

Purine, 6-(p-tolythio)-

Inchi:	InChI=1S/C12H10N4S/c1-8-2-4-9(5-3-8)17-12-10-11(14-6-13-10)15-7-16-12/h2-7H,1H3,
InchiKey:	PVQBKEDASIBTAR-UHFFFAOYSA-N
Formula:	C12H10N4S
SMILES:	Cc1ccc(Sc2ncnc3nc[nH]c23)cc1
Mol. weight [g/mol]:	242.30
CAS:	5444-08-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.68		Crippen Method
logp	2.331		Crippen Method
mcvol	173.530	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=C5444086&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/28-117-1/Purine-6-p-tolythio.pdf>

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