

# 2-Propanol, 3-(6-chloro-9h-purin-9-yl)-1-(n,n-diethylamino)-

**Inchi:** InChI=1S/C12H18ClN5O/c1-3-17(4-2)5-9(19)6-18-8-16-10-11(13)14-7-15-12(10)18/h7-9  
**InchiKey:** XFSNASAQSFOOHW-UHFFFAOYSA-N  
**Formula:** C12H18ClN5O  
**SMILES:** CCN(CC)CC(O)Cn1cnc2c(Cl)ncnc21  
**Mol. weight [g/mol]:** 283.76  
**CAS:** 19270-70-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	1.182		Crippen Method
mcvol	209.030	ml/mol	McGowan Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C19270703&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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>

## Legend

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

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