

# 4H-cyclopenteno[2,3-e]pyrido[1,2-a]pyrimidin-4-one 6,7,8,9-tetrahydro

InChI: O=C1CCNC2CC3C(CN12)CCC3  
InChIKey: MFHROBCSVBZPALM-UHFFFAOYSA-N

Formula: C<sub>11</sub>H<sub>10</sub>N<sub>2</sub>O

SMILES: O=c1ccnc2cc3c(cn12)CCC3

Mol. weight [g/mol]: 186.21

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	1.183		Crippen Method
mcvol	137.600	ml/mol	McGowan Method
rinpola	1961.00		NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R64194&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R64194&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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