9H-purine-9-acetamide, 1,6-dihydro-6-thioxo-

Inchi: InChI=1S/C7H7N5OS/c8-4(13)1-12-3-11-5-6(12)9-2-10-7(5)14/h2-3H,1H2,(H2,8,13)(H,9
InchiKey: LIPKOJGCDKVCOB-UHFFFAOYSA-N
Formula: C7H7N5OS
SMILES: NC(=O)Cn1cnc2c(=S)[nH]cnc21
Mol. weight [g/mol]: 209.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.35		Crippen Method
logp	-0.508		Crippen Method
mcvol	138.390	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=B6008271&Units=SI

Legend

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