

Isosemicarbazide, 3-(9h-purin-6-yl)-3-thio-

Inchi: InChI=1S/C6H7N7S/c7-6(13-8)14-5-3-4(10-1-9-3)11-2-12-5/h1-2H,8H2,(H2,7,13)(H,9,10)
InchiKey: NXWQVTORELUAPM-UHFFFAOYSA-N
Formula: C6H7N7S
SMILES: NN=C(N)Sc1ncnc2[nH]cnc12
Mol. weight [g/mol]: 209.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.55		Crippen Method
logp	-0.848		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.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=B6008032&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/15-924-9/Isosemicarbazide-3-9h-purin-6-yl-3-thio.pdf>

Generated by Cheméo on 2024-04-20 15:58:23.74087335 +0000 UTC m=+15917952.661450666.

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