

1H-Purine-2,6-dione, 3,7-dihydro-1-methyl-

Other names:	Xanthine, 1-methyl- 1-Methylxanthine 2,6-Dihydroxy-1-methylpurine 3,7-dihydro-1-methyl-1H-purine-2,6-dione
Inchi:	InChI=1S/C6H6N4O2/c1-10-5(11)3-4(8-2-7-3)9-6(10)12/h2H,1H3,(H,7,8)(H,9,12)
InchiKey:	MVOYJPOZRLFTCP-UHFFFAOYSA-N
Formula:	C6H6N4O2
SMILES:	<chem>Cn1c(=O)[nH]c2nc[nH]c2c1=O</chem>
Mol. weight [g/mol]:	166.14
CAS:	6136-37-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.61		Crippen Method
logp	-2.014		Crippen Method
mcvol	108.140	ml/mol	McGowan Method

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=C6136374&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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