

1H-Purine, 6-(methylthio)-

Other names:	Purine, 6-(methylthio)- S-Methyl-6-mercaptapurine SQ 8343 6-(Methylthio)purine 6-Methylmercaptapurine 6-Methyl MP NSC 20105
Inchi:	InChI=1S/C6H6N4S/c1-11-6-4-5(8-2-7-4)9-3-10-6/h2-3H,1H3,(H,7,8,9,10)
InchiKey:	UIJIQXGRFSPYQW-UHFFFAOYSA-N
Formula:	C6H6N4S
SMILES:	CSc1ncnc2nc[nH]c12
Mol. weight [g/mol]:	166.20
CAS:	50-66-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	0.593		Crippen Method
mvol	112.750	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50668&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/55-386-3/1H-Purine-6-methylthio.pdf>

Generated by Cheméo on 2024-04-27 03:18:22.373137218 +0000 UTC m=+16477151.293714530.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.