

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:	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

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