

2,6-Dihydroxy-7-methylpurine

Other names:	7-Methylxanthine 1H-Purine-2,6-dione, 3,7-dihydro-7-methyl- Heteroxanthin Heteroxanthine Xanthine, 7-methyl- 7-Methylxanthin 3,7-dihydro-7-methyl-1H-purine-2,6-dione
Inchi:	InChI=1S/C6H6N4O2/c1-10-2-7-4-3(10)5(11)9-6(12)8-4/h2H,1H3,(H2,8,9,11,12)
InchiKey:	PFWLFWPASULGAN-UHFFFAOYSA-N
Formula:	C6H6N4O2
SMILES:	Cn1cnc2[nH]c(=O)[nH]c(=O)c21
Mol. weight [g/mol]:	166.14
CAS:	552-62-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.61		Crippen Method
logp	-2.014		Crippen Method
mcvol	108.140	ml/mol	McGowan Method
rinpol	2089.00		NIST Webbook
rinpol	2089.00		NIST Webbook

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=C552625&Units=SI

Legend

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

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