

# 9H-purine-6(1h)-thione, 9-benzyl-1-[2-(p-tolylthio)ethyl]-

**Inchi:** InChI=1S/C21H20N4S2/c1-16-7-9-18(10-8-16)27-12-11-24-15-23-20-19(21(24)26)22-14  
**InchiKey:** ARMFOOZLBXKIGK-UHFFFAOYSA-N  
**Formula:** C21H20N4S2  
**SMILES:** Cc1ccc(SCCn2cnc3c(ncn3Cc3ccccc3)c2=S)cc1  
**Mol. weight [g/mol]:** 392.54  
**CAS:** 97432-20-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.93		Crippen Method
logp	5.111		Crippen Method
mcvol	292.930	ml/mol	McGowan Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C97432207&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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