

9H-purine-6(1h)-thione, 1-[3-(p-tolylthio)propyl]-

Inchi:	InChI=1S/C15H16N4S2/c1-11-3-5-12(6-4-11)21-8-2-7-19-10-18-14-13(15(19)20)16-9-17
InchiKey:	ZGHGQLKAPIEWIT-UHFFFAOYSA-N
Formula:	C15H16N4S2
SMILES:	Cc1ccc(SCCCn2cnc3[nH]cnc3c2=S)cc1
Mol. weight [g/mol]:	316.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.01		Crippen Method
logp	3.498		Crippen Method
mcvol	232.150	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008677&Units=SI
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

Legend

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

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