4H-Cyclopenteno[2,3-e]pyrido[1,2-a]pyrimidin-4-one, 6-methyl

Inchi: InChI=1S/C12H10N2O/c1-8-5-6-14-11(7-8)13-10-4-2-3-9(10)12(14)15/h3-7H,2H2,1H3
InchiKey: BNCKUBBIJACNOY-UHFFFAOYSA-N
Formula: C12H10N2O
SMILES: Cc1ccn2c(=O)c3c(nc2c1)=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	2020.00		NIST Webbook
rinpol	2020.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R64247&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.