

cis-Zeatin, permethylated

Inchi: InChI=1S/C13H19N5O/c1-10(7-19-4)5-6-17(2)12-11-13(15-8-14-12)18(3)9-16-11/h5,8-9
InchiKey: DPZJINNFLYQJJE-YHYXMXQVSA-N
Formula: C13H19N5O
SMILES: COCC(C)=CCN(C)c1ncnc2c1ncn2C
Mol. weight [g/mol]: 261.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.80		Crippen Method
logp	1.392		Crippen Method
mcvol	206.580	ml/mol	McGowan Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R270265&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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