

Adenosine, 2',3'-O-(1-methylethylidene)-

Other names:	Adenosine, 2',3'-O-isopropylidene- 2',3'-Isopropylideneadenosine 2',3'-O-Isopropylideneadenosine
Inchi:	InChI=1S/C13H17N5O4/c1-13(2)21-8-6(3-19)20-12(9(8)22-13)18-5-17-7-10(14)15-4-16-
InchiKey:	LCCLUOXEZHUNS-UHFFFAOYSA-N
Formula:	C13H17N5O4
SMILES:	CC1(C)OC2C(CO)OC(n3cnc4c(N)ncnc43)C2O1
Mol. weight [g/mol]:	307.31
CAS:	362-75-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	-0.182		Crippen Method
mcvol	206.770	ml/mol	McGowan Method

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=C362754&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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