

P-toluenesulfonamide, alpha-9h-purin-9-yl-

Inchi:	InChI=1S/C12H11N5O2S/c13-20(18,19)10-3-1-9(2-4-10)6-17-8-16-11-5-14-7-15-12(11)1
InchiKey:	JXDTYUUIZURCBJ-UHFFFAOYSA-N
Formula:	C12H11N5O2S
SMILES:	NS(=O)(=O)c1ccc(Cn2cnc3cncnc32)cc1
Mol. weight [g/mol]:	289.31
CAS:	19270-99-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.83		Crippen Method
logp	0.522		Crippen Method
mcvol	195.250	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19270996&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/85-595-8/P-toluenesulfonamide-alpha-9h-purin-9-yl.pdf>

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