

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: OUPWFDSCVTSSI-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

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