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/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=C78958619&Units=SI

Legend

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