

# 3H-v-triazolo[4,5-d]pyrimidine, 5-amino-3-ethyl-7-hydroxy-

Inchi:	InChI=1S/C6H8N6O/c1-2-12-4-3(10-11-12)5(13)9-6(7)8-4/h2H2,1H3,(H3,7,8,9,13)
InchiKey:	RRLFIBUKUXPMJU-UHFFFAOYSA-N
Formula:	C6H8N6O
SMILES:	CCn1nnc2c(O)nc(N)nc21
Mol. weight [g/mol]:	180.17
CAS:	5457-90-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.78		Crippen Method
logp	-0.471		Crippen Method
mcvol	122.230	ml/mol	McGowan Method

## Sources

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>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5457909&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5457909&amp;Units=SI</a>

## Legend

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

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