

[2H3]Dihydrozeatin nucleotide, permethylated

Other names:	Dihydrozeatin nucleotide, permethylated
Inchi:	InChI=1S/C19H31N5O4/c1-13(9-25-3)6-7-23(2)18-17-19(21-11-20-18)24(12-22-17)16-8
InchiKey:	ZLSKKBGHDLNFFW-QDIHITRGSA-N
Formula:	C19H31N5O4
SMILES:	COCC(C)CCN(C)c1ncnc2c1ncn2C1CC(OC)C(COC)O1
Mol. weight [g/mol]:	393.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	1.884		Crippen Method
mcvol	302.170	ml/mol	McGowan Method
rinpol	2999.00		NIST Webbook
rinpol	2997.00		NIST Webbook
rinpol	2998.00		NIST Webbook
rinpol	2998.00		NIST Webbook
rinpol	2998.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R270205&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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