TRIMETHYLZEATIN

Other names: N-[(2E)-4-Methoxy-3-methyl-2-butenyl]-N,9-dimethyl-9H-purin-6-amine
trans-Zeatin, permethylated
9H-Purin-6-amine, N-(4-methoxy-3-methyl-2-butenyl)-N,9-dimethyl-, (E)-
trans-Zeatin, N,9-dimethyl-, methyl ether
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/h5,8-9H
InchiKey: DPZJINNFLYQJJE-BJMVGYQFSA-N
Formula: C13H19N5O
SMILES: COC/C(C)=C/CN(C)c1ncnc2c1ncn2C
Mol. weight [g/mol]: 261.33

Physical Properties

Property code	Value	Unit	Source
logp	1.392		Crippen Method
mcvol	206.580	ml/mol	McGowan Method
rinpol	2299.00		NIST Webbook
rinpol	2304.00		NIST Webbook
rinpol	2304.00		NIST Webbook
rinpol	2299.00		NIST Webbook

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C62747813&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices