

# 3H-Pyrimidin-4-one, 2,3:5,6-bis-trimethyleno

**Other names:** 1,2,3,5,6,7-Hexahydro-3a,8-diaza-s-indacen-4-one  
**Inchi:** InChI=1S/C10H12N2O/c13-10-7-3-1-4-8(7)11-9-5-2-6-12(9)10/h1-6H2  
**InchiKey:** BRFWYALXFLAMPV-UHFFFAOYSA-N  
**Formula:** C10H12N2O  
**SMILES:** O=c1c2c(nc3n1CCC3)CCC2  
**Mol. weight [g/mol]:** 176.22

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	0.678		Crippen Method
mcvol	132.110	ml/mol	McGowan Method
rinpol	1870.00		NIST Webbook
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rinpol	1870.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R119754&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## 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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