

Scopolamine

Other names:	Benzeneacetic acid, «alpha»-(hydroxymethyl)-, 9-methyl-3-oxa-9-azatricyclo[3.3.1.0(2,4)]non-7-yl ester, 1«alpha»H,5«alpha»H-Propan-3«alpha»-ol, 6«beta»,7«beta»-epoxy-, (-)-tropate (ester) (S)-[1«alpha»,2«beta»,4«beta»,5«alpha»,7«beta»]-(-)-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.O(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)c3cccc3)CC1C1OC12
Mol. weight [g/mol]:	303.35
CAS:	51-34-3

Physical Properties

Property code	Value	Unit	Source
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log10ws	-2.03		Crippen Method
logp	0.918		Crippen Method
mcvol	223.210	ml/mol	McGowan Method
rinpol	2290.00		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	2280.00		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
rinpol	2310.00		NIST Webbook
rinpol	2263.00		NIST Webbook
rinpol	2315.00		NIST Webbook

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=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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