

# p-Toluenesulfonamide, alpha-[6-(methylthio)-9H-purin-9-yl]-

**Other names:** «alpha»-[[6-Methylthio]-9H-purine-9-yl]-p-toluenesulfonamide

**Inchi:** InChI=1S/C13H13N5O2S2/c1-21-13-11-12(15-7-16-13)18(8-17-11)6-9-2-4-10(5-3-9)22(1

**InchiKey:** AXRCREXQEFXELO-UHFFFAOYSA-N

**Formula:** C13H13N5O2S2

**SMILES:** CSc1ncnc2c1ncn2Cc1ccc(S(N)(=O)=O)cc1

**Mol. weight [g/mol]:** 335.40

**CAS:** 21268-01-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.58		Crippen Method
logp	1.244		Crippen Method
mcvol	225.690	ml/mol	McGowan Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C21268019&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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