

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

InChI: InChI=1S/C12H12N2O/c1-8-2-3-9-7-14-11(6-10(8)9)13-5-4-12(14)15/h4-8H,2-3H2,1H3
InChIKey: FJBUDJHFRMAFAC-UHFFFAOYSA-N

Formula: C12H12N2O
SMILES: CC1CCc2cn3c(=O)ccnc3cc21
Mol. weight [g/mol]: 200.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	1.744		Crippen Method
mcvol	151.690	ml/mol	McGowan Method
rinpol	1978.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R64233&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: 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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