

Purin-8(9h)-one, 6-amino-7-(2-hydroxyethyl)-

Inchi:	InChI=1S/C7H9N5O2/c8-5-4-6(10-3-9-5)11-7(14)12(4)1-2-13/h3,13H,1-2H2,(H3,8,9,10,1
InchiKey:	ZHDVCCDFLSHZQJ-UHFFFAOYSA-N
Formula:	C7H9N5O2
SMILES:	Nc1ncnc2[nH]c(=O)n(CCO)c12
Mol. weight [g/mol]:	195.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.61		Crippen Method
logp	-1.788		Crippen Method
mcvol	132.210	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009821&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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