

1-(2-Quinolyyl)hexahydro-2h-azepin-2-one-

Inchi:	InChI=1S/C15H16N2O/c18-15-8-2-1-5-11-17(15)14-10-9-12-6-3-4-7-13(12)16-14/h3-4,6
InchiKey:	LSHBLYASVGFZEX-UHFFFAOYSA-N
Formula:	C15H16N2O
SMILES:	O=C1CCCCCN1c1ccc2ccccc2n1
Mol. weight [g/mol]:	240.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.29		Crippen Method
logp	3.142		Crippen Method
mcvol	189.660	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=B6007568&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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