13-Epihydroxyisolupanine

Inchi:	InChI=1S/C15H24N2O2/c18-12-4-5-13-11-6-10(7-16(13)9-12)14-2-1-3-15(19)17(14)8-11
InchiKey:	JZFWYXLNISKIRH-UHFFFAOYSA-N
Formula:	C15H24N2O2
SMILES:	O=C1CCCC2C3CC(CN12)C1CCC(O)CN1C3
Mol. weight [g/mol]:	264.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.71		Crippen Method
logp	0.842		Crippen Method
mcvol	206.170	ml/mol	McGowan Method
rinpol	2345.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R263935&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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