

1H-Purine, 8-(methylthio)-

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]:	166.20
CAS:	33426-53-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	0.593		Crippen Method
mcvol	112.750	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=C33426538&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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