

Adenine, 6-n-benzyl-9-cyclopentyl-

Inchi:	InChI=1S/C17H19N5/c1-2-6-13(7-3-1)10-18-16-15-17(20-11-19-16)22(12-21-15)14-8-4-5
InchiKey:	XBJJYCQQGSHMNQ-UHFFFAOYSA-N
Formula:	C17H19N5
SMILES:	c1ccc(CNc2ncnc3c2ncn3C2CCCC2)cc1
Mol. weight [g/mol]:	293.37
CAS:	35966-95-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.07		Crippen Method
logp	3.554		Crippen Method
mcvol	226.750	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=C35966951&Units=SI

Legend

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

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