

Retrorsine

Other names:	Retrorsine [1,6]Dioxacyclododecino[2,3,4-gh]pyrrolizine-2,7-dione, 3-ethylidene-3,4,5,6,9,11,13,14,14a,14b-decahydro-6-hydroxy-6-(hydroxymethyl)-5-methoxy-1,2,18-dihydroxysecofianan-11,16-dione (3Z,5R,6S,14aR,14bR)
Inchi:	InChI=1S/C18H25NO6/c1-3-12-8-11(2)18(23,10-20)17(22)24-9-13-4-6-19-7-5-14(15(13)16)
InchiKey:	BCJMNZRQJAVDLD-CQRYIUNCSA-N
Formula:	C18H25NO6
SMILES:	CC=C1CC(C)C(O)(CO)C(=O)OCC2=CCN3CCC(OC1=O)C23
Mol. weight [g/mol]:	351.39
CAS:	480-54-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.66		Crippen Method
logp	0.165		Crippen Method
mcvol	259.900	ml/mol	McGowan Method
rinpol	2548.00		NIST Webbook
rinpol	2515.00		NIST Webbook
rinpol	2525.00		NIST Webbook
rinpol	2580.00		NIST Webbook
rinpol	2539.00		NIST Webbook
rinpol	2548.00		NIST Webbook
rinpol	2580.00		NIST Webbook
rinpol	2518.00		NIST Webbook
rinpol	2515.00		NIST Webbook
rinpol	2548.00		NIST Webbook
rinpol	2580.00		NIST Webbook
rinpol	2539.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C480546&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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