Thiopurine, 8-methyl-

Other names:	Purine, 8-(methylthio)- 8-(Methylthio)purine 9H-Purine, 8-(methylthio)- Thiopurine, 8-methyl-
Inchi:	InChI=1S/C6H6N4S/c1-11-6-9-4-2-7-3-8-5(4)10-6/h2-3H,1H3,(H,7,8,9,10)
InchiKey:	OOUSHFSJKWPYDZ-UHFFFAOYSA-N
Formula:	C6H6N4S
SMILES:	CSc1nc2ncncc2[nH]1
Mol. weight [g/mol]:	166.21

Physical Properties

Property code	Value	Unit	Source
logp	0.593		Crippen Method
mcvol	112.750	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33426538&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume