

# Paraxanthine, n-propyl derivative

<b>Inchi:</b>	InChI=1S/C10H14N4O2/c1-4-5-14-8-7(12(2)6-11-8)9(15)13(3)10(14)16/h6H,4-5H2,1-3H3
<b>InchiKey:</b>	DHYGGYFMXYRIGJ-UHFFFAOYSA-N
<b>Formula:</b>	C10H14N4O2
<b>SMILES:</b>	CCCN1c(=O)n(C)c(=O)c2c1ncn2C
<b>Mol. weight [g/mol]:</b>	222.24

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Crippen Method
logp	-0.156		Crippen Method
mcvol	164.500	ml/mol	McGowan Method
rinpol	1999.00		NIST Webbook

## 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>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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=R270938&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R270938&amp;Units=SI</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
<b>rinpol:</b>	Non-polar retention indices

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