

9H-purine, 6-ethyl-9-(beta-d-ribofuranosyl)-

Inchi:	InChI=1S/C12H16N4O4/c1-2-6-8-11(14-4-13-6)16(5-15-8)12-10(19)9(18)7(3-17)20-12/h
InchiKey:	AGKGZTUSZIPPRS-UHFFFAOYSA-N
Formula:	C12H16N4O4
SMILES:	CCc1ncnc2c1ncn2C1OC(CO)C(O)C1O
Mol. weight [g/mol]:	280.28
CAS:	16006-62-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.46		Crippen Method
logp	-1.000		Crippen Method
mcvol	193.560	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=C16006625&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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