

Adenine, n,n-bis(2-hydroxyethyl)-

Inchi:	InChI=1S/C9H13N5O2/c15-3-1-14(2-4-16)9-7-8(11-5-10-7)12-6-13-9/h5-6,15-16H,1-4H2
InchiKey:	HDFTZBLKBXGFGD-UHFFFAOYSA-N
Formula:	C9H13N5O2
SMILES:	OCCN(CCO)c1ncnc2[nH]cnc12
Mol. weight [g/mol]:	223.23
CAS:	6312-66-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.06		Crippen Method
logp	-1.338		Crippen Method
mcvol	160.390	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6312669&Units=SI
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

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/34-473-9/Adenine-n-n-bis-2-hydroxyethyl.pdf>

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