

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/h5,8-9**InchiKey:** DPZJINNFLYQJJE-BJMVGYQFSA-N**Formula:** C13H19N5O**SMILES:** COCC(C)=CCN(C)c1ncnc2c1ncn2C**Mol. weight [g/mol]:** 261.32**CAS:** 62747-81-3

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	2299.00		NIST Webbook
rinpol	2304.00		NIST Webbook
rinpol	2304.00		NIST Webbook
rinpol	2299.00		NIST Webbook

Sources

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=C62747813&Units=SI>**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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