

Adenine, n-butyl-

Inchi:	InChI=1S/C9H13N5/c1-2-3-4-10-8-7-9(12-5-11-7)14-6-13-8/h5-6H,2-4H2,1H3,(H2,10,11,
InchiKey:	CRYKTDPNUYNOTI-UHFFFAOYSA-N
Formula:	C9H13N5
SMILES:	CCCCNc1ncnc2[nH]cnc12
Mol. weight [g/mol]:	191.23
CAS:	5451-41-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	1.083		Crippen Method
mcvol	148.650	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=C5451412&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/57-504-9/Adenine-n-butyl.pdf>

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