

Adenine, 2-(methylthio)-

Inchi:	InChI=1S/C6H7N5S/c1-12-6-10-4(7)3-5(11-6)9-2-8-3/h2H,1H3,(H3,7,8,9,10,11)
InchiKey:	FXGXEFXCWDTSQK-UHFFFAOYSA-N
Formula:	C6H7N5S
SMILES:	CSc1nc(N)c2[nH]cnc2n1
Mol. weight [g/mol]:	181.22
CAS:	1198-83-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	0.175		Crippen Method
mcvol	122.730	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=C1198830&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

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<https://www.chemeo.com/cid/57-874-9/Adenine-2-methylthio.pdf>

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