2H-azepin-2-one, hexahydro-1-(2-pyridyl)-

Inchi: InChI=1S/C11H14N2O/c14-11-7-2-1-5-9-13(11)10-6-3-4-8-12-10/h3-4,6,8H,1-2,5,7,9H2
InchiKey: JRMTZHXHEXFTMZ-UHFFFAOYSA-N
Formula: C11H14N2O
SMILES: O=C1CCCCCN1c1ccccn1
Mol. weight [g/mol]: 190.24
CAS: 51263-32-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	1.989		Crippen Method
mcvol	152.760	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51263322&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