1-Methyl-2,3-dihydro-1H-pyrrolo[2,1-b]quinazolin-

Inchi: InChI=1S/C12H12N2O/c1-8-6-7-11-13-10-5-3-2-4-9(10)12(15)14(8)11/h2-5,8H,6-7H2,1H
InchiKey: DCRZVWIQIPZWER-UHFFFAOYSA-N
Formula: C12H12N2O
SMILES: CC1CCc2nc3ccccc3c(=O)n21
Mol. weight [g/mol]: 200.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	1.904		Crippen Method
mcvol	151.690	ml/mol	McGowan Method
rinpol	1942.00		NIST Webbook
rinpol	1942.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R173570&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.