

9H-purine, 6-[4-methyl-3-thiosemicarbazido]-

Inchi:	InChI=1S/C7H9N7S/c1-8-7(15)14-13-6-4-5(10-2-9-4)11-3-12-6/h2-3H,1H3,(H2,8,14,15)(
InchiKey:	LTOKJKRIIICZQR-UHFFFAOYSA-N
Formula:	C7H9N7S
SMILES:	CNC(=S)NNc1ncnc2[nH]cnc12
Mol. weight [g/mol]:	223.26
CAS:	78958-61-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	-0.708		Crippen Method
mcvol	152.480	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=C78958619&Units=SI

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.chemeo.com/cid/28-379-1/9H-purine-6-4-methyl-3-thiosemicarbazido.pdf>

Generated by Cheméo on 2024-04-25 13:57:35.426553717 +0000 UTC m=+16342704.347131081.

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