

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/ci9903071>
Crippen Method: https://www.cheméo.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

Latest version available from:

<https://www.cheméo.com/cid/38-569-9/9H-purine-9-acetamide-1-6-dihydro-6-thioxo.pdf>

Generated by Cheméo on 2024-04-26 04:31:07.040219236 +0000 UTC m=+16395115.960796548.

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