

# Urea, 1-[2-(6-hydroxy-9h-purin-9-yl)ethyl]-3-methyl-

Inchi:	InChI=1S/C9H12N6O2/c1-10-9(17)11-2-3-15-5-14-6-7(15)12-4-13-8(6)16/h4-5H,2-3H2,1
InchiKey:	ZXIYRCLBZRLJHI-UHFFFAOYSA-N
Formula:	C9H12N6O2
SMILES:	CNC(=O)NCCn1cnc2c(O)ncnc21
Mol. weight [g/mol]:	236.23
CAS:	90674-44-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.35		Crippen Method
logp	-0.539		Crippen Method
mvol	166.070	ml/mol	McGowan Method

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C90674445&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C90674445&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

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

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