

# 1,3,8-trimethyl-7-(2-methylpropyl)purine-2,6-dione

<b>Inchi:</b>	InChI=1S/C12H18N4O2/c1-7(2)6-16-8(3)13-10-9(16)11(17)15(5)12(18)14(10)4/h7H,6H2
<b>InchiKey:</b>	VUYNLAZRVSUFDB-UHFFFAOYSA-N
<b>Formula:</b>	C12H18N4O2
<b>SMILES:</b>	<chem>Cc1nc2c(c(=O)n(C)c(=O)n2C)n1CC(C)C</chem>
<b>Mol. weight [g/mol]:</b>	250.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.60		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.398		Crippen Method
mcvol	192.680	ml/mol	McGowan Method

## Sources

<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>Aqueous and cosolvent solubility data for drug-like organic compounds:</b>	<a href="https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/">https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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