11H-Pyrido[2,1-b]quinazolin-11-one, 1,2,3,4,6,7,8,9-octahydro

Inchi: InChI=1S/C12H18N2O/c15-12-9-5-1-2-6-10(9)13-11-7-3-4-8-14(11)12/h9-10H,1-8H2
InchiKey: JMPLADLXJPQANY-UHFFFAOYSA-N
Formula: C12H18N2O
SMILES: O=C1C2CCCCC2N=C2CCCCN12
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Crippen Method
logp	1.970		Crippen Method
mcvol	164.590	ml/mol	McGowan Method
rinpol	2059.00		NIST Webbook
rinpol	2059.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R64108&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.