

9H-adenine, n⁶-(3,3-dimethyl-4-hydroxy-n-butyl)-

Other names:	9H-adenine, n
Inchi:	InChI=1S/C11H17N5O/c1-11(2,5-17)3-4-12-9-8-10(14-6-13-8)16-7-15-9/h6-7,17H,3-5H2
InchiKey:	DHFKVLLVIVQUGC-UHFFFAOYSA-N
Formula:	C11H17N5O
SMILES:	CC(C)(CO)CCNc1nc[nH]c2ncnc1-2
Mol. weight [g/mol]:	235.29
CAS:	116295-96-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.13		Crippen Method
logp	0.643		Crippen Method
mcvol	182.700	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=C116295966&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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