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/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices