# P-toluenesulfonamide, alpha-(1,6-dihydro-6-oxo-9h-purin-9-yl)-

**Inchi:** InChI=1S/C12H11N5O3S/c13-21(19,20)9-3-1-8(2-4-9)5-17-7-16-10-11(17)14-6-15-12(10

**InchiKey:** RWRNFFKEPARPQR-UHFFFAOYSA-N

**Formula:** C12H11N5O3S

**SMILES:** NS(=O)(=O)c1ccc(Cn2cnc3c(=O)[nH]cnc32)cc1

**Mol. weight [g/mol]:** 305.31

**CAS:** 21267-97-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -2.71 | | Crippen Method |
| logp | -0.667 | | Crippen Method |
| mcvol | 201.120 | ml/mol | McGowan Method |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** 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=C21267970&Units=SI

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume