10-Methyl-7,8,9,10-tetrahydro-6H-azepino[2,1-b]qu

Inchi: InChI=1S/C14H16N2O/c1-10-6-2-5-9-13-15-12-8-4-3-7-11(12)14(17)16(10)13/h3-4,7-8,1
InchiKey: SXCZYKXWTKWHAM-UHFFFAOYSA-N
Formula: C14H16N2O
SMILES: CC1CCCCc2nc3ccccc3c(=O)n21
Mol. weight [g/mol]: 228.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.22		Crippen Method
logp	2.684		Crippen Method
mcvol	179.870	ml/mol	McGowan Method
rinpol	2123.00		NIST Webbook
rinpol	2123.00		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=R173565&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.