

Adenine, 3-benzyl-2-methyl-

Inchi:	InChI=1S/C13H13N5/c1-9-17-12(14)11-13(16-8-15-11)18(9)7-10-5-3-2-4-6-10/h2-6,8H,7
InchiKey:	NUYGSLZXEIGTAP-UHFFFAOYSA-N
Formula:	C13H13N5
SMILES:	Cc1nc(N)c2ncnc-2n1Cc1ccccc1
Mol. weight [g/mol]:	239.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.46		Crippen Method
logp	1.717		Crippen Method
mcvol	181.250	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=B6008221&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/67-007-0/Adenine-3-benzyl-2-methyl.pdf>

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