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

Inchi: InChI=1S/C12H12N2O/c1-8-2[illegible]3-9-7[illegible]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