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

Inchi: InChI=1S/C11H10N2O/c14-11-4-5-12-10-6-8-2-1-3-9(8)7-13(10)11/h4-7H,1-3H2
InchiKey: MHKOBCSVBZFALM-UHFFFAOYSA-N
Formula: C11H10N2O
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
rinpol	1961.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R64194&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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