

[2H6]Isopentenyladenine nucleotide, permethylated

Other names: Isopentenyladenine nucleotide, permethylated
Inchi: InChI=1S/C18H27N5O3/c1-12(2)6-7-22(3)17-16-18(20-10-19-17)23(11-21-16)15-8-13(2)
InchiKey: TYFJYRPUUSPCUJL-JVIGXAJISA-N
Formula: C18H27N5O3
SMILES: COCC1OC(n2cnc3c(N(C)CC=C(C)C)ncnc32)CC1OC
Mol. weight [g/mol]: 361.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	2.178		Crippen Method
mcvol	277.910	ml/mol	McGowan Method
rinpol	2882.00		NIST Webbook
rinpol	2882.00		NIST Webbook
rinpol	2876.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R270245&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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