

# 2(1H)Pyrimidinone,4-(dimethylamino)-1-methyl-

**Inchi:** InChI=1S/C7H11N3O/c1-9(2)6-4-5-10(3)7(11)8-6/h4-5H,1-3H3  
**InchiKey:** DHGBSOMRGXWRSE-UHFFFAOYSA-N  
**Formula:** C7H11N3O  
**SMILES:** CN(C)c1ccn(C)c(=O)n1  
**Mol. weight [g/mol]:** 153.18  
**CAS:** 2228-27-5

## Physical Properties

Property code	Value	Unit	Source
ie	8.70 ± 0.10	eV	NIST Webbook
log10ws	-1.86		Crippen Method
logp	-0.154		Crippen Method
mcvol	121.540	ml/mol	McGowan Method
rinpol	2035.00		NIST Webbook
rinpol	2035.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2228275&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

**ie:** Ionization energy  
**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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