

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

**Inchi:** InChI=1S/2C8H12N6O/c2\*1-2-3-4-14-6-5(12-13-14)7(15)11-8(9)10-6/h2\*2-4H2,1H3,(H3,  
**InchiKey:** MZMKZJMTDOEBDJ-UHFFFAOYSA-N  
**Formula:** C16H24N12O2  
**SMILES:** CCCCN1nnc2c(O)nc(=N)[nH]c21.CCCCN1nnc2c(O)nc(=N)[nH]c21  
**Mol. weight [g/mol]:** 416.44

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.15		Crippen Method
logp	-0.685		Crippen Method
mcvol	300.820	ml/mol	McGowan Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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=B6009901&Units=SI>

## Legend

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

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