6H-Purine-6-thione, 1,7-dihydro-8-methyl-

Other names:	Purine-6(1H)-thione, 8-methyl-
	8-Methyl-6-thiopurine
	8-Methyl-6-thioxopurine
	9H-Purine-6-thiol, 8-methyl-
Inchi:	InChI=1S/C6H6N4S/c1-3-9-4-5(10-3)7-2-8-6(4)11/h2H,1H3,(H2,7,8,9,10,11)
InchiKey:	VIVHKHHYZLMJQH-UHFFFAOYSA-N
Formula:	C6H6N4S
SMILES:	Cc1nc2nc[nH]c(=S)c2[nH]1
Mol. weight [g/mol]:	166.20
CAS:	1126-23-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	0.360		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=C1126234&Units=SI

Legend

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

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