4H-Cyclopenteno[2,3-e]pyrido[1,2-a]pyrimidin-4-one, 9-methyl

Inchi: InChI=1S/C12H12N2O/c1-8-7-9-3-2-4-10(9)14-11(15)5-6-13-12(8)14/h5-7H,2-4H2,1H3

InchiKey: OUPOWFDSCVTSSI-UHFFFAOYSA-N

Formula: C12H12N2O

SMILES: Cc1cc2c(n3c(=O)ccnc13)CCC2

Mol. weight [g/mol]: 200.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	1.492		Crippen Method
mcvol	151.690	ml/mol	McGowan Method
rinpol	2023.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R318208&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