

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

Latest version available from:

<https://www.chemeo.com/cid/115-951-8/Uric-acid-1-methyl.pdf>

Generated by Cheméo on 2025-12-24 08:04:53.49569614 +0000 UTC m=+6311691.025736794.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.