

# Ethanol, 2,2'-[(9-benzyl-9h-purin-6-yl)imino]di-

**Inchi:** InChI=1S/C16H19N5O2/c22-8-6-20(7-9-23)15-14-16(18-11-17-15)21(12-19-14)10-13-4-2  
**InchiKey:** ZESQOPFONWMIQO-UHFFFAOYSA-N  
**Formula:** C16H19N5O2  
**SMILES:** OCCN(CCO)c1ncnc2c1ncn2Cc1ccccc1  
**Mol. weight [g/mol]:** 313.35

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Crippen Method
logp	0.666		Crippen Method
mcvol	235.260	ml/mol	McGowan Method

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=B6008696&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

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

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