

# Imidazolo[1,2-a]pyrimidine-2,5(1H,3H)-dione, 3,7-dimethyl-

**Other names:** 3,7-Dimethylimidazo[1,2-a]pyrimidine-2,5(1H,3H)-dione  
**Inchi:** InChI=1S/C8H9N3O2/c1-4-3-6(12)11-5(2)7(13)10-8(11)9-4/h3,5H,1-2H3,(H,9,10,13)  
**InchiKey:** VNLCDRYHJYBFMO-UHFFFAOYSA-N  
**Formula:** C8H9N3O2  
**SMILES:** Cc1cc(=O)n2c(n1)NC(=O)C2C  
**Mol. weight [g/mol]:** 179.18  
**CAS:** 53854-19-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.04		Crippen Method
logp	0.065		Crippen Method
mcvol	126.340	ml/mol	McGowan Method
rinpol	1806.00		NIST Webbook
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rinpol	1806.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C53854196&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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