

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

Inchi: InChI=1S/C13H14N2O/c1-9-5-4-8-12-14-11-7-3-2-6-10(11)13(16)15(9)12/h2-3,6-7,9H,4-
InchiKey: YUNQTDWKCHAMBY-UHFFFAOYSA-N
Formula: C13H14N2O
SMILES: CC1CCCCc2nc3ccccc3c(=O)n21
Mol. weight [g/mol]: 214.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	2.294		Crippen Method
mcvol	165.780	ml/mol	McGowan Method
rinpol	2123.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R64180&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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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