

cis-Zeatin riboside, permethylated

Inchi: InChI=1S/C20H31N5O5/c1-13(9-26-3)7-8-24(2)18-15-19(22-11-21-18)25(12-23-15)20-17
InchiKey: PJXJSJFRHKGAAI-SYMZOSGVSA-N
Formula: C20H31N5O5
SMILES: COCC(C)=CCN(C)c1ncnc2c1ncn2C1OC(COC)C(OC)C1OC
Mol. weight [g/mol]: 421.49

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.33 | | Crippen Method |
| logp | 1.429 | | Crippen Method |
| mcvol | 317.830 | ml/mol | McGowan Method |
| rinpol | 3065.00 | | NIST Webbook |
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| rinpol | 3065.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R270270&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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<https://www.chemeo.com/cid/40-793-7/cis-Zeatin-riboside-permethylated.pdf>

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