

Adenine, 9-(2-hydroxycyclohexyl)-, trans-

Inchi:	InChI=1S/C11H15N5O/c12-10-9-11(14-5-13-10)16(6-15-9)7-3-1-2-4-8(7)17/h5-8,17H,1-4
InchiKey:	YNEOLWHNIDWTLC-UHFFFAOYSA-N
Formula:	C11H15N5O
SMILES:	Nc1ncnc2c1ncn2C1CCCCC1O
Mol. weight [g/mol]:	233.27
CAS:	954-62-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.38		Crippen Method
logp	0.885		Crippen Method
mcvol	171.840	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C954621&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/91-694-1/Adenine-9-2-hydroxycyclohexyl-trans.pdf>

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