

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=C1CCCCCN1c1ccccc1
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

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