Hydroxytetrahydrorhombifoline

Inchi:	InChI=1S/C15H24N2O2/c1-2-3-7-16-9-11-8-12(10-16)15(19)17-13(11)5-4-6-14(17)18/h2
InchiKey:	AGDMYJKLTLCVIY-UHFFFAOYSA-N
Formula:	C15H24N2O2
SMILES:	C=CCCN1CC2CC(C1)C1CCCC(=O)N1C2O
Mol. weight [g/mol]:	264.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.05		Crippen Method
logp	1.214		Crippen Method
mcvol	212.730	ml/mol	McGowan Method
rinpol	2138.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R264250&Units=SI
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

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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