4H-Cyclopenteno[2,3-e]pyrido[1,2-a]pyrimidin-4-o 6,7,8,9-tetrahydro, 8-methyl

Inchi: InChI=1S/C12H12N2O/c1-8-4-9-6-11-13-3-2-12(15)14(11)7-10(9)5-8/h2-3,6-8H,4-5H2,1H

InchiKey: NZAQPUOGROXAPV-UHFFFAOYSA-N

Formula: C12H12N2O

SMILES: CC1Cc2cc3nccc(=O)n3cc2C1

Mol. weight [g/mol]: 200.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	1.429		Crippen Method
mcvol	151.690	ml/mol	McGowan Method
rinpol	2000.00		NIST Webbook
rinpol	2000.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R64229&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

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