

2H-Pyrido[2,1-b]quinazolin-6-one, 1,3,4,6,7,8,9,10-octahydro-8-methyl

Inchi: InChI=1S/C12H17N3O/c1-8-3-4-10-9(7-8)11(16)15-6-2-5-13-12(15)14-10/h8H,2-7H2,1H
InchiKey: HITNTEVFYQXCJG-UHFFFAOYSA-N
Formula: C12H17N3O
SMILES: CC1CCC2=C(C1)C(=O)N1CCCN=C1N2
Mol. weight [g/mol]: 219.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.33		Crippen Method
logp	1.252		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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=R119729&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

Latest version available from:

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