

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/ci9903071
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

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