

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

Inchi: InChI=1S/C13H18N2O/c1-9-5-4-6-10-12(9)14-11-7-2-3-8-15(11)13(10)16/h9H,2-8H2,1H
InchiKey: WYULMVGNAVLFTQ-UHFFFAOYSA-N
Formula: C13H18N2O
SMILES: CC1CCCc2c1nc1n(c2=O)CCCC1
Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.50		Crippen Method
logp	2.019		Crippen Method
mcvol	174.380	ml/mol	McGowan Method
rinpol	2045.00		NIST Webbook
rinpol	2045.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R121049&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

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