6H-Purin-6-one, 1,7-dihydro-1-methyl-

Other names: Hypoxanthine, 1-methyl-
1-Methylhypoxanthine
Purin-6(1H)-one, 1-methyl
Inchi: InChI=1S/C6H6N4O/c1-10-3-9-5-4(6(10)11)7-2-8-5/h2-3H,1H3,(H,7,8)
InchiKey: KIQMCGMHGVXDFW-UHFFFAOYSA-N
Formula: C6H6N4O
SMILES: Cn1cnc2[nH]cnc2c1=O
Mol. weight [g/mol]: 150.14
CAS: 1125-39-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.74		Crippen Method
logp	-0.825		Crippen Method
mcvol	102.270	ml/mol	McGowan Method
rinpol	1969.00		NIST Webbook

Sources

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=C1125399&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices