4H-Cyclopenteno[2,3-e]pyrido[1.2-a]pyrimidin-4-o

Inchi: InChI=1S/C11H8N2O/c14-11-8-4-3-5-9(8)12-10-6-1-2-7-13(10)11/h1-2,4-7H,3H2
InchiKey: PLWKWPJLRNBJIH-UHFFFAOYSA-N
Formula: C11H8N2O
SMILES: O=c1c2c(nc3ccccn13)=CCC=2
Mol. weight [g/mol]: 184.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.39		Crippen Method
logp	-0.341		Crippen Method
mcvol	133.300	ml/mol	McGowan Method
rinpol	1968.00		NIST Webbook
rinpol	1968.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R64283&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: 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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