Uric acid, 1-methyl

Other names: 7,9-dihydro-1-methyl-1H-purine-2,6,8(3H)-trione
Inchi: InChI=1S/C6H6N4O3/c1-10-4(11)2-3(9-6(10)13)8-5(12)7-2/h1H3,(H,9,13)(H2,7,8,12)
InchiKey: QFDRTQONISXGJA-UHFFFAOYSA-N
Formula: C6H6N4O3
SMILES: Cn1c(=O)[nH]c2[nH]c(=O)[nH]c2c1=O
Mol. weight [g/mol]: 182.14
CAS: 708-79-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.49		Crippen Method
logp	-3.203		Crippen Method
mcvol	114.010	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=C708792&Units=SI

Legend

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