

4H-Cyclopenteno[2,3-e]pyrido[1,2-a]pyrimidin-4-one-8-methyl

InChI: InChI=1S/C12H10N2O/c1-8-4-2-7-11-13-10-6-3-5-9(10)12(15)14(8)11/h2,4-7H,3H2,1H3
InChIKey: QHFQWYDIEYIDOX-UHFFFAOYSA-N
Formula: C12H10N2O
SMILES: Cc1cccc2nc3c(c(=O)n12)=CCC=3
Mol. weight [g/mol]: 198.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.87		Crippen Method
logp	-0.032		Crippen Method
mcvol	147.390	ml/mol	McGowan Method
rinpol	2089.00		NIST Webbook
rinpol	2089.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R64265&Units=SI>

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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