

Uric acid, 3-methyl

Other names:	4,9-dihydro-3-methyl-1H-purine-2,6,8(3H)-trione 7,9-Dihydro-3-methyl-1h-purine-2,6,8(3h)-trione
Inchi:	InChI=1S/C6H6N4O3/c1-10-3-2(7-5(12)8-3)4(11)9-6(10)13/h1H3,(H2,7,8,12)(H,9,11,13)
InchiKey:	ODCYDGXXCHTFIR-UHFFFAOYSA-N
Formula:	C6H6N4O3
SMILES:	Cn1c(=O)[nH]c(=O)c2[nH]c(=O)[nH]c21
Mol. weight [g/mol]:	182.14
CAS:	605-99-2

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/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=C605992&Units=SI

Legend

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

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