

# Ethanol, 2-[2-(9h-purin-6-ylamino)ethylthio]-

**Inchi:** InChI=1S/C9H13N5OS/c15-2-4-16-3-1-10-8-7-9(12-5-11-7)14-6-13-8/h5-6,15H,1-4H2,(H  
**InchiKey:** KZIWLQWHCOIOQO-UHFFFAOYSA-N  
**Formula:** C9H13N5OS  
**SMILES:** OCCSCCNc1ncnc2[nH]cnc12  
**Mol. weight [g/mol]:** 239.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	0.008		Crippen Method
mcvol	170.870	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=B6008358&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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