

1,2,3,4,5,6-hexahydro-(7H)-cyclopentapyridine-7-one

Inchi:	InChI=1S/C8H13NO/c10-8-5-4-7-3-1-2-6-9(7)8/h7H,1-6H2
InchiKey:	IZKATSCDUREBRD-UHFFFAOYSA-N
Formula:	C8H13NO
SMILES:	O=C1CCC2CCCCN12
Mol. weight [g/mol]:	139.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.42		Crippen Method
logp	1.161		Crippen Method
mcvol	113.410	ml/mol	McGowan Method
rinpol	1440.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R231017&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

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