

4-P-tolylsulfonylhydrazo-6-methyl-1,3,3a,7-tetraza

Inchi:	InChI=1S/C13H14N6O2S/c1-9-3-5-11(6-4-9)22(20,21)18-17-12-7-10(2)16-13-14-8-15-19
InchiKey:	KXEQGRAFBLUOGG-UHFFFAOYSA-N
Formula:	C13H14N6O2S
SMILES:	<chem>Cc1ccc(S(=O)(=O)NNc2cc(C)nc3ncnn23)cc1</chem>
Mol. weight [g/mol]:	318.35
CAS:	109445-77-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.36		Crippen Method
logp	1.047		Crippen Method
mcvol	219.320	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=C109445774&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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