

Uric acid, 1,7-dimethyl

Other names:	7,9-dihydro-1,7-dimethyl-1H-purine-2,6,8(3H)-trione
Inchi:	InChI=1S/C7H8N4O3/c1-10-3-4(8-6(10)13)9-7(14)11(2)5(3)12/h1-2H3,(H,8,13)(H,9,14)
InchiKey:	NOFNCLGCUJJPKU-UHFFFAOYSA-N
Formula:	C7H8N4O3
SMILES:	Cn1c(=O)[nH]c2[nH]c(=O)n(C)c2c1=O
Mol. weight [g/mol]:	196.16
CAS:	33868-03-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	-2.710		Crippen Method
mcvol	128.100	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33868030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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