7,8,9,10-Tetrahydro-6H-azepino[2,1-b]quinazolin-1

Other names: 3H-Quinazolin-4-one, 2,3-pentamethyleno
Inchi: InChI=1S/C13H14N2O/c16-13-10-6-3-4-7-11(10)14-12-8-2-1-5-9-15(12)13/h3-4,6-7H,1-2
InchiKey: HTLIIBRHXAULMB-UHFFFAOYSA-N
Formula: C13H14N2O
SMILES: O=c1c2ccccc2nc2n1CCCCC2
Mol. weight [g/mol]: 214.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	2.123		Crippen Method
mcvol	165.780	ml/mol	McGowan Method
rinpol	2101.00		NIST Webbook
rinpol	2101.00		NIST Webbook
rinpol	2101.00		NIST Webbook
rinpol	2101.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R119803&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

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