

# Lumazine, 6,7-dimethyl- (keto form)

<b>Other names:</b>	Lumazine, 6,7-dimethyl-
<b>Inchi:</b>	InChI=1S/C8H8N4O2/c1-3-4(2)10-6-5(9-3)7(13)12-8(14)11-6/h1-2H3,(H2,10,11,12,13,14)
<b>InchiKey:</b>	YVGIYQOPTPWNER-UHFFFAOYSA-N
<b>Formula:</b>	C8H8N4O2
<b>SMILES:</b>	Cc1nc2nc(O)nc(O)c2nc1C
<b>Mol. weight [g/mol]:</b>	192.17
<b>CAS:</b>	5774-32-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	0.448		Crippen Method
mcvol	132.020	ml/mol	McGowan Method

## Sources

<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=C5774323&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5774323&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>

## 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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