	C11H16N2O2
SMILES:	CCC1C(=O)OCC1Cc1cncn1C
Mol. weight [g/mol]:	208.26
CAS:	92-13-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.69		Crippen Method
logp	1.162		Crippen Method
mcvol	162.930	ml/mol	McGowan Method
rinpol	2060.00		NIST Webbook
rinpol	2014.00		NIST Webbook
rinpol	2060.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92137&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
rinpol:	Non-polar retention indices

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