Scopolamine

Other names:	Benzeneacetic acid, «alpha»-(hydroxymethyl)-, 9-methyl-3-oxa-9-azatricyclo[3.3.1.0(2,4)]non-7-yl ester, [7(S)-(1«alpha»,2«beta»,4«beta»,5«alpha»,7«beta»)]-
	1«alpha»H,5«alpha»H-Tropan-3«alpha»-ol, 6«beta»,7«beta»-epoxy-, (-)-tropate (ester)
	(-)-Hyoscine
	Atrochin
	Atroquin
	Hyosceine
	Hyoscine
	Scopine tropate
	Skopolamin
	SEE
	6,7-Epoxytropine tropate
	6-«beta»,7-«beta»-Epoxy-3-«alpha»-tropanyl S-(-)-tropate
	Epoxytropine tropate
	Hyosol
	Oscine
	3-Oxa-9-azatricyclo(3.3.1.O(2,4))nonan-7-ol, 9-methyl-, tropate
	Tropic acid, ester with scopine
	Tropic acid, 9-methyl-3-oxa-9-azatricyclo(3.3.1.O(2,4))non-7-yl ester
	9-Methyl-3-oxa-9-azatricyclo[3.3.1.0(2,4)]nonan-7-ol (-)-tropate
	l-Scopolamine
	Transderm-Scop
	6«beta»,7«beta»-Epoxy-1«alpha»H,5«alpha»H-tropan-3«alpha»-ol (-)-tropate (ester)
	Scop
	Scopoderm-TTS
	Transcop
	(-)-Scopolamine
	Scopine (-)-tropate
Inchi:	InChI=1S/C17H21NO4/c1-18-13-7-11(8-14(18)16-15(13)22-16)21-17(20)12(9-19)10-5-3-
InchiKey:	STECJAGHUSJQJN-MBBCWDQXSA-N
Formula:	C17H21NO4
SMILES:	CN1C2CC(OC(=O)C(CO)c3ccccc3)CC1C1OC12
Mol. weight [g/mol]:	303.35
CAS:	51-34-3

Physical Properties

Property code	Value	Unit	Source

log10ws	-2.03		Crippen Method
logp	0.918		Crippen Method
mcvol	223.210	ml/mol	McGowan Method
rinpol	2315.00		NIST Webbook
rinpol	2263.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2280.00		NIST Webbook
rinpol	2286.00		NIST Webbook
rinpol	2261.00		NIST Webbook
rinpol	2315.00		NIST Webbook
rinpol	2395.40		NIST Webbook
rinpol	2303.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2320.00		NIST Webbook
rinpol	2292.00		NIST Webbook
rinpol	2303.00		NIST Webbook
rinpol	2286.00		NIST Webbook
rinpol	2280.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C51343&Units=SI

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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