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: Cc1ccc(S(=O)(=O)NNc2cc(C)nc3ncnn23)cc1

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