6H-Purine-6-thione, 1,9-dihydro-9-methyl-

Other names:	9H-Purine-6(1H)-thione, 9-methyl- 6-Mercapto-9-methylpurine 9-Methyl-6-thiopurine
Inchi:	InChI=1S/C6H6N4S/c1-10-3-9-4-5(10)7-2-8-6(4)11/h2-3H,1H3,(H,7,8,11)
InchiKey:	HDAZBCXPLJHIIY-UHFFFAOYSA-N
Formula:	C6H6N4S
SMILES:	Cn1cnc2c(=S)[nH]cnc21
Mol. weight [g/mol]:	166.20
CAS:	1006-20-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.17		Crippen Method
logp	0.544		Crippen Method
mcvol	112.750	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1006208&Units=SI

Legend

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