

# 1,3,7-Trimethyluric acid

<b>Other names:</b>	1H-Purine-2,6,8(3H)-trione, 7,9-dihydro-1,3,7-trimethyl-Ba 2753 Uric acid, 1,3,7-trimethyl-7,9-dihydro-1,3,7-trimethyl-1H-purine-2,6,8(3H)-trione
<b>Inchi:</b>	InChI=1S/C8H10N4O3/c1-10-4-5(9-7(10)14)11(2)8(15)12(3)6(4)13/h1-3H3,(H,9,14)
<b>InchiKey:</b>	BYXCFUMGEBZDDI-UHFFFAOYSA-N
<b>Formula:</b>	C8H10N4O3
<b>SMILES:</b>	<chem>Cn1c(=O)c2c([nH]c(=O)n2C)n(C)c1=O</chem>
<b>Mol. weight [g/mol]:</b>	210.19
<b>CAS:</b>	5415-44-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.63		Crippen Method
logp	-2.218		Crippen Method
mcvol	142.190	ml/mol	McGowan Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5415441&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5415441&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

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

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