

9H-purine, 6-amino-2-(methylamino)-9-beta-d-ribofuranosyl-

Inchi:	InChI=1S/C11H16N6O4/c1-13-11-15-8(12)5-9(16-11)17(3-14-5)10-7(20)6(19)4(2-18)21-
InchiKey:	UZWXAPMSNDKDNK-UHFFFAOYSA-N
Formula:	C11H16N6O4
SMILES:	CN=c1nc2c(ncn2C2OC(CO)C(O)C2O)c(N)[nH]1
Mol. weight [g/mol]:	296.28
CAS:	13364-95-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.40		Crippen Method
logp	-2.998		Crippen Method
mcvol	199.430	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=C13364959&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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