

Adenosine, 5'-S-methyl-5'-thio-

Other names:	«beta»-D-Ribofuranose, 1-(6-amino-9H-purin-9-yl)-1-deoxy-5-S-methyl-5-thio-Methylthioadenosine 5'-(Methylthio)-5'-deoxyadenosine 5'-Deoxy-5'-(methylthio)adenosine 5'-S-Methyl-5'-thioadenosine
Inchi:	InChI=1S/C11H15N5O3S/c1-20-2-5-7(17)8(18)11(19-5)16-4-15-6-9(12)13-3-14-10(6)16/
InchiKey:	WUUGFSXJNOTRMR-IOSLPCCCSA-N
Formula:	C11H15N5O3S
SMILES:	CSCC1OC(n2cnc3c(N)ncnc32)C(O)C1O
Mol. weight [g/mol]:	297.33
CAS:	2457-80-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.33		Crippen Method
logp	-0.609		Crippen Method
mcvol	199.930	ml/mol	McGowan Method

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=C2457809&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

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<https://www.chemeo.com/cid/20-401-3/Adenosine-5-S-methyl-5-thio.pdf>

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