

# 1H-Purine-2,6-dione, 7-ethyl-3,7-dihydro-1,3-dimethyl-

<b>Other names:</b>	7-Ethyl-1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione 7-Ethyl-1,3-dimethylxanthine 7-Ethyltheophylline Ethylteofyllin Ethyltheophylline NSC 515485 Theophylline, 7-ethyl-
<b>Inchi:</b>	InChI=1S/C9H12N4O2/c1-4-13-5-10-7-6(13)8(14)12(3)9(15)11(7)2/h5H,4H2,1-3H3
<b>InchiKey:</b>	RPOQNHMXOPWCEK-UHFFFAOYSA-N
<b>Formula:</b>	C9H12N4O2
<b>SMILES:</b>	CCn1cnc2c1c(=O)n(C)c(=O)n2C
<b>Mol. weight [g/mol]:</b>	208.22
<b>CAS:</b>	23043-88-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.76		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-0.546		Crippen Method
mcvol	150.410	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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C23043881&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23043881&amp;Units=SI</a>

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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